



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:22 PM GMT

PDB ID : 1JZ2
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-F-GALACTOSYL-
ENZYME INTERMEDIATE (ORTHORHOMBIC)
Authors : Juers, D.H.; McCarter, J.D.; Mackenzie, L.; Withers, S.G.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

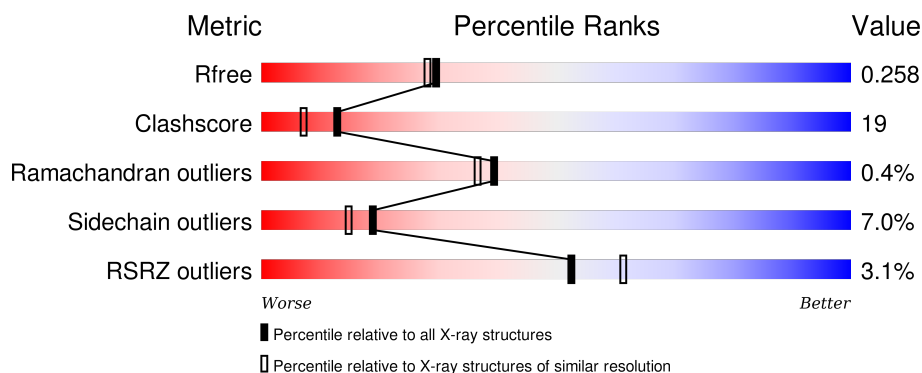
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>3%</div> <div>53% 36% 9% ..</div> </div>
1	B	1023	<div> <div>3%</div> <div>55% 34% 9% ..</div> </div>
1	C	1023	<div> <div>3%</div> <div>55% 35% 8% ..</div> </div>
1	D	1023	<div> <div>3%</div> <div>57% 34% 7% ..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2FG	A	2001	X	-	-	-
2	2FG	B	2001	X	-	-	-
2	2FG	C	2001	X	-	-	-
2	2FG	D	2001	X	-	-	-
3	MG	B	3002	-	-	-	X
5	DMS	A	8402	-	-	-	X
5	DMS	A	8403	-	-	-	X
5	DMS	A	8406	-	-	X	X
5	DMS	A	8407	-	-	-	X
5	DMS	A	8412	-	-	-	X
5	DMS	A	8414	-	-	X	-
5	DMS	A	8417	-	X	-	X
5	DMS	A	8419	-	-	-	X
5	DMS	A	8423	-	-	-	X
5	DMS	A	8502	-	-	-	X
5	DMS	A	8504	-	-	-	X
5	DMS	B	8405	-	-	-	X
5	DMS	B	8406	-	-	-	X
5	DMS	B	8407	-	-	-	X
5	DMS	B	8411	-	-	-	X
5	DMS	B	8417	-	-	X	-
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8504	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	B	8508	-	-	-	X
5	DMS	C	8403	-	-	-	X
5	DMS	C	8404	-	-	-	X
5	DMS	C	8419	-	-	-	X
5	DMS	C	8421	-	-	X	-
5	DMS	D	8406	-	-	-	X
5	DMS	D	8408	-	-	-	X
5	DMS	D	8423	-	-	-	X
6	BTB	B	2002	-	-	X	X
6	BTB	D	2002	-	-	-	X

2 Entry composition [i](#)

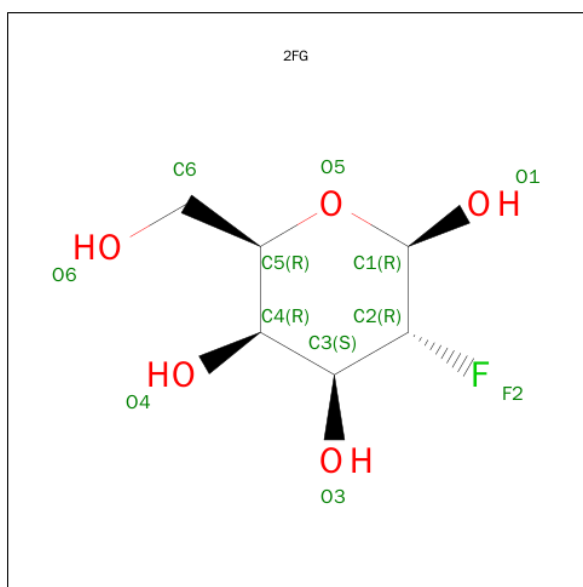
There are 7 unique types of molecules in this entry. The entry contains 35825 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

- Molecule 2 is SUGAR (2-FLUORO-2-DEOXY-BETA-D-GALACTOPYRANOSE) (three-letter code: 2FG) (formula: $C_6H_{11}FO_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	F	O	0	0
			11	6	1	4		
2	B	1	Total	C	F	O	0	0
			11	6	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	F	O	0	0
			11	6	1	4		
2	D	1	Total	C	F	O	0	0
			11	6	1	4		

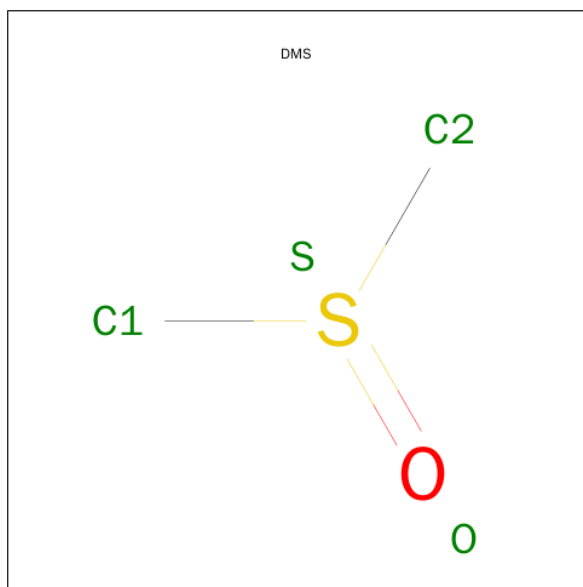
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		
3	D	2	Total	Mg	0	0
			2	2		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	3	Total	Na	0	0
			3	3		
4	A	3	Total	Na	0	0
			3	3		
4	D	3	Total	Na	0	0
			3	3		
4	C	3	Total	Na	0	0
			3	3		

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	A	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	A	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0

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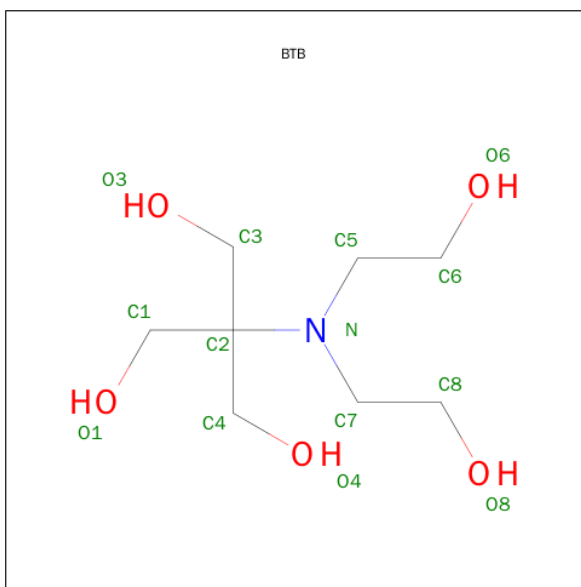
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	C	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0
5	D	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 6 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

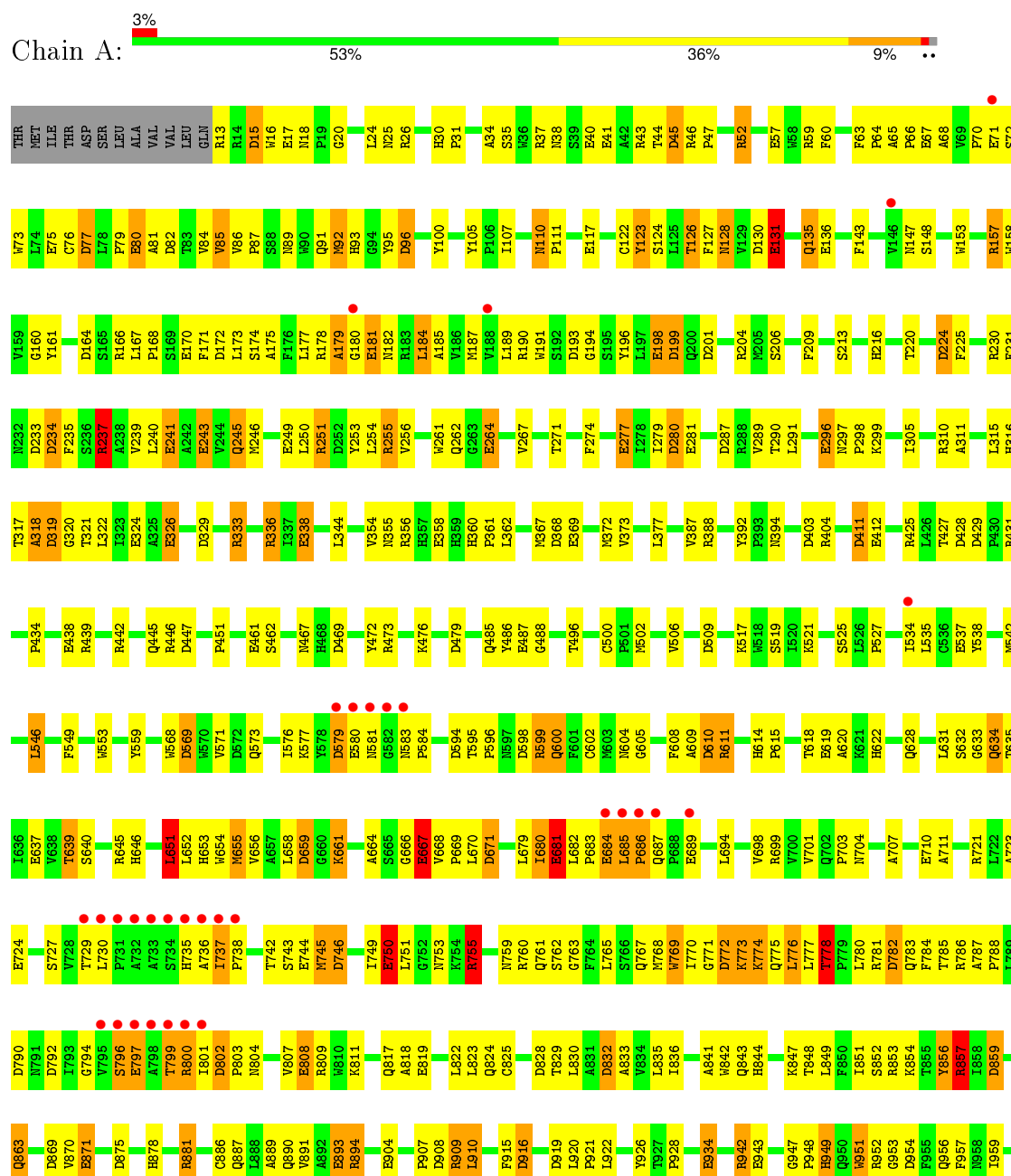
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	753	Total	O	0	0
			753	753		
7	B	734	Total	O	0	0
			734	734		
7	C	716	Total	O	0	0
			716	716		
7	D	754	Total	O	0	0
			754	754		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Beta-Galactosidase









4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.50Å 167.70Å 201.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.60 – 2.10 27.59 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.0 (27.60-2.10) 92.1 (27.59-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 2.10Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.167 , 0.270 0.165 , 0.258	Depositor DCC
R_{free} test set	3979 reflections (1.47%)	DCC
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 131.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 273807 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	35825	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.88 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4330e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MG, DMS, 2FG, BTB

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.02	52/8367 (0.6%)	1.65	148/11415 (1.3%)
1	B	1.01	50/8367 (0.6%)	1.64	173/11415 (1.5%)
1	C	1.00	49/8367 (0.6%)	1.64	161/11415 (1.4%)
1	D	1.02	45/8367 (0.5%)	1.65	187/11415 (1.6%)
All	All	1.01	196/33468 (0.6%)	1.65	669/45660 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
1	D	1	0
All	All	2	0

All (196) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	8.54	1.35	1.25
1	C	198	GLU	CD-OE2	8.05	1.34	1.25
1	C	529	GLU	CD-OE2	7.99	1.34	1.25
1	B	117	GLU	CD-OE2	7.95	1.34	1.25
1	D	667	GLU	CD-OE2	7.55	1.33	1.25
1	D	326	GLU	CD-OE2	7.53	1.33	1.25
1	B	41	GLU	CD-OE2	7.50	1.33	1.25
1	A	296	GLU	CD-OE2	7.49	1.33	1.25
1	D	241	GLU	CD-OE2	7.45	1.33	1.25
1	D	893	GLU	CD-OE2	7.41	1.33	1.25
1	B	71	GLU	CD-OE2	7.40	1.33	1.25
1	C	744	GLU	CD-OE2	7.40	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	264	GLU	CD-OE2	7.40	1.33	1.25
1	C	580	GLU	CD-OE2	7.29	1.33	1.25
1	C	819	GLU	CD-OE2	7.27	1.33	1.25
1	C	969	GLU	CD-OE2	7.20	1.33	1.25
1	B	198	GLU	CD-OE2	7.19	1.33	1.25
1	A	71	GLU	CD-OE2	7.16	1.33	1.25
1	C	71	GLU	CD-OE2	7.13	1.33	1.25
1	B	580	GLU	CD-OE2	7.09	1.33	1.25
1	C	689	GLU	CD-OE2	7.06	1.33	1.25
1	B	326	GLU	CD-OE2	7.04	1.33	1.25
1	C	304	GLU	CD-OE2	7.03	1.33	1.25
1	C	537	GLU	CD-OE2	7.03	1.33	1.25
1	D	131	GLU	CD-OE2	7.03	1.33	1.25
1	C	136	GLU	CD-OE2	6.99	1.33	1.25
1	C	710	GLU	CD-OE2	6.99	1.33	1.25
1	C	797	GLU	CD-OE2	6.97	1.33	1.25
1	B	710	GLU	CD-OE2	6.95	1.33	1.25
1	C	338	GLU	CD-OE2	6.95	1.33	1.25
1	D	689	GLU	CD-OE2	6.93	1.33	1.25
1	A	243	GLU	CD-OE2	6.92	1.33	1.25
1	A	181	GLU	CD-OE2	6.89	1.33	1.25
1	A	170	GLU	CD-OE2	6.88	1.33	1.25
1	A	358	GLU	CD-OE2	6.88	1.33	1.25
1	C	934	GLU	CD-OE2	6.85	1.33	1.25
1	A	80	GLU	CD-OE2	6.85	1.33	1.25
1	A	684	GLU	CD-OE2	6.84	1.33	1.25
1	A	980	GLU	CD-OE2	6.80	1.33	1.25
1	B	893	GLU	CD-OE2	6.79	1.33	1.25
1	D	136	GLU	CD-OE2	6.76	1.33	1.25
1	B	979	GLU	CD-OE2	6.76	1.33	1.25
1	D	797	GLU	CD-OE2	6.75	1.33	1.25
1	C	249	GLU	CD-OE2	6.75	1.33	1.25
1	A	131	GLU	CD-OE2	6.74	1.33	1.25
1	B	819	GLU	CD-OE2	6.70	1.33	1.25
1	A	689	GLU	CD-OE2	6.69	1.33	1.25
1	A	580	GLU	CD-OE2	6.68	1.32	1.25
1	C	117	GLU	CD-OE2	6.66	1.32	1.25
1	B	689	GLU	CD-OE2	6.65	1.32	1.25
1	A	75	GLU	CD-OE2	6.65	1.32	1.25
1	D	117	GLU	CD-OE2	6.64	1.32	1.25
1	A	904	GLU	CD-OE2	6.62	1.32	1.25
1	A	277	GLU	CD-OE2	6.60	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	GLU	CD-OE2	6.56	1.32	1.25
1	C	75	GLU	CD-OE2	6.56	1.32	1.25
1	A	537	GLU	CD-OE2	6.53	1.32	1.25
1	D	681	GLU	CD-OE2	6.52	1.32	1.25
1	B	181	GLU	CD-OE2	6.50	1.32	1.25
1	C	243	GLU	CD-OE2	6.50	1.32	1.25
1	C	979	GLU	CD-OE2	6.49	1.32	1.25
1	D	537	GLU	CD-OE2	6.49	1.32	1.25
1	C	667	GLU	CD-OE2	6.47	1.32	1.25
1	A	136	GLU	CD-OE2	6.46	1.32	1.25
1	B	667	GLU	CD-OE2	6.44	1.32	1.25
1	A	264	GLU	CD-OE2	6.43	1.32	1.25
1	C	684	GLU	CD-OE2	6.43	1.32	1.25
1	A	819	GLU	CD-OE2	6.43	1.32	1.25
1	B	934	GLU	CD-OE2	6.42	1.32	1.25
1	B	980	GLU	CD-OE2	6.42	1.32	1.25
1	C	181	GLU	CD-OE2	6.42	1.32	1.25
1	A	241	GLU	CD-OE2	6.41	1.32	1.25
1	B	277	GLU	CD-OE2	6.40	1.32	1.25
1	B	744	GLU	CD-OE2	6.39	1.32	1.25
1	D	980	GLU	CD-OE2	6.38	1.32	1.25
1	C	170	GLU	CD-OE2	6.38	1.32	1.25
1	D	744	GLU	CD-OE2	6.36	1.32	1.25
1	C	980	GLU	CD-OE2	6.36	1.32	1.25
1	D	710	GLU	CD-OE2	6.33	1.32	1.25
1	D	181	GLU	CD-OE2	6.33	1.32	1.25
1	B	241	GLU	CD-OE2	6.31	1.32	1.25
1	B	684	GLU	CD-OE2	6.30	1.32	1.25
1	A	710	GLU	CD-OE2	6.30	1.32	1.25
1	C	296	GLU	CD-OE2	6.28	1.32	1.25
1	D	338	GLU	CD-OE2	6.27	1.32	1.25
1	D	819	GLU	CD-OE2	6.26	1.32	1.25
1	D	57	GLU	CD-OE2	6.23	1.32	1.25
1	B	461	GLU	CD-OE2	6.21	1.32	1.25
1	D	75	GLU	CD-OE2	6.21	1.32	1.25
1	C	487	GLU	CD-OE2	6.21	1.32	1.25
1	A	681	GLU	CD-OE2	6.21	1.32	1.25
1	C	893	GLU	CD-OE2	6.21	1.32	1.25
1	D	249	GLU	CD-OE2	6.21	1.32	1.25
1	D	198	GLU	CD-OE2	6.21	1.32	1.25
1	B	296	GLU	CD-OE2	6.19	1.32	1.25
1	B	650	GLU	CD-OE2	6.19	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	943	GLU	CD-OE2	6.18	1.32	1.25
1	B	637	GLU	CD-OE2	6.17	1.32	1.25
1	D	637	GLU	CD-OE2	6.16	1.32	1.25
1	A	893	GLU	CD-OE2	6.15	1.32	1.25
1	A	117	GLU	CD-OE2	6.14	1.32	1.25
1	C	650	GLU	CD-OE2	6.12	1.32	1.25
1	C	264	GLU	CD-OE2	6.10	1.32	1.25
1	D	529	GLU	CD-OE2	6.10	1.32	1.25
1	D	170	GLU	CD-OE2	6.09	1.32	1.25
1	D	808	GLU	CD-OE2	6.08	1.32	1.25
1	B	537	GLU	CD-OE2	6.08	1.32	1.25
1	B	529	GLU	CD-OE2	6.06	1.32	1.25
1	B	40	GLU	CD-OE2	6.03	1.32	1.25
1	B	131	GLU	CD-OE2	6.03	1.32	1.25
1	B	487	GLU	CD-OE2	6.03	1.32	1.25
1	A	871	GLU	CD-OE2	6.02	1.32	1.25
1	D	296	GLU	CD-OE2	6.02	1.32	1.25
1	B	264	GLU	CD-OE2	6.02	1.32	1.25
1	C	277	GLU	CD-OE2	6.01	1.32	1.25
1	B	797	GLU	CD-OE2	6.01	1.32	1.25
1	B	136	GLU	CD-OE2	5.98	1.32	1.25
1	C	808	GLU	CD-OE2	5.98	1.32	1.25
1	D	324	GLU	CD-OE2	5.97	1.32	1.25
1	D	684	GLU	CD-OE2	5.95	1.32	1.25
1	A	17	GLU	CD-OE2	5.94	1.32	1.25
1	A	667	GLU	CD-OE2	5.94	1.32	1.25
1	B	1006	GLU	CD-OE2	5.92	1.32	1.25
1	A	369	GLU	CD-OE2	5.91	1.32	1.25
1	D	750	GLU	CD-OE2	5.88	1.32	1.25
1	A	461	GLU	CD-OE2	5.88	1.32	1.25
1	D	41	GLU	CD-OE2	5.87	1.32	1.25
1	D	80	GLU	CD-OE2	5.86	1.32	1.25
1	C	131	GLU	CD-OE2	5.84	1.32	1.25
1	C	326	GLU	CD-OE2	5.83	1.32	1.25
1	B	681	GLU	CD-OE2	5.83	1.32	1.25
1	A	637	GLU	CD-OE2	5.81	1.32	1.25
1	C	1006	GLU	CD-OE2	5.78	1.32	1.25
1	C	637	GLU	CD-OE2	5.77	1.32	1.25
1	D	580	GLU	CD-OE2	5.74	1.31	1.25
1	D	731	PRO	N-CD	5.74	1.55	1.47
1	D	969	GLU	CD-OE2	5.73	1.31	1.25
1	D	487	GLU	CD-OE2	5.72	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	41	GLU	CD-OE2	5.71	1.31	1.25
1	A	487	GLU	CD-OE2	5.70	1.31	1.25
1	D	334	GLU	CD-OE2	5.69	1.31	1.25
1	C	41	GLU	CD-OE2	5.68	1.31	1.25
1	A	750	GLU	CD-OE2	5.67	1.31	1.25
1	C	724	GLU	CD-OE2	5.67	1.31	1.25
1	D	277	GLU	CD-OE2	5.65	1.31	1.25
1	B	508	GLU	CD-OE2	5.64	1.31	1.25
1	A	326	GLU	CD-OE2	5.64	1.31	1.25
1	A	412	GLU	CD-OE2	5.64	1.31	1.25
1	A	324	GLU	CD-OE2	5.63	1.31	1.25
1	A	797	GLU	CD-OE2	5.63	1.31	1.25
1	C	750	GLU	CD-OE2	5.63	1.31	1.25
1	C	681	GLU	CD-OE2	5.61	1.31	1.25
1	B	57	GLU	CD-OE2	5.61	1.31	1.25
1	C	57	GLU	CD-OE2	5.61	1.31	1.25
1	D	17	GLU	CD-OE2	5.59	1.31	1.25
1	A	1006	GLU	CD-OE2	5.56	1.31	1.25
1	A	67	GLU	CD-OE2	5.55	1.31	1.25
1	C	438	GLU	CD-OE2	5.55	1.31	1.25
1	C	871	GLU	CD-OE2	5.52	1.31	1.25
1	A	57	GLU	CD-OE2	5.52	1.31	1.25
1	B	304	GLU	CD-OE2	5.52	1.31	1.25
1	C	281	GLU	CD-OE2	5.52	1.31	1.25
1	B	969	GLU	CD-OE2	5.51	1.31	1.25
1	A	438	GLU	CD-OE2	5.51	1.31	1.25
1	C	619	GLU	CD-OE2	5.50	1.31	1.25
1	A	808	GLU	CD-OE2	5.49	1.31	1.25
1	A	198	GLU	CD-OE2	5.49	1.31	1.25
1	B	358	GLU	CD-OE2	5.48	1.31	1.25
1	D	358	GLU	CD-OE2	5.48	1.31	1.25
1	D	438	GLU	CD-OE2	5.43	1.31	1.25
1	A	979	GLU	CD-OE2	5.41	1.31	1.25
1	B	412	GLU	CD-OE2	5.40	1.31	1.25
1	A	943	GLU	CD-OE2	5.38	1.31	1.25
1	B	80	GLU	CD-OE2	5.37	1.31	1.25
1	B	369	GLU	CD-OE2	5.34	1.31	1.25
1	A	724	GLU	CD-OE2	5.32	1.31	1.25
1	A	338	GLU	CD-OE2	5.30	1.31	1.25
1	B	338	GLU	CD-OE2	5.28	1.31	1.25
1	B	243	GLU	CD-OE2	5.27	1.31	1.25
1	B	75	GLU	CD-OE2	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	GLU	CD-OE2	5.25	1.31	1.25
1	A	969	GLU	CD-OE2	5.24	1.31	1.25
1	B	170	GLU	CD-OE2	5.23	1.31	1.25
1	D	641	GLU	CD-OE1	-5.23	1.20	1.25
1	C	241	GLU	CD-OE2	5.21	1.31	1.25
1	A	281	GLU	CD-OE2	5.20	1.31	1.25
1	A	744	GLU	CD-OE2	5.18	1.31	1.25
1	C	641	GLU	CD-OE2	5.17	1.31	1.25
1	D	40	GLU	CD-OE2	5.17	1.31	1.25
1	A	934	GLU	CD-OE2	5.15	1.31	1.25
1	B	724	GLU	CD-OE2	5.15	1.31	1.25
1	C	943	GLU	CD-OE2	5.14	1.31	1.25
1	B	314	GLU	CD-OE2	5.12	1.31	1.25
1	B	943	GLU	CD-OE2	5.08	1.31	1.25
1	B	904	GLU	CD-OE2	5.07	1.31	1.25
1	C	40	GLU	CD-OE2	5.05	1.31	1.25

All (669) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	685	LEU	C-N-CD	-18.06	80.87	120.60
1	D	881	ARG	NE-CZ-NH1	16.92	128.76	120.30
1	C	917	ARG	NE-CZ-NH1	-14.85	112.88	120.30
1	A	909	ARG	NE-CZ-NH1	14.21	127.41	120.30
1	D	237	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	569	ASP	CB-CG-OD2	-13.38	106.25	118.30
1	D	687	GLN	C-N-CD	-12.88	92.28	120.60
1	B	853	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	B	802	ASP	CB-CG-OD2	-12.12	107.39	118.30
1	A	172	ASP	CB-CG-OD2	-11.72	107.75	118.30
1	D	255	ARG	NE-CZ-NH1	11.71	126.15	120.30
1	D	630	ARG	NE-CZ-NH1	11.69	126.14	120.30
1	D	43	ARG	NE-CZ-NH1	11.62	126.11	120.30
1	C	255	ARG	NE-CZ-NH1	11.56	126.08	120.30
1	A	569	ASP	CB-CG-OD1	11.49	128.64	118.30
1	D	856	TYR	CB-CG-CD2	-11.19	114.28	121.00
1	B	594	ASP	CB-CG-OD2	-11.10	108.31	118.30
1	A	237	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	C	43	ARG	NE-CZ-NH1	11.00	125.80	120.30
1	B	255	ARG	NE-CZ-NH1	10.93	125.77	120.30
1	D	448	ARG	NE-CZ-NH2	-10.92	114.84	120.30
1	B	473	ARG	NE-CZ-NH1	10.64	125.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	610	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	B	853	ARG	NE-CZ-NH2	-10.45	115.07	120.30
1	A	439	ARG	NE-CZ-NH1	10.33	125.47	120.30
1	C	178	ARG	NE-CZ-NH1	10.31	125.45	120.30
1	C	233	ASP	CB-CG-OD2	-10.22	109.10	118.30
1	C	954	ASP	CB-CG-OD2	-10.22	109.11	118.30
1	A	997	ASP	CB-CG-OD2	-10.18	109.14	118.30
1	D	479	ASP	CB-CG-OD2	-10.16	109.15	118.30
1	B	802	ASP	CB-CG-OD1	10.03	127.33	118.30
1	C	403	ASP	CB-CG-OD2	-10.00	109.30	118.30
1	C	594	ASP	CB-CG-OD2	-9.95	109.35	118.30
1	B	164	ASP	CB-CG-OD1	9.89	127.20	118.30
1	D	448	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	D	233	ASP	CB-CG-OD1	9.84	127.16	118.30
1	C	997	ASP	CB-CG-OD2	-9.84	109.45	118.30
1	D	439	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	B	448	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	651	LEU	CB-CA-C	9.75	128.73	110.20
1	C	572	ASP	CB-CG-OD1	9.70	127.03	118.30
1	B	288	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	B	282	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	632	SER	N-CA-CB	9.61	124.91	110.50
1	C	917	ARG	NE-CZ-NH2	9.57	125.09	120.30
1	A	234	ASP	CB-CG-OD2	-9.56	109.69	118.30
1	B	178	ARG	NE-CZ-NH1	9.53	125.07	120.30
1	A	610	ASP	CB-CG-OD2	-9.52	109.74	118.30
1	B	954	ASP	CB-CG-OD2	-9.43	109.81	118.30
1	D	428	ASP	CB-CG-OD2	-9.39	109.85	118.30
1	D	809	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	D	630	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	157	ARG	NE-CZ-NH1	9.29	124.94	120.30
1	C	363	HIS	CA-CB-CG	-9.21	97.94	113.60
1	D	479	ASP	CB-CG-OD1	9.19	126.57	118.30
1	C	469	ASP	CB-CG-OD1	9.17	126.55	118.30
1	C	224	ASP	CB-CG-OD1	9.15	126.53	118.30
1	A	404	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	B	13	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	B	579	ASP	CB-CG-OD2	-9.07	110.13	118.30
1	A	336	ARG	NE-CZ-NH1	9.06	124.83	120.30
1	C	671	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	B	908	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	B	832	ASP	CB-CG-OD2	-9.03	110.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	881	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	D	45	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	B	411	ASP	CB-CG-OD2	-8.96	110.23	118.30
1	D	559	TYR	CB-CG-CD2	-8.93	115.64	121.00
1	C	199	ASP	CB-CG-OD1	8.90	126.31	118.30
1	B	388	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	C	287	ASP	CB-CG-OD1	8.86	126.28	118.30
1	C	492	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	909	ARG	NE-CZ-NH2	-8.83	115.88	120.30
1	C	557	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	A	611	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	579	ASP	CB-CG-OD2	-8.76	110.42	118.30
1	C	572	ASP	CB-CG-OD2	-8.75	110.43	118.30
1	B	255	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	594	ASP	CB-CG-OD1	8.68	126.11	118.30
1	D	699	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	C	469	ASP	CB-CG-OD2	-8.64	110.52	118.30
1	A	255	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	832	ASP	CB-CG-OD1	8.58	126.03	118.30
1	C	610	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	D	233	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	D	144	ASP	CB-CG-OD1	8.55	126.00	118.30
1	D	659	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	B	800	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	C	832	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	C	473	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	B	997	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	C	610	ASP	CB-CG-OD1	8.47	125.92	118.30
1	C	908	ASP	CB-CG-OD1	8.46	125.91	118.30
1	D	559	TYR	CB-CG-CD1	8.45	126.07	121.00
1	C	237	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	D	954	ASP	CB-CG-OD1	8.43	125.88	118.30
1	A	52	ARG	NE-CZ-NH1	8.41	124.51	120.30
1	B	411	ASP	CB-CG-OD1	8.41	125.87	118.30
1	B	648	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	A	234	ASP	CB-CG-OD1	8.38	125.84	118.30
1	A	997	ASP	CB-CG-OD1	8.37	125.83	118.30
1	A	45	ASP	CB-CG-OD1	8.36	125.83	118.30
1	C	857	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	D	469	ASP	CB-CG-OD1	8.34	125.80	118.30
1	B	310	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	A	45	ASP	CB-CG-OD2	-8.24	110.88	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	875	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	610	ASP	CB-CG-OD1	8.22	125.69	118.30
1	C	172	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	A	82	ASP	CB-CG-OD2	-8.19	110.93	118.30
1	C	792	ASP	CB-CG-OD1	8.17	125.65	118.30
1	D	199	ASP	CB-CG-OD2	-8.16	110.95	118.30
1	D	792	ASP	CB-CG-OD1	8.15	125.63	118.30
1	B	509	ASP	CB-CG-OD1	8.13	125.62	118.30
1	C	224	ASP	CB-CG-OD2	-8.13	110.98	118.30
1	D	919	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	429	ASP	CB-CG-OD1	8.06	125.56	118.30
1	B	611	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	233	ASP	CB-CG-OD1	8.04	125.53	118.30
1	B	908	ASP	CB-CG-OD1	8.03	125.53	118.30
1	D	746	ASP	CB-CA-C	-8.02	94.36	110.40
1	C	280	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	D	237	ARG	CD-NE-CZ	8.00	134.79	123.60
1	A	509	ASP	CB-CG-OD1	7.99	125.49	118.30
1	A	856	TYR	CB-CG-CD2	-7.99	116.21	121.00
1	D	572	ASP	CB-CG-OD2	-7.98	111.12	118.30
1	D	648	ASP	CB-CG-OD2	-7.97	111.12	118.30
1	C	442	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	B	166	ARG	NE-CZ-NH1	7.95	124.28	120.30
1	B	492	ASP	CB-CG-OD1	7.95	125.45	118.30
1	D	610	ASP	CB-CG-OD1	7.95	125.45	118.30
1	B	13	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	B	280	ASP	CB-CG-OD1	7.94	125.44	118.30
1	D	292	ARG	NE-CZ-NH1	7.93	124.27	120.30
1	D	204	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	772	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	579	ASP	CB-CG-OD1	7.90	125.41	118.30
1	A	479	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	A	746	ASP	CB-CG-OD2	-7.87	111.21	118.30
1	B	919	ASP	CB-CG-OD2	-7.87	111.22	118.30
1	A	172	ASP	CB-CG-OD1	7.84	125.36	118.30
1	A	509	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	630	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	C	594	ASP	CB-CG-OD1	7.78	125.31	118.30
1	A	479	ASP	CB-CG-OD1	7.77	125.29	118.30
1	C	599	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	C	828	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	D	908	ASP	CB-CG-OD2	-7.76	111.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	ASP	CB-CG-OD1	7.76	125.29	118.30
1	A	908	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	C	356	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	D	336	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	D	255	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	B	45	ASP	CB-CG-OD1	7.73	125.26	118.30
1	D	469	ASP	CB-CG-OD2	-7.73	111.34	118.30
1	D	199	ASP	CB-CG-OD1	7.72	125.25	118.30
1	C	429	ASP	CB-CG-OD2	-7.72	111.36	118.30
1	D	497	ASP	CB-CG-OD1	7.70	125.23	118.30
1	B	579	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	233	ASP	CB-CG-OD1	7.67	125.20	118.30
1	B	610	ASP	CB-CG-OD2	-7.67	111.40	118.30
1	D	288	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	224	ASP	CB-CG-OD1	7.65	125.18	118.30
1	A	233	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	B	671	ASP	CB-CG-OD2	-7.64	111.43	118.30
1	D	204	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	178	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	130	ASP	CB-CG-OD2	-7.62	111.45	118.30
1	A	954	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	D	356	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	782	ASP	CB-CG-OD1	7.58	125.12	118.30
1	A	786	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	D	802	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	411	ASP	CB-CG-OD2	-7.53	111.52	118.30
1	A	201	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	428	ASP	CB-CG-OD1	7.51	125.06	118.30
1	D	492	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	D	569	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	C	473	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	C	671	ASP	CB-CG-OD1	7.49	125.04	118.30
1	B	356	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	D	429	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	B	598	ASP	CB-CG-OD1	7.46	125.01	118.30
1	C	15	ASP	CB-CG-OD2	-7.46	111.59	118.30
1	B	997	ASP	CB-CG-OD1	7.44	125.00	118.30
1	C	319	ASP	CB-CG-OD1	7.42	124.98	118.30
1	D	429	ASP	CB-CG-OD1	7.41	124.97	118.30
1	C	287	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	538	TYR	CB-CG-CD1	-7.41	116.56	121.00
1	C	954	ASP	CB-CG-OD1	7.40	124.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	800	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	C	403	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	553	TRP	CA-CB-CG	-7.38	99.67	113.70
1	A	954	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	85	VAL	CB-CA-C	-7.37	97.40	111.40
1	B	869	ASP	CB-CG-OD1	7.37	124.93	118.30
1	B	287	ASP	CB-CG-OD1	7.36	124.92	118.30
1	D	428	ASP	CB-CG-OD1	7.35	124.92	118.30
1	D	909	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	B	144	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	318	ALA	CB-CA-C	-7.33	99.10	110.10
1	C	741	THR	CA-CB-CG2	-7.33	102.14	112.40
1	B	448	ARG	NE-CZ-NH2	-7.32	116.64	120.30
1	B	531	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	477	SER	N-CA-CB	-7.30	99.55	110.50
1	A	769	TRP	CB-CA-C	-7.30	95.80	110.40
1	C	442	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	D	252	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	46	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	333	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	C	881	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	782	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	B	77	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	B	782	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	B	52	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	482	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	D	772	ASP	N-CA-CB	-7.21	97.62	110.60
1	C	916	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	D	201	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	336	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	D	77	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	D	796	SER	N-CA-CB	7.16	121.24	110.50
1	B	185	ALA	N-CA-CB	7.15	120.11	110.10
1	B	919	ASP	CB-CG-OD1	7.15	124.73	118.30
1	D	319	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	B	746	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	D	287	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	942	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	D	126	THR	CA-CB-CG2	-7.10	102.45	112.40
1	B	610	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	280	ASP	CB-CG-OD1	7.09	124.69	118.30
1	C	772	ASP	CB-CG-OD1	7.09	124.68	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	828	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	185	ALA	N-CA-CB	7.08	120.02	110.10
1	B	368	ASP	CB-CG-OD2	-7.05	111.95	118.30
1	C	59	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	659	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	699	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	C	832	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	987	ASP	CB-CG-OD1	7.00	124.60	118.30
1	A	707	ALA	CB-CA-C	-7.00	99.60	110.10
1	C	685	LEU	O-C-N	7.00	134.40	121.10
1	B	509	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	C	336	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	1018	LEU	CB-CA-C	-6.98	96.93	110.20
1	B	319	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	C	199	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	15	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	C	853	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	639	THR	CA-CB-CG2	-6.97	102.64	112.40
1	A	26	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	D	875	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	B	329	ASP	CB-CG-OD2	-6.94	112.05	118.30
1	B	561	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	857	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	659	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	B	916	ASP	CB-CG-OD1	6.94	124.54	118.30
1	C	987	ASP	CB-CG-OD2	-6.94	112.06	118.30
1	D	311	ALA	N-CA-CB	6.94	119.81	110.10
1	A	594	ASP	CB-CG-OD2	-6.93	112.06	118.30
1	D	147	ASN	N-CA-CB	-6.93	98.13	110.60
1	C	569	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	952	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	82	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	908	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	611	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	A	442	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	251	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	C	310	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	B	569	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	C	772	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	B	447	ASP	CB-CG-OD1	6.87	124.48	118.30
1	A	973	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	472	TYR	CB-CG-CD2	-6.86	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	ASP	CB-CG-OD1	6.83	124.45	118.30
1	D	368	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	D	792	ASP	CB-CG-OD2	-6.83	112.16	118.30
1	D	659	ASP	CB-CG-OD1	6.82	124.44	118.30
1	D	755	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	B	199	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	648	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	45	ASP	CB-CG-OD1	6.81	124.43	118.30
1	B	233	ASP	CB-CG-OD2	-6.80	112.18	118.30
1	B	469	ASP	CB-CG-OD1	6.80	124.42	118.30
1	A	318	ALA	CA-C-O	6.79	134.37	120.10
1	A	431	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	579	ASP	CB-CG-OD1	6.79	124.41	118.30
1	C	329	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	B	140	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	C	43	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	A	859	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	916	ASP	CB-CG-OD1	6.76	124.38	118.30
1	A	96	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	D	706	THR	CA-CB-CG2	-6.74	102.96	112.40
1	D	45	ASP	CB-CG-OD1	6.72	124.34	118.30
1	D	439	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	237	ARG	CD-NE-CZ	6.70	132.97	123.60
1	A	446	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	429	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	B	237	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	869	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	144	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	D	769	TRP	CB-CA-C	-6.64	97.11	110.40
1	C	987	ASP	CB-CG-OD1	6.64	124.27	118.30
1	B	164	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	B	507	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	C	769	TRP	CB-CA-C	-6.63	97.14	110.40
1	D	856	TYR	CB-CG-CD1	6.62	124.97	121.00
1	A	553	TRP	CA-CB-CG	-6.62	101.13	113.70
1	B	403	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	869	ASP	CB-CG-OD1	6.58	124.23	118.30
1	B	996	ASP	CB-CG-OD1	6.58	124.22	118.30
1	D	15	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	D	15	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	772	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	59	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	B	553	TRP	CA-CB-CG	-6.55	101.25	113.70
1	A	802	ASP	CB-CG-OD2	-6.55	112.40	118.30
1	C	429	ASP	CB-CG-OD1	6.55	124.19	118.30
1	A	329	ASP	CB-CG-OD1	6.54	124.19	118.30
1	D	954	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	772	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	D	782	ASP	CB-CG-OD1	6.54	124.19	118.30
1	C	172	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	193	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	D	237	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	D	130	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	329	ASP	CB-CG-OD1	6.52	124.17	118.30
1	C	996	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	D	594	ASP	CB-CG-OD2	-6.52	112.44	118.30
1	D	251	ARG	CD-NE-CZ	6.51	132.72	123.60
1	B	280	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	598	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	201	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	C	828	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	894	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	C	952	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	15	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	997	ASP	CB-CG-OD1	6.45	124.10	118.30
1	B	96	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	916	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	B	252	ASP	CA-CB-CG	-6.41	99.29	113.40
1	A	469	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	809	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	388	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	C	919	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	230	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	630	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	C	82	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	A	1018	LEU	CB-CA-C	-6.34	98.15	110.20
1	C	854	LYS	CB-CA-C	-6.34	97.71	110.40
1	D	648	ASP	CB-CG-OD1	6.34	124.00	118.30
1	A	280	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	916	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	D	77	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	280	ASP	CB-CG-OD2	-6.33	112.61	118.30
1	B	77	ASP	CB-CG-OD1	6.32	123.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	204	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	D	782	ASP	CB-CG-OD2	-6.31	112.62	118.30
1	B	685	LEU	N-CA-CB	6.30	123.00	110.40
1	A	52	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	746	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	D	224	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	77	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	C	569	ASP	CB-CG-OD1	6.26	123.94	118.30
1	B	252	ASP	CB-CG-OD2	-6.26	112.66	118.30
1	D	13	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	46	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	C	916	ASP	CB-CG-OD1	6.23	123.91	118.30
1	C	661	LYS	N-CA-CB	6.23	121.81	110.60
1	D	869	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	43	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	472	TYR	CB-CG-CD2	-6.22	117.27	121.00
1	A	164	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	B	405	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	A	356	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	952	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	792	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	A	942	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	C	319	ASP	CB-CG-OD2	-6.18	112.74	118.30
1	C	659	ASP	CB-CG-OD1	6.18	123.86	118.30
1	B	234	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	D	388	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	319	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	375	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	B	746	ASP	CB-CA-C	-6.16	98.09	110.40
1	B	82	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	648	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	952	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	746	ASP	CB-CA-C	-6.14	98.13	110.40
1	C	211	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	538	TYR	CB-CG-CD2	6.11	124.67	121.00
1	B	204	ARG	NE-CZ-NH2	-6.11	117.25	120.30
1	D	368	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	411	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	219	THR	CA-CB-CG2	-6.09	103.87	112.40
1	C	482	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	973	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	C	280	ASP	CB-CG-OD1	6.07	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	599	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	B	233	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	790	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	123	TYR	CB-CG-CD2	-6.04	117.37	121.00
1	C	230	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	185	ALA	CB-CA-C	6.03	119.14	110.10
1	A	310	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	772	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	875	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	690	SER	N-CA-CB	6.01	119.52	110.50
1	D	388	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	45	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	C	201	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	598	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	958	ASN	N-CA-CB	6.00	121.39	110.60
1	D	719	GLN	CB-CA-C	-5.99	98.42	110.40
1	D	741	THR	CA-CB-CG2	-5.99	104.02	112.40
1	C	204	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	166	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	469	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	15	ASP	CB-CG-OD1	5.98	123.68	118.30
1	A	77	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	802	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	405	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	A	659	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	280	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	C	802	ASP	N-CA-CB	5.95	121.30	110.60
1	B	946	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	C	492	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	D	492	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	59	ARG	NE-CZ-NH2	-5.93	117.34	120.30
1	A	781	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	252	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	B	199	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	199	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	D	287	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	B	486	TYR	CB-CG-CD1	-5.88	117.47	121.00
1	C	411	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	C	507	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	D	82	ASP	CB-CG-OD1	5.87	123.58	118.30
1	D	329	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	909	ARG	NE-CZ-NH1	5.86	123.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	569	ASP	CB-CG-OD1	5.86	123.57	118.30
1	D	881	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	318	ALA	CA-C-N	-5.85	104.34	117.20
1	B	183	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	164	ASP	CB-CG-OD1	5.84	123.56	118.30
1	D	251	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	505	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	B	531	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	C	472	TYR	CB-CG-CD1	5.81	124.49	121.00
1	A	856	TYR	CB-CG-CD1	5.81	124.49	121.00
1	C	917	ARG	CD-NE-CZ	-5.80	115.48	123.60
1	A	184	LEU	CB-CA-C	-5.79	99.19	110.20
1	B	920	LEU	CB-CA-C	-5.79	99.19	110.20
1	D	288	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	B	82	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	973	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	469	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	C	611	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	C	648	ASP	CB-CG-OD2	-5.75	113.13	118.30
1	D	838	THR	CA-CB-CG2	-5.74	104.36	112.40
1	B	859	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	C	792	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	D	43	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	919	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	D	820	ALA	N-CA-CB	5.72	118.11	110.10
1	D	110	ASN	N-CA-CB	-5.71	100.31	110.60
1	B	333	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	C	746	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	980	GLU	C-N-CA	-5.70	110.33	122.30
1	D	591	ASP	CB-CG-OD1	5.70	123.42	118.30
1	B	869	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	D	21	VAL	CA-CB-CG2	-5.69	102.37	110.90
1	D	553	TRP	CA-CB-CG	-5.69	102.89	113.70
1	A	425	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	172	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	B	792	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	329	ASP	CB-CG-OD1	5.66	123.40	118.30
1	A	411	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	690	SER	N-CA-C	5.64	126.23	111.00
1	B	210	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	689	GLU	N-CA-C	-5.64	95.78	111.00
1	B	781	ARG	NE-CZ-NH2	-5.64	117.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	193	ASP	CB-CG-OD1	5.63	123.36	118.30
1	A	828	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	210	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	95	TYR	CA-CB-CG	-5.62	102.73	113.40
1	D	891	VAL	CA-CB-CG2	-5.61	102.48	110.90
1	C	30	HIS	CA-CB-CG	-5.61	104.06	113.60
1	A	52	ARG	CB-CA-C	-5.61	99.19	110.40
1	A	130	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	234	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	368	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	B	230	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	D	221	GLN	N-CA-CB	-5.59	100.53	110.60
1	D	252	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	671	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	368	ASP	CB-CG-OD1	5.59	123.33	118.30
1	C	360	HIS	CA-CB-CG	-5.59	104.10	113.60
1	D	958	ASN	N-CA-CB	5.58	120.64	110.60
1	C	178	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	598	ASP	CB-CG-OD1	5.58	123.32	118.30
1	B	43	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	187	MET	CA-CB-CG	-5.57	103.83	113.30
1	C	479	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	B	15	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	A	317	THR	CA-CB-CG2	-5.57	104.60	112.40
1	A	951	TRP	N-CA-CB	5.57	120.62	110.60
1	A	881	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	996	ASP	CB-CG-OD2	-5.57	113.29	118.30
1	C	509	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	A	949	HIS	CB-CA-C	-5.55	99.31	110.40
1	C	164	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	828	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	721	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	130	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	123	TYR	CB-CG-CD2	-5.53	117.69	121.00
1	B	363	HIS	CA-CB-CG	-5.53	104.21	113.60
1	A	859	ASP	CB-CG-OD1	5.52	123.27	118.30
1	C	356	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	598	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	179	ALA	N-CA-CB	5.50	117.80	110.10
1	A	659	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	781	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	428	ASP	CB-CG-OD1	5.48	123.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	537	GLU	N-CA-CB	5.47	120.45	110.60
1	D	1020	TRP	CB-CG-CD2	-5.47	119.49	126.60
1	B	507	ASP	CB-CG-OD1	5.47	123.22	118.30
1	D	630	ARG	N-CA-CB	5.47	120.44	110.60
1	C	859	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	D	786	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	D	100	TYR	N-CA-CB	5.46	120.43	110.60
1	B	804	ASN	CA-CB-CG	-5.45	101.41	113.40
1	D	509	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	D	472	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	C	75	GLU	CB-CA-C	5.45	121.29	110.40
1	B	211	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	403	ASP	CB-CG-OD2	-5.43	113.42	118.30
1	A	193	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	569	ASP	CB-CG-OD1	5.42	123.18	118.30
1	D	333	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	857	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	D	144	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	425	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	337	ILE	CA-CB-CG1	-5.40	100.73	111.00
1	D	446	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	96	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	33	PHE	CB-CA-C	-5.40	99.60	110.40
1	C	477	SER	N-CA-CB	-5.39	102.41	110.50
1	D	757	GLN	CA-CB-CG	-5.39	101.54	113.40
1	D	425	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	D	161	TYR	CB-CG-CD2	-5.37	117.78	121.00
1	D	859	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	96	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	252	ASP	CA-CB-CG	-5.37	101.59	113.40
1	A	333	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	594	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	239	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	C	848	THR	CA-CB-CG2	-5.36	104.90	112.40
1	B	1005	ALA	N-CA-CB	5.35	117.59	110.10
1	D	980	GLU	C-N-CA	-5.34	111.08	122.30
1	D	802	ASP	C-N-CD	-5.34	108.85	120.60
1	C	920	LEU	CB-CA-C	-5.34	100.06	110.20
1	D	100	TYR	CB-CG-CD1	-5.33	117.80	121.00
1	D	183	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	1013	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	863	GLN	CA-CB-CG	-5.32	101.69	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1020	TRP	CG-CD2-CE3	-5.32	129.11	133.90
1	B	165	SER	CB-CA-C	-5.32	99.99	110.10
1	C	721	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	C	77	ASP	CB-CG-OD1	5.32	123.08	118.30
1	D	832	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	D	772	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	C	946	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	D	220	THR	CA-CB-CG2	-5.30	104.98	112.40
1	D	116	THR	CA-CB-CG2	-5.30	104.98	112.40
1	A	96	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	919	ASP	CB-CG-OD1	5.29	123.06	118.30
1	D	572	ASP	CB-CG-OD1	5.29	123.06	118.30
1	C	908	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	172	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	D	130	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	588	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	C	308	LEU	CB-CG-CD1	-5.27	102.04	111.00
1	C	746	ASP	CB-CG-OD1	5.27	123.05	118.30
1	D	201	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	729	THR	CA-C-N	-5.26	105.62	117.20
1	B	719	GLN	CB-CA-C	-5.26	99.88	110.40
1	D	997	ASP	CB-CG-OD1	5.26	123.03	118.30
1	D	679	LEU	CA-CB-CG	-5.25	103.22	115.30
1	D	96	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	492	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	779	PRO	N-CA-CB	5.24	109.58	103.30
1	B	106	PRO	N-CA-CB	5.24	109.58	103.30
1	D	133	TRP	CA-CB-CG	-5.23	103.75	113.70
1	B	769	TRP	CB-CA-C	-5.23	99.93	110.40
1	D	1006	GLU	N-CA-CB	5.22	120.00	110.60
1	D	166	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	C	52	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	802	ASP	N-CA-CB	5.22	119.99	110.60
1	C	457	SER	N-CA-CB	5.22	118.33	110.50
1	B	987	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	755	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	729	THR	C-N-CA	5.20	134.71	121.70
1	C	45	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	A	800	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	412	GLU	N-CA-CB	-5.19	101.26	110.60
1	B	237	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	997	ASP	CB-CG-OD2	-5.18	113.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	157	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	D	329	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	760	ARG	NE-CZ-NH2	5.17	122.89	120.30
1	D	875	ASP	CB-CG-OD1	5.17	122.95	118.30
1	A	224	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	52	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	B	909	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	221	GLN	CB-CA-C	-5.15	100.10	110.40
1	A	832	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	577	LYS	N-CA-CB	5.14	119.86	110.60
1	B	255	ARG	CB-CA-C	-5.14	100.13	110.40
1	C	67	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	A	598	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	746	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	246	MET	CG-SD-CE	-5.13	92.00	100.20
1	C	509	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	287	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	376	ILE	CA-CB-CG2	5.12	121.14	110.90
1	D	782	ASP	CB-CA-C	-5.12	100.17	110.40
1	B	282	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	836	ILE	CB-CA-C	-5.09	101.42	111.60
1	B	875	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	C	927	THR	CA-CB-CG2	-5.09	105.28	112.40
1	D	157	ARG	N-CA-CB	5.09	119.76	110.60
1	D	416	GLU	CG-CD-OE1	5.08	128.47	118.30
1	D	638	VAL	CB-CA-C	-5.08	101.75	111.40
1	C	942	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	D	172	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	760	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	D	538	TYR	CB-CG-CD2	5.07	124.04	121.00
1	C	746	ASP	N-CA-CB	-5.07	101.48	110.60
1	A	559	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	A	656	VAL	CA-CB-CG2	-5.06	103.30	110.90
1	D	961	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	D	247	CYS	N-CA-CB	5.06	119.71	110.60
1	C	77	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	98	PRO	N-CA-C	-5.06	98.95	112.10
1	D	724	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	A	311	ALA	N-CA-CB	5.05	117.17	110.10
1	D	157	ARG	CB-CA-C	5.05	120.50	110.40
1	A	778	THR	N-CA-CB	5.05	119.89	110.30
1	C	432	TRP	N-CA-CB	-5.04	101.52	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	686	PRO	C-N-CA	-5.04	109.10	121.70
1	A	110	ASN	C-N-CD	-5.04	109.52	120.60
1	A	987	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	651	LEU	CB-CA-C	5.03	119.76	110.20
1	D	881	ARG	NH1-CZ-NH2	-5.03	113.86	119.40
1	D	1020	TRP	CE2-CD2-CE3	5.03	124.74	118.70
1	B	859	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	786	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	A	996	ASP	CB-CG-OD1	5.03	122.82	118.30
1	C	826	THR	CA-CB-CG2	-5.02	105.37	112.40
1	A	671	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	B	100	TYR	N-CA-CB	5.02	119.63	110.60
1	C	184	LEU	CB-CA-C	-5.01	100.68	110.20
1	D	473	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	D	854	LYS	CB-CA-C	-5.01	100.38	110.40
1	D	546	LEU	N-CA-CB	5.01	120.41	110.40
1	B	632	SER	N-CA-CB	5.00	118.00	110.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	690	SER	CA
1	D	157	ARG	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8125	0	7716	342	0
1	B	8125	0	7716	320	0
1	C	8125	0	7716	322	0
1	D	8125	0	7716	248	0
2	A	11	0	8	1	0
2	B	11	0	8	0	0
2	C	11	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	11	0	9	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	3	0	0	0	0
4	B	3	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
5	A	76	0	114	26	0
5	B	80	0	120	26	0
5	C	60	0	90	11	0
5	D	60	0	90	4	0
6	B	14	0	19	7	0
6	D	14	0	19	6	0
7	A	753	0	0	22	0
7	B	734	0	0	11	0
7	C	716	0	0	17	0
7	D	754	0	0	18	0
All	All	35825	0	31349	1234	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:GLN:N	1:C:634:GLN:HE21	1.45	1.13
1:B:687:GLN:HG3	1:B:688:PRO:HD2	1.21	1.12
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.33	1.11
1:C:634:GLN:NE2	1:C:634:GLN:H	1.49	1.09
1:A:655:MET:HB3	1:A:699:ARG:HH12	0.95	1.09
1:B:655:MET:HE2	1:B:665:SER:HB3	1.12	1.07
1:B:133:TRP:HA	5:B:8504:DMS:H11	1.39	1.04
1:A:797:GLU:HG2	1:A:799:THR:HG23	1.33	1.03
1:C:843:GLN:HG2	1:C:848:THR:HA	1.40	1.02
1:A:651:LEU:HD11	1:A:667:GLU:HB2	1.37	1.01
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.45	0.97
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.29	0.97
1:B:418:HIS:HE2	6:B:2002:BTB:HO3	1.11	0.96
1:B:822:LEU:HD12	1:B:823:LEU:N	1.82	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:822:LEU:HD12	1:B:823:LEU:H	1.28	0.95
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.02	0.95
1:A:655:MET:HB3	1:A:699:ARG:NH1	1.81	0.95
1:B:830:LEU:HD13	1:B:857:ARG:HH21	1.29	0.94
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.33	0.93
1:C:778:THR:HG23	1:C:887:GLN:CB	1.99	0.92
1:B:46:ARG:HB3	1:B:47:PRO:HD2	1.52	0.92
1:D:651:LEU:HD11	1:D:667:GLU:HG3	1.52	0.92
1:D:720:TRP:HA	5:D:8427:DMS:H13	1.53	0.91
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.06	0.91
1:A:797:GLU:HG2	1:A:799:THR:CG2	2.00	0.90
1:A:634:GLN:HG2	1:A:682:LEU:HB2	1.54	0.90
1:A:765:LEU:HD21	1:A:768:MET:CE	2.02	0.89
1:C:135:GLN:HE21	1:C:135:GLN:HA	1.36	0.89
1:A:599:ARG:HH11	1:A:600:GLN:HE22	1.17	0.89
1:A:224:ASP:HB3	1:A:245:GLN:HG3	1.54	0.88
1:A:290:THR:HB	5:A:8412:DMS:C2	2.04	0.86
1:B:133:TRP:HA	5:B:8504:DMS:C1	2.06	0.86
1:A:765:LEU:HD21	1:A:768:MET:HE2	1.57	0.86
1:D:635:THR:CG2	1:D:679:LEU:HD22	2.05	0.86
1:C:49:GLN:NE2	1:C:49:GLN:H	1.74	0.86
1:B:796:SER:HA	1:B:801:ILE:O	1.75	0.85
1:C:858:ILE:HD12	1:C:864:MET:HA	1.58	0.85
1:A:600:GLN:H	1:A:600:GLN:HE21	1.25	0.84
5:A:8501:DMS:H22	7:A:8912:HOH:O	1.77	0.84
1:B:336:ARG:HB3	5:B:8409:DMS:S	2.18	0.84
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.43	0.83
1:B:843:GLN:HG3	1:B:848:THR:HA	1.60	0.83
1:B:46:ARG:HG3	1:B:46:ARG:HH11	1.43	0.83
1:B:655:MET:CE	1:B:665:SER:HB3	2.03	0.83
1:B:581:ASN:HB2	1:B:583:ASN:ND2	1.93	0.82
1:A:778:THR:HG23	1:A:887:GLN:CB	2.10	0.82
1:A:131:GLU:O	1:A:135:GLN:HG2	1.79	0.82
1:B:658:LEU:O	1:B:661:LYS:HG3	1.80	0.82
1:C:262:GLN:HG3	1:C:309:TYR:CE2	2.14	0.81
1:A:237:ARG:NH1	1:A:237:ARG:HB3	1.96	0.81
1:A:68:ALA:O	1:A:70:PRO:HD3	1.81	0.81
1:A:599:ARG:NH1	1:A:600:GLN:NE2	2.29	0.80
1:C:334:GLU:OE1	1:C:336:ARG:HD3	1.81	0.80
1:C:745:MET:HA	1:C:761:GLN:HE22	1.47	0.80
1:B:687:GLN:HG3	1:B:688:PRO:CD	2.09	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.64	0.80
1:B:79:PRO:HD2	1:B:80:GLU:OE2	1.82	0.80
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.17	0.80
1:D:720:TRP:HA	5:D:8427:DMS:C1	2.12	0.79
1:A:320:GLY:HA2	5:A:8406:DMS:H11	1.61	0.79
1:D:802:ASP:OD1	1:D:803:PRO:HD2	1.83	0.79
1:D:635:THR:HG22	1:D:679:LEU:HD22	1.65	0.78
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.64	0.78
1:D:857:ARG:HG2	1:D:857:ARG:HH11	1.46	0.78
1:A:615:PRO:O	1:A:618:THR:HG22	1.83	0.78
1:C:738:PRO:HA	1:C:751:LEU:HD12	1.66	0.77
1:B:830:LEU:HD13	1:B:857:ARG:NH2	1.99	0.77
1:B:131:GLU:O	1:B:135:GLN:HG2	1.84	0.77
1:D:835:LEU:C	1:D:836:ILE:HD13	2.04	0.77
1:A:599:ARG:NH1	1:A:600:GLN:HE22	1.82	0.77
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.65	0.77
1:B:1020:TRP:HD1	1:B:1021:CYS:N	1.81	0.77
1:A:730:LEU:HD21	1:B:823:LEU:O	1.85	0.77
1:A:775:GLN:C	1:A:776:LEU:HD23	2.04	0.77
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.00	0.76
1:D:370:GLN:HG2	7:D:8955:HOH:O	1.84	0.76
1:C:285:TYR:HB3	1:C:288:ARG:HG3	1.65	0.76
1:C:843:GLN:HG2	1:C:848:THR:CA	2.15	0.76
1:C:824:GLN:HG3	1:C:825:CYS:N	2.00	0.75
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.69	0.75
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.51	0.75
1:C:857:ARG:C	1:C:858:ILE:HD13	2.07	0.74
1:C:316:HIS:HA	1:C:323:ILE:HG13	1.66	0.74
1:D:773:LYS:HG2	1:D:775:GLN:HE22	1.52	0.74
1:B:890:GLN:HG3	1:B:891:VAL:N	2.02	0.74
1:C:952:ARG:HH11	1:C:952:ARG:HG3	1.52	0.74
1:A:79:PRO:HD2	1:A:80:GLU:OE1	1.88	0.74
1:A:797:GLU:O	1:A:801:ILE:HD13	1.88	0.73
1:C:355:ASN:OD1	1:C:388:ARG:HD3	1.87	0.73
1:B:843:GLN:CG	1:B:848:THR:HA	2.18	0.73
1:A:774:LYS:HB2	1:A:774:LYS:HZ3	1.53	0.73
1:C:858:ILE:HD11	1:C:864:MET:HG3	1.69	0.73
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.70	0.73
1:A:290:THR:HB	5:A:8412:DMS:H22	1.70	0.73
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.24	0.73
1:C:625:GLN:NE2	7:C:8715:HOH:O	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.25	0.72
1:C:759:ASN:OD1	1:C:761:GLN:N	2.23	0.72
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.71	0.72
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.04	0.72
1:D:599:ARG:HB3	7:D:9126:HOH:O	1.89	0.72
1:C:79:PRO:HD2	1:C:80:GLU:OE2	1.90	0.72
1:C:579:ASP:OD1	1:C:583:ASN:N	2.22	0.72
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.72	0.72
1:A:527:PRO:HB3	1:B:339:ASN:O	1.90	0.71
1:A:890:GLN:HG3	1:A:891:VAL:N	2.04	0.71
1:B:102:ASN:HD22	5:B:8506:DMS:H13	1.56	0.71
1:A:703:PRO:O	1:A:711:ALA:HB1	1.91	0.71
1:A:38:ASN:OD1	1:A:40:GLU:HB3	1.91	0.71
1:C:887:GLN:NE2	1:C:980:GLU:O	2.22	0.71
1:A:767:GLN:NE2	1:A:774:LYS:HD2	2.06	0.71
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.06	0.71
1:B:75:GLU:HA	1:B:75:GLU:OE1	1.90	0.71
1:C:595:THR:HA	1:C:596:PRO:C	2.11	0.71
1:C:400:THR:O	1:C:404:ARG:HG3	1.90	0.71
1:B:639:THR:OG1	1:B:677:LYS:HD3	1.91	0.71
1:A:131:GLU:HG3	1:A:179:ALA:HB2	1.72	0.71
1:C:237:ARG:NH1	1:C:296:GLU:HG3	2.05	0.71
1:B:1023:LYS:HD3	1:B:1023:LYS:H	1.55	0.71
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.22	0.70
1:D:853:ARG:HH12	1:D:871:GLU:HG3	1.57	0.70
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.73	0.70
1:D:658:LEU:O	1:D:661:LYS:HD2	1.91	0.70
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.26	0.70
1:C:358:GLU:HB3	1:C:367:MET:CG	2.21	0.70
1:A:290:THR:HB	5:A:8412:DMS:H23	1.73	0.70
1:D:629:PHE:C	1:D:630:ARG:HD3	2.11	0.70
1:A:634:GLN:HG2	1:A:682:LEU:HD12	1.74	0.70
1:C:782:ASP:HA	1:C:884:LEU:HD23	1.74	0.70
1:C:577:LYS:O	1:C:584:PRO:HA	1.91	0.69
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.06	0.69
1:B:102:ASN:HD22	5:B:8506:DMS:C1	2.05	0.69
1:C:94:GLY:HA3	5:C:8421:DMS:C1	2.22	0.69
1:C:94:GLY:HA3	5:C:8421:DMS:H13	1.74	0.69
1:B:133:TRP:CA	5:B:8504:DMS:H11	2.20	0.69
1:C:145:GLY:HA3	1:C:210:ARG:HB2	1.74	0.69
1:D:36:TRP:CD1	1:D:48:SER:HB2	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:770:ILE:HD12	1:D:775:GLN:NE2	2.08	0.69
1:C:358:GLU:HB3	1:C:367:MET:HG2	1.74	0.69
1:C:78:LEU:HB3	1:C:80:GLU:OE1	1.93	0.69
1:A:320:GLY:HA2	5:A:8406:DMS:C1	2.22	0.69
1:B:237:ARG:HG3	1:B:237:ARG:NH1	2.06	0.69
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.08	0.69
1:B:822:LEU:O	1:B:823:LEU:HD23	1.93	0.69
1:B:843:GLN:HG2	1:B:847:LYS:C	2.13	0.69
1:B:600:GLN:H	1:B:600:GLN:HE21	1.41	0.68
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.06	0.68
1:D:878:HIS:HD2	7:D:8606:HOH:O	1.77	0.68
1:B:822:LEU:HD11	1:B:824:GLN:O	1.93	0.68
1:A:778:THR:HG23	1:A:887:GLN:HB2	1.72	0.68
1:A:599:ARG:HH11	1:A:600:GLN:NE2	1.86	0.68
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.77	0.67
1:C:178:ARG:NH1	1:C:181:GLU:O	2.26	0.67
1:B:746:ASP:CA	1:B:760:ARG:HG3	2.24	0.67
1:D:757:GLN:HG3	1:D:758:PHE:N	2.08	0.67
1:A:853:ARG:HH12	1:A:871:GLU:HG3	1.59	0.67
1:C:858:ILE:N	1:C:858:ILE:HD13	2.07	0.67
1:D:577:LYS:NZ	1:D:591:ASP:O	2.27	0.67
1:A:658:LEU:O	1:A:661:LYS:HG3	1.94	0.67
1:A:131:GLU:HB3	1:A:135:GLN:NE2	2.09	0.67
1:C:684:GLU:O	1:C:686:PRO:HD3	1.94	0.67
1:A:128:ASN:OD1	1:A:180:GLY:HA2	1.95	0.67
1:A:797:GLU:N	1:A:800:ARG:O	2.27	0.67
1:B:1020:TRP:CD1	1:B:1021:CYS:N	2.63	0.67
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.60	0.67
1:B:801:ILE:HG22	1:B:802:ASP:H	1.58	0.67
1:A:628:GLN:NE2	5:A:8402:DMS:O	2.27	0.67
1:D:651:LEU:HD21	1:D:653:HIS:HE1	1.60	0.67
1:A:1020:TRP:HD1	1:A:1021:CYS:N	1.93	0.66
1:B:79:PRO:HG2	1:B:80:GLU:HG3	1.76	0.66
1:A:128:ASN:HA	1:A:180:GLY:O	1.95	0.66
1:B:46:ARG:CG	1:B:46:ARG:HH11	2.09	0.66
1:C:17:GLU:HG2	1:C:113:PHE:HA	1.78	0.66
1:B:86:VAL:HG13	1:B:87:PRO:HA	1.77	0.66
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:C:738:PRO:CA	1:C:751:LEU:HD12	2.25	0.66
1:B:37:ARG:NH2	1:B:218:PRO:HD3	2.10	0.66
1:C:375:ASP:O	1:C:379:MET:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:GLU:OE2	1:D:245:GLN:NE2	2.27	0.66
1:C:896:ASN:HB3	1:C:945:ASN:HB2	1.78	0.66
1:C:797:GLU:OE1	1:C:800:ARG:HB2	1.96	0.66
1:A:759:ASN:OD1	1:A:761:GLN:N	2.29	0.66
1:A:759:ASN:OD1	1:A:762:SER:N	2.27	0.66
1:A:776:LEU:HD23	1:A:776:LEU:N	2.09	0.66
1:C:730:LEU:HD21	1:D:823:LEU:O	1.95	0.66
5:C:8417:DMS:H21	7:C:9028:HOH:O	1.95	0.66
1:D:629:PHE:O	1:D:630:ARG:HD3	1.96	0.66
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.78	0.66
1:D:634:GLN:NE2	1:D:683:PRO:O	2.29	0.66
1:A:319:ASP:HB2	7:A:9169:HOH:O	1.96	0.65
1:B:801:ILE:HG22	1:B:802:ASP:N	2.11	0.65
1:D:965:GLN:O	1:D:969:GLU:HG3	1.95	0.65
1:D:782:ASP:HA	1:D:884:LEU:HD23	1.78	0.65
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.27	0.65
1:A:800:ARG:HB2	1:A:800:ARG:HH11	1.61	0.65
1:B:237:ARG:NE	1:B:296:GLU:OE1	2.29	0.65
1:D:128:ASN:HA	1:D:180:GLY:O	1.96	0.65
1:C:38:ASN:OD1	1:C:41:GLU:HG3	1.97	0.65
1:A:73:TRP:CZ2	1:A:122:CYS:HB3	2.31	0.65
1:A:869:ASP:OD1	1:A:1015:HIS:ND1	2.23	0.65
1:A:887:GLN:NE2	1:A:980:GLU:O	2.29	0.65
1:C:822:LEU:HD12	1:C:824:GLN:H	1.62	0.65
1:A:157:ARG:HD3	7:A:9138:HOH:O	1.96	0.65
1:A:256:VAL:O	1:A:271:THR:HA	1.97	0.65
1:C:858:ILE:HD12	1:C:864:MET:CA	2.26	0.64
1:B:36:TRP:CD1	1:B:48:SER:HB2	2.31	0.64
1:A:843:GLN:HG2	1:A:848:THR:HA	1.78	0.64
1:B:52:ARG:HG3	1:B:214:LEU:HB2	1.79	0.64
1:A:765:LEU:HD21	1:A:768:MET:HE1	1.78	0.64
1:C:128:ASN:HB2	1:C:181:GLU:OE1	1.97	0.64
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.33	0.64
1:C:847:LYS:NZ	1:D:724:GLU:O	2.30	0.64
1:D:635:THR:HG21	1:D:679:LEU:HD22	1.80	0.64
1:C:822:LEU:HD12	1:C:823:LEU:N	2.12	0.64
1:D:577:LYS:O	1:D:584:PRO:HA	1.97	0.64
1:B:233:ASP:HA	5:B:8417:DMS:H11	1.78	0.64
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.29	0.64
1:D:486:TYR:CE2	1:D:488:GLY:HA3	2.32	0.64
1:B:948:PRO:O	1:B:1022:GLN:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ARG:HB3	1:B:47:PRO:CD	2.27	0.64
1:B:795:VAL:O	1:B:800:ARG:NH2	2.30	0.64
1:D:88:SER:HA	1:D:366:VAL:HG21	1.80	0.64
1:A:651:LEU:HD21	1:A:653:HIS:NE2	2.13	0.64
1:A:965:GLN:O	1:A:969:GLU:HG3	1.98	0.64
1:C:961:ARG:NH2	1:C:979:GLU:O	2.29	0.64
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.80	0.63
1:A:907:PRO:HG2	1:A:990:HIS:O	1.99	0.63
1:A:599:ARG:HB2	1:A:600:GLN:HE21	1.63	0.63
1:B:802:ASP:H	1:B:803:PRO:HD3	1.61	0.63
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.97	0.63
1:B:615:PRO:O	1:B:618:THR:HG22	1.97	0.63
1:A:194:GLY:O	1:A:198:GLU:HG3	1.99	0.63
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.29	0.63
1:C:940:GLY:HA2	7:C:9022:HOH:O	1.98	0.63
1:C:237:ARG:CG	1:C:237:ARG:HH11	2.11	0.63
1:B:759:ASN:OD1	1:B:761:GLN:N	2.30	0.63
1:C:685:LEU:HD23	1:C:686:PRO:HD2	1.81	0.63
1:D:785:THR:O	1:D:881:ARG:HD2	1.99	0.63
1:B:595:THR:HA	1:B:596:PRO:C	2.19	0.63
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.33	0.62
1:A:769:TRP:HA	1:A:773:LYS:O	1.99	0.62
1:B:252:ASP:OD2	1:B:252:ASP:N	2.30	0.62
1:C:858:ILE:CD1	1:C:864:MET:HA	2.29	0.62
1:C:858:ILE:CD1	1:C:864:MET:HG3	2.30	0.62
1:D:277:GLU:OE1	1:D:277:GLU:HA	1.96	0.62
1:B:237:ARG:HH11	1:B:237:ARG:CG	2.13	0.62
1:B:78:LEU:HD22	1:B:80:GLU:OE2	2.00	0.62
1:D:634:GLN:O	1:D:682:LEU:N	2.29	0.62
1:B:746:ASP:HA	1:B:760:ARG:CG	2.24	0.62
1:C:746:ASP:HA	1:C:760:ARG:HG2	1.81	0.62
1:A:878:HIS:HD2	7:A:8576:HOH:O	1.81	0.62
1:C:777:LEU:CD1	1:C:980:GLU:HB3	2.30	0.62
1:A:655:MET:HE3	1:A:664:ALA:O	2.00	0.62
1:B:78:LEU:HB3	1:B:80:GLU:OE2	2.00	0.62
1:A:847:LYS:NZ	1:B:724:GLU:O	2.33	0.62
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.35	0.62
1:D:86:VAL:HG13	1:D:87:PRO:HA	1.82	0.62
1:B:178:ARG:NH1	1:B:181:GLU:O	2.23	0.62
1:C:802:ASP:OD1	1:C:803:PRO:HD2	2.00	0.62
1:A:784:PHE:HA	1:A:881:ARG:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:HB2	1:A:209:PHE:CE2	2.35	0.62
1:B:88:SER:HA	1:B:366:VAL:HG21	1.82	0.62
1:B:71:GLU:H	1:B:71:GLU:CD	2.03	0.62
1:C:145:GLY:CA	1:C:210:ARG:HB2	2.29	0.61
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.65	0.61
1:D:646:HIS:HB2	7:D:9165:HOH:O	1.98	0.61
1:D:835:LEU:O	1:D:836:ILE:HD13	1.99	0.61
1:D:420:MET:HE2	1:D:425:ARG:HB3	1.80	0.61
1:A:802:ASP:OD1	1:A:803:PRO:HD2	2.00	0.61
1:C:581:ASN:HB3	1:C:583:ASN:HD22	1.66	0.61
1:C:660:GLY:O	1:C:662:PRO:HD3	1.99	0.61
1:D:595:THR:HA	1:D:596:PRO:C	2.20	0.61
1:A:774:LYS:HB2	1:A:774:LYS:NZ	2.15	0.61
1:A:502:MET:O	1:A:517:LYS:HE3	1.99	0.61
1:C:130:ASP:OD2	1:C:132:SER:N	2.31	0.61
1:C:721:ARG:NE	7:C:8891:HOH:O	2.25	0.61
1:C:278:ILE:N	1:C:278:ILE:HD13	2.15	0.61
1:A:736:ALA:CB	1:A:751:LEU:HD11	2.31	0.61
1:A:595:THR:HA	1:A:596:PRO:C	2.21	0.61
1:D:580:GLU:HA	1:D:580:GLU:OE1	2.00	0.60
1:C:339:ASN:O	1:D:527:PRO:HB3	2.01	0.60
1:D:272:ALA:HB1	1:D:273:PRO:HD2	1.82	0.60
1:A:737:ILE:HD13	1:A:738:PRO:HD2	1.82	0.60
1:C:696:LEU:HD12	1:C:697:THR:N	2.16	0.60
1:D:393:PRO:HD3	1:D:412:GLU:O	2.00	0.60
1:B:128:ASN:HA	1:B:180:GLY:O	2.01	0.60
1:B:502:MET:SD	6:B:2002:BTB:H62	2.42	0.60
1:B:237:ARG:HG3	1:B:237:ARG:HH11	1.67	0.60
1:B:233:ASP:HA	5:B:8417:DMS:C1	2.31	0.60
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.82	0.60
1:D:1006:GLU:HG2	1:D:1007:PHE:CD1	2.36	0.60
1:B:738:PRO:CA	1:B:751:LEU:HD12	2.31	0.60
1:A:749:ILE:O	1:A:755:ARG:HB3	2.01	0.60
1:C:88:SER:HA	1:C:366:VAL:HG21	1.84	0.60
1:B:769:TRP:CZ2	1:B:774:LYS:HE3	2.37	0.60
1:C:740:LEU:HB3	7:C:9005:HOH:O	2.01	0.60
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.84	0.60
1:B:216:HIS:CG	5:B:8504:DMS:H12	2.37	0.60
1:A:746:ASP:HA	1:A:760:ARG:HG3	1.84	0.60
1:A:736:ALA:HB3	1:A:751:LEU:HD11	1.84	0.60
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.33	0.60
1:D:893:GLU:HG3	1:D:894:ARG:HG2	1.84	0.60
1:D:178:ARG:NE	1:D:181:GLU:O	2.30	0.60
1:B:822:LEU:HD12	1:B:824:GLN:H	1.67	0.59
1:B:1017:GLN:HB3	7:B:9181:HOH:O	2.01	0.59
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.38	0.59
1:A:367:MET:HB3	1:A:372:MET:HE3	1.84	0.59
1:C:36:TRP:CD1	1:C:48:SER:HB2	2.37	0.59
1:A:646:HIS:NE2	1:A:671:ASP:OD1	2.29	0.59
1:D:853:ARG:NH1	7:D:8876:HOH:O	2.30	0.59
1:A:737:ILE:CD1	1:A:738:PRO:HD2	2.32	0.59
1:A:287:ASP:N	1:A:287:ASP:OD1	2.34	0.59
1:C:706:THR:HG1	1:C:709:SER:HG	1.50	0.59
1:C:858:ILE:HD11	1:C:864:MET:CG	2.33	0.59
1:A:738:PRO:HB3	1:A:751:LEU:HB2	1.84	0.59
6:B:2002:BTB:H32	6:B:2002:BTB:H61	1.83	0.59
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.36	0.59
1:C:666:GLY:C	1:C:667:GLU:HG3	2.24	0.59
1:C:843:GLN:CG	1:C:848:THR:HA	2.23	0.58
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.85	0.58
1:D:62:TRP:CD1	1:D:95:TYR:HB3	2.38	0.58
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.38	0.58
1:D:873:ALA:O	1:D:876:THR:HG22	2.03	0.58
1:A:234:ASP:O	1:A:235:PHE:HB2	2.03	0.58
1:A:1017:GLN:HG2	7:A:9178:HOH:O	2.02	0.58
1:C:73:TRP:CZ2	1:C:122:CYS:HB3	2.39	0.58
1:B:895:VAL:O	1:B:919:ASP:HA	2.03	0.58
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.84	0.58
1:B:914:CYS:HB2	7:B:8862:HOH:O	2.04	0.58
1:C:696:LEU:HD12	1:C:697:THR:H	1.69	0.58
1:B:377:LEU:HD22	1:B:708:TRP:CA	2.32	0.58
1:D:240:LEU:HD23	1:D:240:LEU:C	2.24	0.58
1:B:795:VAL:HG12	7:B:9213:HOH:O	2.04	0.58
1:C:782:ASP:OD1	1:C:842:TRP:HH2	1.87	0.58
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.86	0.58
1:C:127:PHE:CD2	1:C:127:PHE:N	2.71	0.58
1:A:948:PRO:HD2	1:A:949:HIS:CD2	2.38	0.58
1:C:836:ILE:O	1:C:856:TYR:N	2.30	0.58
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.39	0.57
1:C:948:PRO:O	1:C:1022:GLN:HA	2.04	0.57
1:D:892:ALA:HB3	1:D:946:TYR:CE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:843:GLN:HA	1:C:847:LYS:O	2.04	0.57
1:D:681:GLU:HA	1:D:681:GLU:OE1	2.03	0.57
1:B:145:GLY:N	1:B:210:ARG:HB2	2.19	0.57
1:C:640:SER:O	1:C:675:GLN:HA	2.04	0.57
1:D:578:TYR:HA	1:D:583:ASN:O	2.04	0.57
6:D:2002:BTB:C8	6:D:2002:BTB:H62	2.34	0.57
1:D:836:ILE:N	1:D:836:ILE:HD13	2.18	0.57
1:A:646:HIS:ND1	7:A:9135:HOH:O	2.33	0.57
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.86	0.57
1:B:878:HIS:HE1	7:B:9063:HOH:O	1.86	0.57
1:A:111:PRO:HA	1:A:196:TYR:CE1	2.38	0.57
1:A:651:LEU:HD12	1:A:668:VAL:C	2.25	0.57
1:A:255:ARG:HG3	1:A:318:ALA:HA	1.86	0.57
1:C:907:PRO:HG2	1:C:990:HIS:O	2.05	0.57
1:B:861:SER:OG	1:B:863:GLN:HG3	2.05	0.57
1:C:762:SER:O	1:C:822:LEU:HD22	2.04	0.57
1:B:494:THR:HB	1:C:473:ARG:NH2	2.19	0.57
1:A:59:ARG:NH2	1:A:81:ALA:HB3	2.20	0.57
1:B:46:ARG:CB	1:B:47:PRO:HD2	2.32	0.57
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.20	0.57
1:A:427:THR:O	1:A:467:ASN:HB2	2.05	0.57
1:D:753:ASN:OD1	1:D:754:LYS:HG3	2.04	0.57
1:B:240:LEU:HD23	1:B:240:LEU:C	2.25	0.57
1:C:118:ASN:O	1:C:119:PRO:C	2.41	0.56
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.87	0.56
1:A:694:LEU:HB2	1:A:723:ALA:O	2.05	0.56
1:A:237:ARG:NH2	1:A:296:GLU:OE2	2.38	0.56
1:C:49:GLN:HE21	1:C:49:GLN:H	1.50	0.56
1:A:853:ARG:HH12	1:A:871:GLU:CG	2.18	0.56
1:B:155:ASN:N	1:B:183:ARG:O	2.28	0.56
1:A:367:MET:HB3	1:A:372:MET:CE	2.35	0.56
1:D:737:ILE:HG13	1:D:738:PRO:N	2.18	0.56
1:C:794:GLY:HA3	7:C:8757:HOH:O	2.04	0.56
1:C:381:GLN:O	1:C:621:LYS:HE3	2.05	0.56
1:A:13:ARG:NH2	1:D:13:ARG:HB2	2.20	0.56
1:C:80:GLU:H	1:C:80:GLU:CD	2.08	0.56
1:B:756:TRP:CE2	1:B:858:ILE:HD12	2.40	0.56
1:D:801:ILE:HG22	1:D:802:ASP:N	2.21	0.56
1:A:85:VAL:N	5:A:8414:DMS:O	2.34	0.56
1:B:769:TRP:NE1	1:B:774:LYS:HE3	2.21	0.56
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLY:O	1:C:198:GLU:HG3	2.05	0.56
1:A:153:TRP:CD1	1:A:158:TRP:HA	2.41	0.56
1:B:878:HIS:HD2	7:B:8595:HOH:O	1.89	0.56
1:A:30:HIS:HB2	1:A:31:PRO:HD2	1.87	0.56
1:C:777:LEU:HD13	1:C:980:GLU:HB3	1.88	0.56
1:D:660:GLY:HA3	7:D:9016:HOH:O	2.05	0.56
1:D:225:PHE:HA	1:D:243:GLU:O	2.06	0.56
1:C:127:PHE:HE2	1:C:184:LEU:HG	1.70	0.56
1:A:37:ARG:HB3	7:A:9101:HOH:O	2.05	0.56
1:B:651:LEU:C	1:B:651:LEU:HD23	2.26	0.56
1:D:153:TRP:CD1	1:D:158:TRP:HA	2.41	0.56
1:D:746:ASP:HA	1:D:760:ARG:HG3	1.87	0.55
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.89	0.55
1:B:734:SER:OG	1:B:860:GLY:HA3	2.05	0.55
1:C:878:HIS:HD2	7:C:8588:HOH:O	1.89	0.55
1:C:749:ILE:O	1:C:755:ARG:HA	2.05	0.55
1:B:338:GLU:HG2	7:B:9111:HOH:O	2.06	0.55
1:A:126:THR:O	1:A:126:THR:HG22	2.06	0.55
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.87	0.55
1:D:531:ARG:HB3	1:D:532:PRO:HD2	1.87	0.55
1:C:78:LEU:HB3	1:C:80:GLU:CD	2.26	0.55
1:B:236:SER:C	1:B:237:ARG:HG2	2.26	0.55
1:B:178:ARG:HD2	1:B:181:GLU:O	2.06	0.55
1:C:240:LEU:HD23	1:C:240:LEU:C	2.27	0.55
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.42	0.55
1:A:40:GLU:OE1	1:A:40:GLU:HA	2.06	0.55
1:B:237:ARG:CG	1:B:237:ARG:NH1	2.68	0.55
1:A:506:VAL:HG12	1:A:521:LYS:HE3	1.89	0.55
1:D:768:MET:O	1:D:775:GLN:N	2.34	0.55
1:C:237:ARG:HG2	1:C:237:ARG:HH11	1.71	0.55
1:A:30:HIS:HB2	1:A:31:PRO:CD	2.36	0.55
1:B:147:ASN:HB2	1:B:209:PHE:CE2	2.42	0.55
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.06	0.55
1:B:763:GLY:HA3	1:B:822:LEU:HD22	1.89	0.55
1:D:465:GLY:O	1:D:468:HIS:HB2	2.07	0.55
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.06	0.55
1:D:658:LEU:O	1:D:659:ASP:C	2.44	0.55
1:A:577:LYS:O	1:A:584:PRO:HA	2.07	0.55
1:A:742:THR:HG22	1:A:743:SER:N	2.21	0.54
1:B:986:ILE:HD11	1:B:1018:LEU:CD2	2.38	0.54
1:A:835:LEU:HD13	1:A:857:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:LEU:HD12	1:A:668:VAL:O	2.07	0.54
1:D:651:LEU:HD21	1:D:653:HIS:CE1	2.41	0.54
1:A:823:LEU:O	1:B:730:LEU:HD11	2.07	0.54
1:B:581:ASN:HB2	1:B:583:ASN:HD21	1.72	0.54
1:D:782:ASP:OD1	1:D:842:TRP:HH2	1.91	0.54
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.42	0.54
1:A:373:VAL:O	1:A:377:LEU:HG	2.07	0.54
1:B:667:GLU:O	1:B:668:VAL:HG23	2.07	0.54
1:D:14:ARG:HG2	1:D:14:ARG:HH11	1.73	0.54
1:A:844:HIS:HE1	7:A:9219:HOH:O	1.90	0.54
1:C:38:ASN:HB3	1:C:41:GLU:HG3	1.88	0.54
1:D:835:LEU:HD12	1:D:856:TYR:O	2.07	0.54
1:A:990:HIS:HD2	1:A:991:MET:O	1.91	0.54
1:B:968:MET:HE3	7:B:9218:HOH:O	2.08	0.54
1:C:610:ASP:O	1:C:611:ARG:HB2	2.07	0.54
1:B:740:LEU:HD12	1:B:748:CYS:O	2.07	0.54
1:B:46:ARG:CG	1:B:46:ARG:NH1	2.70	0.54
1:B:769:TRP:CE2	1:B:774:LYS:HE3	2.43	0.54
1:B:60:PHE:HA	1:B:122:CYS:O	2.07	0.54
1:D:687:GLN:HE21	1:D:687:GLN:HA	1.72	0.54
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.42	0.54
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.08	0.54
1:D:139:THR:OG1	1:D:216:HIS:HD2	1.91	0.54
1:D:970:THR:CG2	1:D:975:LEU:HB2	2.38	0.54
1:B:896:ASN:HA	1:B:918:TRP:O	2.07	0.54
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.72	0.53
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.34	0.53
1:A:808:GLU:OE1	1:A:811:LYS:HE2	2.08	0.53
1:C:786:ARG:HD3	1:C:880:ALA:HB1	1.90	0.53
1:C:890:GLN:HG3	1:C:891:VAL:N	2.23	0.53
1:D:749:ILE:N	1:D:749:ILE:HD12	2.23	0.53
1:C:367:MET:HB3	1:C:372:MET:CE	2.38	0.53
1:A:1020:TRP:CD1	1:A:1021:CYS:N	2.75	0.53
1:A:619:GLU:HG2	1:A:909:ARG:HG3	1.90	0.53
1:A:52:ARG:O	1:A:213:SER:HB2	2.09	0.53
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.90	0.53
1:C:576:ILE:HD12	1:C:584:PRO:HB2	1.90	0.53
1:D:486:TYR:CZ	1:D:488:GLY:HA3	2.43	0.53
1:D:14:ARG:HG2	1:D:14:ARG:NH1	2.22	0.53
1:D:98:PRO:HB2	1:D:203:TRP:CE3	2.43	0.53
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:907:PRO:HG2	1:D:990:HIS:O	2.08	0.53
1:C:658:LEU:O	1:C:659:ASP:C	2.46	0.53
1:A:320:GLY:O	5:A:8406:DMS:H13	2.08	0.53
1:A:737:ILE:HD12	1:A:737:ILE:C	2.29	0.53
1:B:756:TRP:CD2	1:B:858:ILE:HD12	2.42	0.53
1:C:867:THR:CG2	1:C:1015:HIS:HE1	2.22	0.53
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.90	0.53
1:D:651:LEU:HD12	1:D:668:VAL:C	2.29	0.53
1:D:769:TRP:HA	1:D:773:LYS:O	2.09	0.53
1:B:110:ASN:N	1:B:111:PRO:HD3	2.24	0.53
1:A:797:GLU:HB3	1:A:800:ARG:H	1.74	0.53
1:A:777:LEU:HG	1:A:889:ALA:HA	1.90	0.53
1:A:573:GLN:HB2	1:A:602:CYS:O	2.08	0.53
1:A:47:PRO:HA	5:A:8501:DMS:O	2.09	0.53
1:D:836:ILE:O	1:D:855:THR:HA	2.08	0.53
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.44	0.53
1:A:59:ARG:NH2	1:A:81:ALA:O	2.41	0.53
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.91	0.53
1:C:96:ASP:HB2	7:C:8851:HOH:O	2.09	0.53
1:B:1023:LYS:HD3	1:B:1023:LYS:N	2.24	0.53
1:A:807:VAL:HG22	1:A:811:LYS:HD3	1.90	0.53
1:D:843:GLN:HA	1:D:847:LYS:O	2.09	0.53
1:B:1013:ARG:NH1	7:B:9015:HOH:O	2.36	0.53
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.43	0.53
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.09	0.53
1:C:891:VAL:HG12	1:C:891:VAL:O	2.08	0.53
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.91	0.53
1:D:654:TRP:CZ3	1:D:656:VAL:HG23	2.44	0.53
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.44	0.53
1:A:797:GLU:CG	1:A:799:THR:HG23	2.24	0.52
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.91	0.52
1:D:347:LYS:HE2	7:D:8783:HOH:O	2.08	0.52
1:D:857:ARG:HH11	1:D:857:ARG:CG	2.20	0.52
1:C:38:ASN:CG	1:C:41:GLU:HG3	2.29	0.52
1:A:942:ARG:HA	1:A:953:GLY:O	2.08	0.52
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.45	0.52
1:A:824:GLN:HG2	1:A:825:CYS:N	2.22	0.52
1:D:352:ARG:HG2	1:D:553:TRP:CH2	2.44	0.52
1:A:750:GLU:HG3	1:A:751:LEU:N	2.24	0.52
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.25	0.52
1:B:947:GLY:O	1:B:1023:LYS:NZ	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:GLY:N	1:C:210:ARG:HB2	2.24	0.52
1:C:246:MET:CE	1:C:250:LEU:HD23	2.39	0.52
1:C:651:LEU:HB2	1:C:669:PRO:HA	1.91	0.52
6:D:2002:BTB:C8	6:D:2002:BTB:C6	2.88	0.52
1:A:571:VAL:CG2	1:A:609:ALA:HA	2.40	0.52
1:C:850:PHE:HA	1:C:871:GLU:O	2.09	0.52
1:C:832:ASP:OD1	1:C:832:ASP:N	2.43	0.52
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.43	0.52
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.24	0.52
1:A:701:VAL:O	1:A:703:PRO:HD3	2.09	0.52
1:C:765:LEU:HD21	1:C:768:MET:SD	2.50	0.52
1:D:814:GLY:HA2	7:D:8854:HOH:O	2.10	0.52
1:B:216:HIS:CD2	5:B:8504:DMS:H12	2.44	0.52
1:A:634:GLN:NE2	1:A:685:LEU:HD12	2.25	0.52
1:A:767:GLN:CG	1:A:774:LYS:HG2	2.41	0.52
1:C:237:ARG:NH1	1:C:296:GLU:OE1	2.43	0.52
1:B:13:ARG:O	1:B:14:ARG:C	2.44	0.52
1:C:135:GLN:NE2	1:C:135:GLN:HA	2.11	0.51
1:C:135:GLN:HE21	1:C:135:GLN:CA	2.15	0.51
1:C:131:GLU:OE2	1:C:135:GLN:OE1	2.29	0.51
1:C:858:ILE:HD12	1:C:864:MET:CB	2.40	0.51
1:A:255:ARG:HB2	1:A:316:HIS:CE1	2.44	0.51
1:B:233:ASP:CA	5:B:8417:DMS:H11	2.40	0.51
1:A:506:VAL:CG1	1:A:521:LYS:HE3	2.40	0.51
5:A:8410:DMS:H12	7:A:9021:HOH:O	2.09	0.51
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.78	0.51
1:A:445:GLN:HG2	7:A:8951:HOH:O	2.09	0.51
1:A:107:ILE:HA	5:A:8419:DMS:C2	2.40	0.51
1:C:777:LEU:HG	1:C:889:ALA:HA	1.92	0.51
1:A:782:ASP:OD1	1:A:842:TRP:HH2	1.93	0.51
1:A:851:ILE:O	1:A:870:VAL:HA	2.10	0.51
1:A:639:THR:HG22	1:A:640:SER:N	2.24	0.51
1:A:654:TRP:CE2	1:A:666:GLY:N	2.78	0.51
1:A:355:ASN:OD1	1:A:388:ARG:HD3	2.10	0.51
1:B:836:ILE:HG22	1:B:837:THR:N	2.26	0.51
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.92	0.51
1:C:581:ASN:HB3	1:C:583:ASN:ND2	2.24	0.51
1:B:965:GLN:O	1:B:969:GLU:HG3	2.10	0.51
1:D:251:ARG:HG3	7:D:9178:HOH:O	2.09	0.51
1:D:794:GLY:HA3	7:D:8771:HOH:O	2.09	0.51
1:A:157:ARG:NH1	1:A:175:ALA:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:472:TYR:O	1:D:476:LYS:HG2	2.11	0.51
1:A:93:HIS:HB3	1:A:95:TYR:CE1	2.46	0.51
1:A:250:LEU:C	1:A:251:ARG:HG2	2.29	0.51
1:D:585:TRP:HA	5:D:8411:DMS:S	2.49	0.51
1:C:740:LEU:HD12	1:C:741:THR:N	2.26	0.51
1:A:85:VAL:HG23	5:A:8414:DMS:O	2.11	0.51
1:C:100:TYR:CE2	1:C:602:CYS:HB3	2.45	0.51
1:A:737:ILE:HD12	1:A:738:PRO:N	2.26	0.51
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.46	0.51
1:D:651:LEU:HD11	1:D:667:GLU:CG	2.33	0.51
1:C:367:MET:HB3	1:C:372:MET:HE3	1.91	0.51
1:B:13:ARG:CZ	1:C:13:ARG:HG3	2.41	0.51
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.45	0.51
1:A:127:PHE:N	1:A:127:PHE:CD2	2.78	0.51
1:A:863:GLN:NE2	1:A:1021:CYS:HB2	2.25	0.50
1:A:804:ASN:ND2	1:A:1001:PRO:HG2	2.26	0.50
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.46	0.50
1:A:89:ASN:HA	1:A:206:SER:O	2.11	0.50
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.47	0.50
1:B:236:SER:O	1:B:237:ARG:HD3	2.10	0.50
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.46	0.50
1:B:701:VAL:O	1:B:703:PRO:HD3	2.12	0.50
1:A:893:GLU:C	1:A:894:ARG:HG2	2.31	0.50
1:D:579:ASP:N	1:D:583:ASN:O	2.40	0.50
1:B:689:GLU:O	1:B:690:SER:HB3	2.12	0.50
1:B:648:ASP:O	5:B:8425:DMS:O	2.29	0.50
1:A:652:LEU:N	1:A:668:VAL:O	2.27	0.50
1:C:103:VAL:HG22	1:C:418:HIS:CE1	2.46	0.50
1:C:46:ARG:HB3	1:C:47:PRO:HD2	1.93	0.50
1:D:747:PHE:CD1	1:D:827:ALA:HB2	2.47	0.50
1:A:809:ARG:HH21	1:A:1001:PRO:HG3	1.77	0.50
1:B:961:ARG:NH2	1:B:979:GLU:O	2.42	0.50
1:B:629:PHE:HA	1:B:637:GLU:O	2.11	0.50
1:C:747:PHE:CD1	1:C:827:ALA:HB2	2.47	0.50
1:B:72:SER:O	1:B:76:CYS:N	2.40	0.50
1:C:739:HIS:O	1:C:749:ILE:HA	2.12	0.50
1:A:360:HIS:CG	1:A:361:PRO:HD2	2.46	0.50
1:D:654:TRP:HZ3	1:D:656:VAL:HG23	1.77	0.50
1:D:142:ILE:HG23	1:D:170:GLU:HG2	1.93	0.50
1:C:630:ARG:HD2	1:C:637:GLU:OE1	2.12	0.50
1:A:92:MET:CE	1:A:92:MET:HA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:930:VAL:O	1:C:932:PRO:HD3	2.11	0.50
1:B:795:VAL:CG1	5:B:8506:DMS:C2	2.90	0.50
1:B:949:HIS:O	1:B:1023:LYS:NZ	2.36	0.50
1:A:745:MET:HE1	1:A:761:GLN:CB	2.42	0.50
1:A:770:ILE:O	1:A:771:GLY:C	2.48	0.50
1:A:599:ARG:HB2	1:A:600:GLN:NE2	2.26	0.50
1:B:100:TYR:O	1:B:597:ASN:HA	2.12	0.50
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.46	0.50
1:B:843:GLN:HG2	1:B:847:LYS:O	2.12	0.49
1:B:769:TRP:HE1	1:B:774:LYS:HE3	1.76	0.49
1:A:158:TRP:CZ2	1:A:160:GLY:HA2	2.47	0.49
1:A:92:MET:HE2	1:A:92:MET:HA	1.94	0.49
1:D:263:GLY:C	1:D:265:THR:H	2.16	0.49
1:D:639:THR:OG1	1:D:677:LYS:HE2	2.12	0.49
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.47	0.49
1:C:94:GLY:HA3	5:C:8421:DMS:H11	1.94	0.49
1:C:740:LEU:HD12	1:C:741:THR:H	1.76	0.49
1:A:646:HIS:HE2	1:A:671:ASP:CG	2.15	0.49
1:A:107:ILE:CA	5:A:8419:DMS:H21	2.42	0.49
5:C:8404:DMS:H21	7:C:8756:HOH:O	2.13	0.49
1:D:416:GLU:OE2	1:D:418:HIS:HB2	2.12	0.49
1:D:157:ARG:NH1	1:D:176:PHE:CD2	2.80	0.49
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.49
1:C:271:THR:HG22	1:C:272:ALA:N	2.27	0.49
1:A:277:GLU:H	1:A:277:GLU:CD	2.14	0.49
1:D:133:TRP:N	1:D:133:TRP:CD1	2.80	0.49
1:B:577:LYS:HD3	1:B:585:TRP:CH2	2.47	0.49
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.43	0.49
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.42	0.49
1:D:963:SER:HB3	1:D:983:TRP:NE1	2.27	0.49
1:C:49:GLN:NE2	1:C:49:GLN:N	2.52	0.49
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.30	0.49
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.93	0.49
1:D:745:MET:HE2	1:D:745:MET:HA	1.93	0.49
1:A:767:GLN:CD	1:A:774:LYS:HG2	2.33	0.49
1:A:225:PHE:HA	1:A:243:GLU:O	2.12	0.49
1:C:86:VAL:CG1	1:C:87:PRO:HA	2.41	0.49
6:D:2002:BTB:H41	7:D:8510:HOH:O	2.10	0.49
1:B:100:TYR:CZ	1:B:602:CYS:HB3	2.47	0.49
1:C:876:THR:OG1	1:C:877:PRO:HD2	2.12	0.49
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:774:LYS:HE2	7:D:9002:HOH:O	2.11	0.49
1:C:237:ARG:NH1	1:C:296:GLU:CG	2.76	0.49
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.79	0.49
1:D:691:ALA:HB1	1:D:727:SER:HB2	1.95	0.49
1:D:757:GLN:HG2	1:D:766:SER:OG	2.13	0.49
1:A:835:LEU:HD12	1:A:856:TYR:O	2.13	0.49
1:C:822:LEU:HD12	1:C:823:LEU:H	1.78	0.49
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.95	0.49
1:A:807:VAL:HG13	1:A:808:GLU:N	2.28	0.49
1:B:920:LEU:HD13	1:B:924:ASP:HB3	1.95	0.49
1:A:18:ASN:OD1	1:A:20:GLY:N	2.42	0.49
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.94	0.49
1:A:525:SER:HB3	1:B:525:SER:HB3	1.94	0.49
1:C:654:TRP:O	1:C:655:MET:HB3	2.12	0.49
1:C:685:LEU:HD23	1:C:686:PRO:CD	2.42	0.49
1:D:784:PHE:HA	1:D:881:ARG:O	2.13	0.49
1:D:157:ARG:HD3	1:D:176:PHE:CD2	2.47	0.49
1:A:500:CYS:HA	1:A:534:ILE:O	2.12	0.49
1:C:59:ARG:NH2	1:C:81:ALA:HB3	2.28	0.49
1:C:573:GLN:HB2	1:C:602:CYS:O	2.13	0.48
1:C:237:ARG:NH2	1:C:296:GLU:OE1	2.46	0.48
1:A:622:HIS:O	5:A:8402:DMS:H11	2.12	0.48
1:A:336:ARG:HH21	1:A:338:GLU:CD	2.16	0.48
1:B:262:GLN:HB2	1:B:267:VAL:HG21	1.93	0.48
1:B:630:ARG:NH2	1:B:637:GLU:OE1	2.47	0.48
1:C:689:GLU:CG	1:C:690:SER:H	2.24	0.48
1:D:130:ASP:OD1	1:D:132:SER:N	2.45	0.48
1:C:125:LEU:HG	1:C:126:THR:N	2.28	0.48
1:B:134:LEU:O	1:B:135:GLN:C	2.48	0.48
1:D:773:LYS:CG	1:D:775:GLN:NE2	2.75	0.48
1:D:176:PHE:N	1:D:176:PHE:CD1	2.81	0.48
1:C:59:ARG:HB2	1:C:124:SER:OG	2.14	0.48
1:D:68:ALA:O	1:D:70:PRO:HD3	2.13	0.48
1:C:635:THR:OG1	1:C:681:GLU:HG2	2.13	0.48
1:B:745:MET:SD	1:B:745:MET:N	2.82	0.48
1:A:634:GLN:NE2	1:A:685:LEU:CD1	2.77	0.48
1:C:334:GLU:CD	1:C:336:ARG:HD3	2.33	0.48
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.94	0.48
1:B:801:ILE:CG2	1:B:802:ASP:N	2.77	0.48
1:A:842:TRP:C	1:A:843:GLN:HG3	2.33	0.48
1:C:416:GLU:OE2	1:C:418:HIS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:GLY:HA2	1:A:998:SER:O	2.13	0.48
1:D:16:TRP:CG	1:D:189:LEU:HD13	2.49	0.48
1:D:651:LEU:CD2	1:D:653:HIS:HE1	2.26	0.48
1:A:322:LEU:HB2	5:A:8406:DMS:C2	2.44	0.48
1:B:930:VAL:O	1:B:932:PRO:HD3	2.14	0.48
1:B:873:ALA:O	1:B:876:THR:HG22	2.14	0.48
1:D:891:VAL:CG2	1:D:981:GLY:HA2	2.44	0.48
1:C:819:GLU:HG2	1:C:819:GLU:H	1.27	0.48
1:A:843:GLN:HB3	1:A:847:LYS:O	2.13	0.48
1:C:869:ASP:OD1	1:C:1015:HIS:ND1	2.42	0.48
1:B:142:ILE:HG12	1:B:170:GLU:CD	2.33	0.48
1:A:809:ARG:NH2	1:A:1001:PRO:CG	2.77	0.48
1:D:833:ALA:HB1	1:D:858:ILE:O	2.12	0.48
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.49	0.48
1:B:216:HIS:CD2	5:B:8504:DMS:C1	2.97	0.48
1:B:138:GLN:N	1:B:217:LYS:O	2.24	0.48
1:B:757:GLN:HG2	1:B:758:PHE:N	2.28	0.48
1:A:853:ARG:NH1	7:A:8845:HOH:O	2.23	0.48
1:A:721:ARG:NH2	7:A:8974:HOH:O	2.46	0.48
1:D:358:GLU:HB3	1:D:367:MET:HG2	1.96	0.48
1:A:655:MET:HG2	1:A:699:ARG:HH22	1.79	0.47
1:B:703:PRO:O	1:B:711:ALA:HB1	2.14	0.47
1:D:972:HIS:HB2	1:D:975:LEU:HG	1.95	0.47
1:D:140:ARG:HB2	1:D:171:PHE:O	2.14	0.47
1:C:797:GLU:HB2	1:C:800:ARG:HB2	1.96	0.47
1:D:131:GLU:HG2	1:D:135:GLN:OE1	2.14	0.47
1:B:52:ARG:HG2	1:B:133:TRP:HH2	1.79	0.47
1:D:767:GLN:CG	1:D:768:MET:N	2.77	0.47
1:D:885:ASN:HB2	1:D:984:LEU:O	2.14	0.47
1:A:947:GLY:O	1:A:1023:LYS:NZ	2.43	0.47
1:C:49:GLN:CD	1:C:49:GLN:H	2.12	0.47
1:C:93:HIS:O	5:C:8421:DMS:H13	2.15	0.47
1:A:957:PHE:HA	1:A:985:ASN:O	2.14	0.47
1:B:342:LEU:O	1:B:348:PRO:HA	2.14	0.47
1:B:546:LEU:HA	7:B:8649:HOH:O	2.14	0.47
1:C:778:THR:HG23	1:C:887:GLN:HB2	1.91	0.47
5:B:8506:DMS:H23	7:B:9213:HOH:O	2.15	0.47
1:B:73:TRP:O	1:B:183:ARG:NH1	2.38	0.47
6:D:2002:BTB:C6	6:D:2002:BTB:H82	2.45	0.47
1:A:143:PHE:O	1:A:168:PRO:HA	2.15	0.47
1:A:830:LEU:N	1:A:833:ALA:O	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:ND2	1:C:21:VAL:HG23	2.30	0.47
1:D:701:VAL:O	1:D:703:PRO:HD3	2.15	0.47
1:A:600:GLN:H	1:A:600:GLN:NE2	2.05	0.47
1:D:635:THR:OG1	1:D:681:GLU:OE1	2.29	0.47
1:A:131:GLU:CG	1:A:135:GLN:NE2	2.77	0.47
1:D:433:LEU:N	1:D:434:PRO:CD	2.77	0.47
1:D:373:VAL:O	1:D:377:LEU:HG	2.15	0.47
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.14	0.47
1:A:635:THR:OG1	1:A:681:GLU:OE2	2.26	0.47
1:B:52:ARG:HG2	1:B:133:TRP:CH2	2.49	0.47
1:C:653:HIS:CE1	1:C:667:GLU:CG	2.98	0.47
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.96	0.47
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.15	0.47
1:C:656:VAL:HA	1:C:695:TRP:O	2.15	0.47
1:A:568:TRP:CH2	2:A:2001:2FG:H3	2.50	0.47
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.77	0.47
1:D:746:ASP:HB3	1:D:757:GLN:HE21	1.80	0.47
1:A:745:MET:O	1:A:760:ARG:HG3	2.14	0.47
1:A:654:TRP:NE1	1:A:666:GLY:HA3	2.29	0.47
1:A:809:ARG:HH21	1:A:1001:PRO:CG	2.28	0.47
1:D:157:ARG:HD3	1:D:176:PHE:HD2	1.80	0.47
1:D:427:THR:HG21	1:D:462:SER:HB3	1.97	0.47
1:B:216:HIS:NE2	5:B:8504:DMS:H13	2.29	0.47
1:D:679:LEU:HA	1:D:679:LEU:HD23	1.58	0.47
1:B:795:VAL:HG12	5:B:8506:DMS:S	2.54	0.47
1:A:737:ILE:HD12	1:A:738:PRO:O	2.14	0.47
1:A:153:TRP:CD1	1:A:158:TRP:CA	2.98	0.47
1:A:274:PHE:HA	1:A:289:VAL:HB	1.97	0.47
1:C:894:ARG:HE	1:C:894:ARG:HB3	1.58	0.47
1:D:801:ILE:CG2	1:D:802:ASP:N	2.78	0.47
1:C:226:HIS:N	1:C:226:HIS:CD2	2.79	0.47
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.80	0.47
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.96	0.46
1:A:15:ASP:OD2	7:A:8674:HOH:O	2.20	0.46
1:D:324:GLU:HG3	1:D:325:ALA:N	2.30	0.46
1:D:827:ALA:HA	1:D:836:ILE:HD12	1.98	0.46
1:C:77:ASP:OD2	1:C:78:LEU:O	2.33	0.46
1:D:965:GLN:HA	1:D:968:MET:HE3	1.98	0.46
1:D:937:LEU:HD12	1:D:957:PHE:O	2.15	0.46
1:B:651:LEU:HD22	1:B:701:VAL:HB	1.96	0.46
1:D:158:TRP:CZ2	1:D:160:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:576:ILE:HD11	5:B:8411:DMS:S	2.54	0.46
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.51	0.46
1:D:808:GLU:OE1	1:D:808:GLU:HA	2.15	0.46
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.97	0.46
1:B:86:VAL:CG1	1:B:87:PRO:HA	2.43	0.46
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.50	0.46
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.15	0.46
1:D:496:THR:O	1:D:496:THR:HG23	2.16	0.46
1:B:742:THR:HG22	1:B:743:SER:N	2.31	0.46
1:A:767:GLN:OE1	1:A:768:MET:O	2.33	0.46
1:C:579:ASP:HB2	1:C:580:GLU:OE2	2.16	0.46
1:A:863:GLN:NE2	1:A:1021:CYS:CB	2.79	0.46
1:C:88:SER:HA	1:C:366:VAL:CG2	2.45	0.46
1:D:972:HIS:HB3	1:D:974:HIS:ND1	2.30	0.46
1:B:110:ASN:N	1:B:111:PRO:CD	2.78	0.46
1:B:220:THR:HA	1:B:248:GLY:HA3	1.98	0.46
1:D:65:ALA:HB1	1:D:67:GLU:OE1	2.15	0.46
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.50	0.46
1:C:458:LEU:HB2	1:C:486:TYR:HB2	1.96	0.46
1:C:653:HIS:ND1	1:C:667:GLU:CG	2.76	0.46
1:D:767:GLN:HG3	1:D:768:MET:N	2.31	0.46
1:C:38:ASN:CB	1:C:41:GLU:HG3	2.46	0.46
1:D:26:ARG:HD2	1:D:169:SER:HA	1.97	0.46
1:B:146:VAL:O	1:B:165:SER:HA	2.16	0.46
1:B:885:ASN:HB2	1:B:984:LEU:O	2.14	0.46
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.14	0.46
1:B:43:ARG:HD2	1:B:261:TRP:CD2	2.50	0.46
1:A:651:LEU:CD2	1:A:653:HIS:NE2	2.78	0.46
1:C:762:SER:C	1:C:822:LEU:HD22	2.37	0.46
1:C:674:PRO:O	1:C:675:GLN:HB2	2.15	0.46
1:B:569:ASP:O	1:B:605:GLY:HA2	2.16	0.46
1:A:809:ARG:HD2	7:A:9019:HOH:O	2.14	0.46
1:A:216:HIS:CE1	5:A:8504:DMS:C1	2.99	0.46
1:B:256:VAL:O	1:B:271:THR:HA	2.15	0.46
1:D:400:THR:O	1:D:403:ASP:HB2	2.16	0.46
1:A:653:HIS:O	1:A:698:VAL:HA	2.16	0.46
1:A:253:TYR:O	1:A:318:ALA:N	2.48	0.46
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.98	0.46
1:B:613:PRO:HB3	1:B:617:LEU:HD23	1.98	0.46
1:B:897:TRP:CZ2	1:B:938:ARG:HG2	2.51	0.46
1:C:784:PHE:HA	1:C:881:ARG:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:ILE:HA	1:A:576:ILE:HD13	1.74	0.46
1:B:133:TRP:CD1	5:B:8504:DMS:H11	2.51	0.45
1:D:801:ILE:CG2	1:D:802:ASP:H	2.29	0.45
1:D:893:GLU:CG	1:D:894:ARG:HG2	2.45	0.45
1:A:542:MET:HA	1:A:604:ASN:HA	1.97	0.45
1:B:421:VAL:HG13	1:C:282:ARG:O	2.15	0.45
1:D:670:LEU:HA	1:D:670:LEU:HD23	1.71	0.45
1:B:254:LEU:HA	1:B:254:LEU:HD23	1.76	0.45
1:A:131:GLU:HG2	1:A:135:GLN:NE2	2.31	0.45
1:B:127:PHE:N	1:B:127:PHE:CD2	2.85	0.45
1:A:972:HIS:HB3	1:A:974:HIS:ND1	2.31	0.45
1:B:391:HIS:ND1	1:B:412:GLU:OE2	2.45	0.45
1:A:297:ASN:N	1:A:298:PRO:CD	2.79	0.45
1:B:63:PHE:CD1	1:B:63:PHE:N	2.84	0.45
1:C:634:GLN:NE2	1:C:635:THR:N	2.64	0.45
1:A:131:GLU:CB	1:A:135:GLN:NE2	2.80	0.45
1:D:857:ARG:NH1	1:D:857:ARG:CG	2.79	0.45
1:B:751:LEU:HD23	1:B:751:LEU:O	2.16	0.45
1:A:427:THR:HG21	1:A:462:SER:HB3	1.98	0.45
1:B:730:LEU:O	1:B:731:PRO:C	2.54	0.45
1:C:611:ARG:HD2	1:C:611:ARG:N	2.31	0.45
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.42	0.45
1:D:237:ARG:NH1	1:D:296:GLU:HG2	2.31	0.45
1:D:177:LEU:HA	1:D:177:LEU:HD23	1.76	0.45
1:B:745:MET:C	1:B:760:ARG:HG3	2.37	0.45
1:C:867:THR:CG2	1:C:1015:HIS:CE1	2.99	0.45
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.16	0.45
1:D:829:THR:O	1:D:830:LEU:HD23	2.17	0.45
1:D:652:LEU:HD11	1:D:698:VAL:HB	1.98	0.45
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.16	0.45
1:C:895:VAL:O	1:C:919:ASP:HA	2.16	0.45
1:B:822:LEU:CD1	1:B:824:GLN:H	2.29	0.45
1:C:836:ILE:O	1:C:855:THR:HA	2.17	0.45
1:C:870:VAL:HG12	1:C:871:GLU:N	2.32	0.45
1:B:640:SER:O	1:B:675:GLN:HA	2.16	0.45
1:D:936:GLY:O	1:D:938:ARG:NH1	2.44	0.45
1:B:571:VAL:HG22	1:B:572:ASP:O	2.16	0.45
1:A:670:LEU:HA	1:A:670:LEU:HD23	1.65	0.45
1:B:802:ASP:HA	1:B:803:PRO:HD2	1.72	0.45
1:D:660:GLY:O	1:D:662:PRO:HD3	2.16	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:HIS:HA	1:B:568:TRP:O	2.17	0.45
1:B:554:GLN:NE2	7:B:8677:HOH:O	2.26	0.45
1:D:540:HIS:CE1	1:D:542:MET:HB2	2.52	0.45
1:B:433:LEU:N	1:B:434:PRO:CD	2.80	0.45
1:A:807:VAL:CG1	1:A:808:GLU:N	2.80	0.45
1:C:278:ILE:N	1:C:278:ILE:CD1	2.77	0.45
1:B:414:ASN:O	1:B:439:ARG:HD3	2.17	0.45
1:D:903:GLN:HB3	7:D:8686:HOH:O	2.16	0.45
1:D:789:LEU:HD11	1:D:993:ILE:HG22	1.98	0.45
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.69	0.45
1:C:135:GLN:NE2	1:C:135:GLN:CA	2.79	0.45
1:A:743:SER:O	1:A:760:ARG:NH1	2.39	0.45
1:C:634:GLN:HE21	1:C:634:GLN:CA	2.25	0.45
1:C:738:PRO:N	1:C:751:LEU:HD12	2.32	0.45
1:A:322:LEU:HB2	5:A:8406:DMS:H22	1.99	0.45
1:C:94:GLY:O	5:C:8421:DMS:H11	2.17	0.45
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.98	0.45
1:B:785:THR:O	1:B:881:ARG:HD2	2.17	0.45
1:C:39:SER:HB3	1:C:314:GLU:OE2	2.17	0.45
1:B:739:HIS:O	1:B:749:ILE:HA	2.17	0.45
1:C:52:ARG:HG2	1:C:133:TRP:CH2	2.52	0.45
1:B:843:GLN:HG2	1:B:848:THR:N	2.31	0.44
1:D:1006:GLU:HG2	1:D:1007:PHE:CE1	2.52	0.44
1:A:823:LEU:HD11	1:A:841:ALA:HB2	1.98	0.44
1:C:292:ARG:HH12	5:C:8412:DMS:C2	2.30	0.44
1:C:914:CYS:HB2	7:C:8858:HOH:O	2.17	0.44
1:A:220:THR:HG22	1:A:315:LEU:HD21	1.99	0.44
1:A:652:LEU:HD12	1:A:699:ARG:O	2.17	0.44
1:B:336:ARG:HH11	5:B:8409:DMS:H11	1.83	0.44
1:B:237:ARG:HH11	1:B:237:ARG:CB	2.30	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.68	0.44
1:A:84:VAL:HA	5:A:8414:DMS:O	2.18	0.44
1:D:832:ASP:O	1:D:833:ALA:HB2	2.17	0.44
1:C:52:ARG:CG	1:C:133:TRP:CH2	2.99	0.44
1:B:942:ARG:HA	1:B:953:GLY:O	2.17	0.44
1:A:486:TYR:CE2	1:A:488:GLY:HA3	2.52	0.44
1:B:856:TYR:CD1	1:B:856:TYR:N	2.85	0.44
1:A:753:ASN:N	1:A:753:ASN:OD1	2.47	0.44
1:B:743:SER:OG	1:B:744:GLU:N	2.50	0.44
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.78	0.44
1:B:756:TRP:CE2	1:B:858:ILE:CD1	2.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:PRO:O	1:D:687:GLN:NE2	2.51	0.44
1:A:107:ILE:CA	5:A:8419:DMS:C2	2.95	0.44
1:C:463:GLY:HA2	7:C:8508:HOH:O	2.16	0.44
1:D:930:VAL:O	1:D:932:PRO:HD3	2.18	0.44
1:D:640:SER:O	1:D:675:GLN:HA	2.17	0.44
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.52	0.44
1:B:773:LYS:HD3	1:B:773:LYS:HA	1.61	0.44
1:A:59:ARG:HH21	1:A:81:ALA:HB3	1.82	0.44
1:A:525:SER:O	1:B:561:ARG:HD3	2.17	0.44
1:B:131:GLU:O	1:B:135:GLN:N	2.48	0.44
1:B:797:GLU:HB2	1:B:798:ALA:H	1.48	0.44
1:D:630:ARG:N	1:D:630:ARG:HD3	2.31	0.44
1:C:111:PRO:HA	1:C:112:PRO:HA	1.40	0.44
1:B:738:PRO:HA	1:B:751:LEU:HD12	1.99	0.44
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.83	0.44
1:D:794:GLY:HA2	1:D:998:SER:O	2.17	0.44
1:A:635:THR:HA	1:A:680:ILE:O	2.18	0.44
1:B:166:ARG:HG3	1:B:392:TYR:HB2	2.00	0.44
1:C:634:GLN:N	1:C:634:GLN:NE2	2.29	0.44
1:C:952:ARG:NH1	1:C:952:ARG:HG3	2.28	0.44
1:C:578:TYR:CE2	1:C:584:PRO:HB3	2.53	0.44
1:B:155:ASN:ND2	1:B:182:ASN:OD1	2.40	0.44
1:C:65:ALA:HB1	1:C:67:GLU:OE1	2.17	0.44
1:C:158:TRP:CZ2	1:C:160:GLY:HA2	2.52	0.44
5:A:8407:DMS:C2	7:A:8736:HOH:O	2.64	0.44
1:C:287:ASP:N	1:C:287:ASP:OD1	2.45	0.44
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.72	0.44
1:C:801:ILE:O	1:C:803:PRO:HD3	2.18	0.44
1:D:895:VAL:O	1:D:919:ASP:HA	2.17	0.44
1:D:899:GLY:HA2	1:D:915:PHE:CD1	2.53	0.44
1:B:473:ARG:O	1:B:477:SER:HB2	2.18	0.44
1:B:578:TYR:N	1:B:578:TYR:CD1	2.85	0.44
1:D:631:LEU:HD12	1:D:632:SER:H	1.82	0.44
1:D:533:LEU:HD23	1:D:533:LEU:C	2.37	0.44
1:B:763:GLY:HA3	1:B:822:LEU:CD2	2.47	0.44
1:B:847:LYS:HE2	1:B:875:ASP:OD1	2.17	0.44
1:A:77:ASP:HB2	7:A:8947:HOH:O	2.17	0.44
1:B:305:ILE:HD11	1:B:645:ARG:HB3	2.00	0.44
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.90	0.44
1:B:581:ASN:CB	1:B:583:ASN:HD21	2.29	0.44
1:C:433:LEU:O	1:C:433:LEU:HD12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:ARG:HH21	5:B:8412:DMS:H23	1.82	0.44
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.53	0.44
1:A:684:GLU:OE2	1:A:685:LEU:O	2.36	0.43
1:A:622:HIS:CE1	5:A:8402:DMS:C1	3.01	0.43
1:A:579:ASP:OD1	1:A:583:ASN:N	2.37	0.43
1:D:674:PRO:C	1:D:675:GLN:HG2	2.38	0.43
1:D:57:GLU:HB3	1:D:83:THR:CG2	2.48	0.43
1:D:137:GLY:HA2	1:D:219:THR:HG23	1.99	0.43
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.53	0.43
1:A:768:MET:O	1:A:775:GLN:N	2.51	0.43
1:A:654:TRP:NE1	1:A:666:GLY:CA	2.81	0.43
1:B:594:ASP:O	1:B:597:ASN:ND2	2.41	0.43
1:D:899:GLY:HA2	1:D:915:PHE:CE1	2.54	0.43
1:B:59:ARG:O	1:B:123:TYR:HA	2.18	0.43
1:A:631:LEU:HD11	1:A:633:GLY:O	2.19	0.43
1:C:382:ASN:O	1:C:383:ASN:HB2	2.17	0.43
1:C:634:GLN:O	1:C:682:LEU:N	2.43	0.43
6:B:2002:BTB:O3	6:B:2002:BTB:O1	2.27	0.43
1:C:652:LEU:O	1:C:667:GLU:HA	2.19	0.43
1:C:823:LEU:HD11	1:C:841:ALA:HB2	2.00	0.43
1:D:659:ASP:O	7:D:9016:HOH:O	2.21	0.43
1:D:580:GLU:C	1:D:582:GLY:H	2.21	0.43
1:B:667:GLU:O	1:B:668:VAL:CG2	2.66	0.43
1:A:216:HIS:CE1	5:A:8504:DMS:H12	2.53	0.43
1:B:441:THR:HG22	1:B:474:TRP:CZ2	2.53	0.43
1:A:190:ARG:HG2	1:A:191:TRP:CE2	2.53	0.43
1:D:147:ASN:HB2	1:D:209:PHE:CE2	2.54	0.43
1:B:377:LEU:HA	1:B:377:LEU:HD23	1.73	0.43
1:A:869:ASP:HB3	7:A:8850:HOH:O	2.18	0.43
1:D:738:PRO:HD3	1:D:860:GLY:HA2	2.00	0.43
1:D:740:LEU:HD12	1:D:741:THR:H	1.83	0.43
1:D:59:ARG:NH2	1:D:81:ALA:HB3	2.34	0.43
1:B:367:MET:HE2	1:B:372:MET:HG2	1.99	0.43
6:B:2002:BTB:H71	6:B:2002:BTB:O4	2.19	0.43
1:B:843:GLN:HA	1:B:847:LYS:O	2.17	0.43
1:C:763:GLY:CA	1:C:822:LEU:HD21	2.48	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.35	0.43
1:A:745:MET:HE1	1:A:761:GLN:HB3	1.99	0.43
6:D:2002:BTB:H32	6:D:2002:BTB:H51	1.49	0.43
1:A:338:GLU:HG2	7:A:9084:HOH:O	2.19	0.43
1:C:559:TYR:CE2	1:D:522:LYS:HA	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:TYR:O	5:C:8419:DMS:O	2.37	0.43
1:A:546:LEU:HA	7:A:8631:HOH:O	2.18	0.43
1:B:482:ARG:HA	1:B:483:PRO:HD3	1.72	0.43
1:A:403:ASP:CG	1:A:451:PRO:HD2	2.39	0.43
1:C:844:HIS:N	1:C:847:LYS:O	2.49	0.43
1:D:667:GLU:C	1:D:668:VAL:HG23	2.39	0.43
1:B:843:GLN:HG2	1:B:848:THR:HA	1.98	0.43
1:C:746:ASP:CA	1:C:760:ARG:HG2	2.48	0.43
5:C:8419:DMS:H22	7:C:8687:HOH:O	2.17	0.43
1:C:839:ALA:HA	1:C:852:SER:O	2.17	0.43
1:B:832:ASP:N	1:B:832:ASP:OD1	2.51	0.43
1:A:131:GLU:HG2	1:A:135:GLN:CD	2.39	0.43
1:B:142:ILE:CG1	1:B:170:GLU:HG2	2.49	0.43
1:C:958:ASN:OD1	1:C:985:ASN:ND2	2.26	0.43
1:C:600:GLN:HB2	1:C:603:MET:CE	2.48	0.43
1:B:446:ARG:NE	1:B:447:ASP:OD1	2.49	0.43
1:A:326:GLU:HA	1:A:326:GLU:OE1	2.18	0.43
1:A:986:ILE:HD13	1:A:986:ILE:HG23	1.74	0.43
1:A:634:GLN:CG	1:A:682:LEU:HD12	2.46	0.43
1:C:896:ASN:OD1	1:C:917:ARG:NH1	2.50	0.43
1:D:63:PHE:CB	1:D:64:PRO:HD2	2.39	0.43
1:A:583:ASN:HA	1:A:584:PRO:HD3	1.92	0.43
1:C:658:LEU:HA	1:C:694:LEU:HD23	2.01	0.43
1:D:261:TRP:HA	1:D:265:THR:O	2.19	0.43
1:C:220:THR:HA	1:C:248:GLY:HA3	2.01	0.43
1:C:634:GLN:NE2	1:C:634:GLN:CA	2.81	0.43
1:A:836:ILE:HB	1:A:856:TYR:HB2	2.01	0.43
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.54	0.43
1:A:824:GLN:CG	1:A:825:CYS:N	2.80	0.43
1:C:569:ASP:O	1:C:605:GLY:HA2	2.18	0.43
1:C:63:PHE:HA	1:C:64:PRO:HD3	1.73	0.43
1:D:101:THR:HG23	1:D:204:ARG:NH2	2.34	0.43
1:D:399:TYR:CE1	1:D:446:ARG:NH2	2.87	0.43
1:D:259:SER:HB2	7:D:8894:HOH:O	2.18	0.43
1:B:167:LEU:HD21	1:B:393:PRO:HG2	2.01	0.43
1:A:34:ALA:O	1:A:35:SER:C	2.57	0.43
1:A:926:TYR:CZ	1:A:928:PRO:HA	2.54	0.43
1:C:796:SER:OG	1:C:808:GLU:OE2	2.28	0.43
1:A:787:ALA:HB3	1:A:934:GLU:N	2.34	0.43
1:B:382:ASN:O	1:B:383:ASN:HB2	2.19	0.43
1:A:485:GLN:HA	1:A:496:THR:OG1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:O	1:B:659:ASP:C	2.56	0.42
1:C:390:SER:HA	1:C:391:HIS:HA	1.77	0.42
1:D:1022:GLN:HG2	1:D:1023:LYS:N	2.21	0.42
1:B:746:ASP:OD1	1:B:759:ASN:HA	2.18	0.42
1:D:856:TYR:CD1	1:D:856:TYR:N	2.87	0.42
1:D:486:TYR:CE2	1:D:488:GLY:CA	3.01	0.42
1:C:36:TRP:CD2	1:C:42:ALA:HA	2.55	0.42
1:C:369:GLU:HB2	1:C:397:LEU:CD2	2.49	0.42
1:A:24:LEU:O	1:A:25:ASN:HB2	2.18	0.42
1:B:599:ARG:HE	1:B:599:ARG:HB3	1.69	0.42
1:B:745:MET:HB2	1:B:746:ASP:OD2	2.18	0.42
1:C:858:ILE:CD1	1:C:864:MET:CG	2.95	0.42
1:C:85:VAL:CG1	1:C:86:VAL:N	2.77	0.42
1:B:833:ALA:HB1	1:B:858:ILE:O	2.19	0.42
1:B:965:GLN:HA	1:B:968:MET:HG2	2.02	0.42
1:B:142:ILE:HG12	1:B:170:GLU:CG	2.49	0.42
1:B:576:ILE:HD11	5:B:8411:DMS:C1	2.49	0.42
1:B:887:GLN:NE2	1:B:980:GLU:O	2.50	0.42
1:A:354:VAL:O	1:A:387:VAL:HA	2.18	0.42
1:B:777:LEU:HA	1:B:777:LEU:HD23	1.68	0.42
1:A:685:LEU:HA	1:A:686:PRO:HD3	1.82	0.42
1:A:63:PHE:CB	1:A:64:PRO:CD	2.97	0.42
1:C:822:LEU:HA	1:C:822:LEU:HD13	1.66	0.42
1:A:85:VAL:HG23	5:A:8414:DMS:S	2.60	0.42
1:C:870:VAL:CG1	1:C:871:GLU:N	2.82	0.42
1:C:13:ARG:O	1:C:14:ARG:C	2.57	0.42
1:D:157:ARG:HH11	1:D:176:PHE:HA	1.85	0.42
1:C:689:GLU:HG3	1:C:690:SER:H	1.84	0.42
1:B:472:TYR:O	1:B:476:LYS:HG2	2.19	0.42
1:C:906:TYR:CZ	1:C:937:LEU:HB2	2.55	0.42
1:A:963:SER:HB3	1:A:983:TRP:CE2	2.54	0.42
1:B:782:ASP:HA	1:B:884:LEU:HD23	2.02	0.42
1:B:18:ASN:HA	1:B:19:PRO:HD2	1.65	0.42
1:A:659:ASP:O	7:A:8988:HOH:O	2.21	0.42
1:C:134:LEU:HD23	1:C:134:LEU:HA	1.76	0.42
1:A:682:LEU:HB3	1:A:683:PRO:HD2	2.01	0.42
1:C:661:LYS:HA	1:C:662:PRO:HD3	1.65	0.42
1:C:742:THR:HG23	1:C:747:PHE:CE2	2.54	0.42
1:B:358:GLU:HB3	1:B:367:MET:HG2	2.02	0.42
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.54	0.42
1:A:231:PHE:N	1:A:231:PHE:CD1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:LEU:HA	1:B:54:LEU:HD23	1.84	0.42
1:C:763:GLY:HA3	1:C:822:LEU:CD2	2.50	0.42
1:A:802:ASP:O	1:A:808:GLU:HG3	2.20	0.42
1:B:542:MET:HA	1:B:604:ASN:HA	2.01	0.42
1:A:124:SER:HA	1:A:184:LEU:O	2.20	0.42
1:B:72:SER:O	1:B:75:GLU:N	2.53	0.42
1:B:738:PRO:N	1:B:751:LEU:HD12	2.35	0.42
1:A:972:HIS:HB2	1:A:975:LEU:HD12	2.01	0.42
1:D:1022:GLN:CG	1:D:1023:LYS:N	2.82	0.42
1:C:301:TRP:CH2	1:C:452:SER:HA	2.54	0.42
1:A:44:THR:O	1:A:45:ASP:HB3	2.20	0.42
1:B:38:ASN:HB3	1:B:41:GLU:HG2	2.00	0.42
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.80	0.42
1:A:291:LEU:HD22	1:A:291:LEU:N	2.35	0.42
1:B:233:ASP:OD1	1:B:234:ASP:N	2.52	0.42
1:D:740:LEU:HD12	1:D:741:THR:N	2.34	0.42
1:B:367:MET:HE2	1:B:372:MET:CG	2.49	0.42
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.48	0.42
1:C:809:ARG:NH2	7:C:8816:HOH:O	2.53	0.42
1:C:173:LEU:HA	1:C:173:LEU:HD23	1.74	0.42
1:C:821:ALA:N	1:C:841:ALA:O	2.52	0.42
1:B:755:ARG:HG3	1:B:756:TRP:N	2.35	0.42
1:D:99:ILE:O	1:D:204:ARG:N	2.43	0.42
1:B:685:LEU:HA	1:B:686:PRO:HD3	1.69	0.42
1:B:505:ARG:O	1:B:519:SER:HA	2.19	0.42
1:C:959:ILE:HG13	1:C:982:THR:HG22	2.02	0.42
1:A:610:ASP:O	1:A:611:ARG:HB2	2.20	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.54	0.42
1:C:147:ASN:HA	1:C:148:SER:HA	1.62	0.42
1:B:464:HIS:HB2	1:B:489:GLY:HA3	2.02	0.42
1:B:900:LEU:CD1	1:B:910:LEU:HD22	2.50	0.42
1:D:896:ASN:HA	1:D:918:TRP:O	2.20	0.42
1:A:634:GLN:HG2	1:A:682:LEU:CD1	2.47	0.42
1:A:774:LYS:NZ	1:A:774:LYS:CB	2.77	0.42
1:B:875:ASP:N	1:B:875:ASP:OD1	2.47	0.42
1:B:797:GLU:N	1:B:800:ARG:O	2.52	0.42
1:C:473:ARG:NH2	7:C:9092:HOH:O	2.39	0.42
1:A:964:GLN:O	1:A:968:MET:HB2	2.19	0.42
1:B:326:GLU:O	1:B:327:ALA:HB2	2.20	0.42
1:D:863:GLN:NE2	1:D:952:ARG:HH22	2.18	0.42
1:A:65:ALA:HB1	1:A:66:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:474:TRP:O	1:C:477:SER:HB3	2.20	0.42
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.54	0.41
1:B:36:TRP:NE1	1:B:48:SER:HB2	2.34	0.41
1:A:13:ARG:HH22	1:D:13:ARG:HB2	1.84	0.41
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.54	0.41
1:C:54:LEU:HA	1:C:54:LEU:HD23	1.82	0.41
1:A:679:LEU:HD23	1:A:679:LEU:HA	1.80	0.41
1:B:743:SER:O	1:B:760:ARG:NH1	2.42	0.41
1:B:745:MET:O	1:B:760:ARG:HG3	2.20	0.41
1:B:58:TRP:HB2	1:B:86:VAL:HG23	2.01	0.41
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.85	0.41
1:A:736:ALA:HB1	1:A:751:LEU:CD1	2.50	0.41
1:A:832:ASP:O	1:A:833:ALA:HB2	2.20	0.41
1:B:473:ARG:HH11	1:B:476:LYS:HB2	1.85	0.41
1:B:851:ILE:O	1:B:870:VAL:HA	2.20	0.41
1:D:694:LEU:HB2	1:D:723:ALA:O	2.20	0.41
1:D:626:PHE:CE1	5:D:8403:DMS:S	3.13	0.41
1:D:767:GLN:CD	1:D:768:MET:H	2.21	0.41
1:C:433:LEU:C	1:C:433:LEU:HD12	2.40	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.41
1:B:986:ILE:CD1	1:B:1018:LEU:CD2	2.98	0.41
1:C:694:LEU:HD23	1:C:694:LEU:HA	1.72	0.41
1:A:92:MET:HE3	1:A:92:MET:N	2.34	0.41
1:C:377:LEU:HD23	1:C:377:LEU:HA	1.87	0.41
1:C:126:THR:HA	1:C:182:ASN:O	2.20	0.41
5:A:8407:DMS:H23	7:A:8736:HOH:O	2.19	0.41
1:C:606:LEU:O	1:C:614:HIS:HB2	2.19	0.41
1:B:153:TRP:HH2	1:B:187:MET:HE2	1.85	0.41
1:B:581:ASN:CB	1:B:583:ASN:ND2	2.75	0.41
1:C:762:SER:CB	7:C:8880:HOH:O	2.68	0.41
1:B:233:ASP:CA	5:B:8417:DMS:C1	2.98	0.41
1:B:494:THR:HB	1:C:473:ARG:HH22	1.84	0.41
1:B:963:SER:HB3	1:B:983:TRP:NE1	2.35	0.41
1:A:972:HIS:HB3	1:A:974:HIS:CE1	2.56	0.41
1:A:910:LEU:HD12	1:A:910:LEU:C	2.41	0.41
6:B:2002:BTB:H81	6:B:2002:BTB:H52	1.65	0.41
1:D:635:THR:HG22	1:D:679:LEU:CD2	2.43	0.41
1:C:738:PRO:CA	1:C:751:LEU:CD1	2.96	0.41
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.55	0.41
1:B:737:ILE:HG13	1:B:738:PRO:N	2.25	0.41
1:A:362:LEU:HD23	1:A:362:LEU:HA	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:HD12	1:A:161:TYR:CB	2.51	0.41
1:C:1017:GLN:HG3	1:C:1018:LEU:N	2.36	0.41
1:A:173:LEU:O	1:A:174:SER:C	2.58	0.41
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.81	0.41
5:A:8404:DMS:H22	7:A:8630:HOH:O	2.20	0.41
1:C:526:LEU:HA	1:C:526:LEU:HD23	1.81	0.41
1:B:857:ARG:HD3	1:B:857:ARG:HH11	1.60	0.41
1:C:952:ARG:HH11	1:C:952:ARG:CG	2.29	0.41
1:D:634:GLN:NE2	1:D:682:LEU:O	2.52	0.41
1:A:569:ASP:O	1:A:605:GLY:HA2	2.21	0.41
1:B:444:VAL:O	1:B:448:ARG:HG2	2.20	0.41
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.02	0.41
1:B:653:HIS:O	1:B:698:VAL:HA	2.20	0.41
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.49	0.41
1:C:110:ASN:N	1:C:111:PRO:CD	2.84	0.41
1:A:785:THR:O	1:A:881:ARG:HD2	2.20	0.41
1:C:66:PRO:HD2	1:C:67:GLU:OE1	2.20	0.41
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.55	0.41
1:C:240:LEU:HD23	1:C:241:GLU:N	2.36	0.41
1:A:43:ARG:HH22	1:A:264:GLU:HG3	1.85	0.41
1:D:694:LEU:HD23	1:D:694:LEU:HA	1.75	0.41
1:C:851:ILE:HG21	1:C:853:ARG:NH1	2.36	0.41
1:C:91:GLN:HG2	1:C:98:PRO:HA	2.02	0.41
1:B:991:MET:HG2	1:B:992:GLY:O	2.20	0.41
1:A:921:PRO:O	1:A:922:LEU:C	2.59	0.41
1:C:724:GLU:HG2	1:C:725:ASN:N	2.35	0.41
1:D:995:GLY:O	1:D:996:ASP:C	2.59	0.41
1:D:801:ILE:HG22	1:D:802:ASP:H	1.84	0.41
1:C:433:LEU:N	1:C:434:PRO:CD	2.83	0.41
1:A:948:PRO:CD	1:A:949:HIS:N	2.84	0.41
1:A:167:LEU:HB3	1:A:168:PRO:HD2	2.03	0.41
1:C:292:ARG:CG	1:C:292:ARG:HH11	2.34	0.41
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.86	0.41
1:D:698:VAL:HG23	1:D:698:VAL:O	2.19	0.41
1:B:277:GLU:CG	5:B:8412:DMS:H21	2.51	0.41
1:B:368:ASP:O	1:B:372:MET:HG3	2.21	0.41
1:D:376:ILE:HG21	1:D:376:ILE:HD13	1.75	0.41
1:B:54:LEU:HD11	1:B:214:LEU:HG	2.03	0.41
1:A:767:GLN:HE21	1:A:774:LYS:HD2	1.84	0.41
1:A:224:ASP:HB3	1:A:245:GLN:CG	2.39	0.41
1:B:843:GLN:HG2	1:B:848:THR:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:ARG:NH2	1:C:338:GLU:OE2	2.54	0.41
1:A:316:HIS:HB2	1:A:321:THR:O	2.21	0.41
1:C:110:ASN:O	1:C:113:PHE:N	2.49	0.41
1:D:178:ARG:N	1:D:182:ASN:OD1	2.52	0.41
1:B:240:LEU:HD13	1:B:260:LEU:HD13	2.02	0.41
1:B:648:ASP:C	5:B:8425:DMS:O	2.59	0.41
1:D:703:PRO:O	1:D:711:ALA:HB1	2.21	0.41
1:C:226:HIS:O	1:C:242:ALA:HA	2.21	0.41
1:C:292:ARG:HH12	5:C:8412:DMS:H23	1.84	0.41
1:D:869:ASP:CG	1:D:1015:HIS:HD1	2.21	0.41
1:C:153:TRP:CD1	1:C:158:TRP:HA	2.56	0.41
1:C:866:ILE:O	1:C:1017:GLN:HA	2.20	0.41
1:A:920:LEU:HB3	1:A:921:PRO:HD2	2.03	0.41
1:B:125:LEU:HD12	5:B:8502:DMS:S	2.61	0.41
1:A:818:ALA:HB2	1:A:849:LEU:HD12	2.03	0.41
1:C:431:ARG:HD2	7:C:9111:HOH:O	2.21	0.41
1:B:631:LEU:HD12	1:B:635:THR:O	2.21	0.41
1:B:80:GLU:HG3	1:B:80:GLU:H	1.16	0.41
1:C:580:GLU:OE1	1:C:581:ASN:N	2.53	0.41
1:C:579:ASP:OD2	1:C:581:ASN:HB2	2.20	0.41
1:A:110:ASN:HA	1:A:111:PRO:HD2	1.90	0.41
1:D:153:TRP:CD1	1:D:158:TRP:CA	3.04	0.41
1:C:878:HIS:HE1	7:C:9056:HOH:O	2.02	0.41
1:A:654:TRP:CE2	1:A:666:GLY:CA	3.04	0.41
1:D:926:TYR:CZ	1:D:928:PRO:HA	2.55	0.41
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.03	0.41
1:A:60:PHE:HE1	1:A:123:TYR:CE1	2.39	0.41
1:A:240:LEU:HD23	1:A:240:LEU:C	2.41	0.41
1:B:62:TRP:CD1	1:B:95:TYR:HB3	2.56	0.41
1:A:915:PHE:CD2	1:A:915:PHE:C	2.95	0.41
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.86	0.41
1:D:363:HIS:HD2	7:D:9026:HOH:O	2.04	0.41
1:D:46:ARG:CB	1:D:47:PRO:CD	2.99	0.40
1:B:651:LEU:C	1:B:651:LEU:CD2	2.90	0.40
1:D:975:LEU:HD23	1:D:975:LEU:HA	1.70	0.40
1:C:52:ARG:HG2	1:C:133:TRP:HH2	1.86	0.40
1:C:888:LEU:O	1:C:981:GLY:HA3	2.21	0.40
1:C:344:LEU:O	1:C:345:ASN:C	2.59	0.40
1:C:542:MET:HA	1:C:604:ASN:HA	2.02	0.40
1:B:65:ALA:HB1	1:B:66:PRO:HD2	2.03	0.40
1:D:368:ASP:OD2	7:D:8918:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:LEU:HD12	1:A:652:LEU:HA	1.76	0.40
1:C:49:GLN:N	1:C:49:GLN:CD	2.74	0.40
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.54	0.40
1:C:262:GLN:CG	1:C:309:TYR:CE2	2.98	0.40
1:A:316:HIS:HB3	1:A:322:LEU:HA	2.03	0.40
1:B:155:ASN:OD1	1:B:183:ARG:N	2.40	0.40
1:B:390:SER:HA	1:B:391:HIS:HA	1.89	0.40
1:A:24:LEU:HD12	1:A:161:TYR:HB3	2.03	0.40
1:D:759:ASN:O	1:D:763:GLY:N	2.50	0.40
1:B:780:LEU:HA	1:B:886:CYS:HB3	2.04	0.40
6:D:2002:BTB:H42	7:D:9211:HOH:O	2.21	0.40
1:B:653:HIS:CD2	1:B:666:GLY:O	2.75	0.40
1:B:977:HIS:O	1:B:977:HIS:CD2	2.75	0.40
1:C:910:LEU:HD12	1:C:910:LEU:C	2.41	0.40
1:D:545:SER:O	1:D:546:LEU:HB2	2.21	0.40
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.56	0.40
6:B:2002:BTB:H41	6:B:2002:BTB:H51	1.94	0.40
1:D:968:MET:HB2	1:D:968:MET:HE2	1.90	0.40
1:A:127:PHE:O	1:A:182:ASN:N	2.37	0.40
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.39	0.40
1:C:337:ILE:HA	1:C:341:LEU:O	2.22	0.40
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.56	0.40
1:D:116:THR:HG23	1:D:116:THR:H	1.66	0.40
1:C:634:GLN:HE21	1:C:634:GLN:H	0.64	0.40
1:C:746:ASP:OD2	1:C:759:ASN:HA	2.22	0.40
1:C:305:ILE:HD11	1:C:645:ARG:CB	2.51	0.40
1:B:845:GLN:OE1	1:B:845:GLN:CA	2.69	0.40
1:A:92:MET:CE	1:A:92:MET:CA	3.00	0.40
1:A:279:ILE:HG13	1:A:280:ASP:N	2.35	0.40
1:C:817:GLN:O	1:C:818:ALA:C	2.59	0.40
1:A:959:ILE:HD13	1:A:959:ILE:HG21	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	957 (95%)	50 (5%)	2 (0%)	52	53
1	B	1009/1023 (99%)	945 (94%)	58 (6%)	6 (1%)	30	24
1	C	1009/1023 (99%)	948 (94%)	54 (5%)	7 (1%)	26	21
1	D	1009/1023 (99%)	957 (95%)	49 (5%)	3 (0%)	46	45
All	All	4036/4092 (99%)	3807 (94%)	211 (5%)	18 (0%)	39	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	732	ALA
1	B	796	SER
1	B	801	ILE
1	B	802	ASP
1	C	686	PRO
1	C	689	GLU
1	C	732	ALA
1	D	688	PRO
1	A	796	SER
1	B	731	PRO
1	D	164	ASP
1	D	546	LEU
1	C	164	ASP
1	C	461	GLU
1	C	832	ASP
1	A	916	ASP
1	C	688	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	802 (93%)	62 (7%)	18	14
1	B	864/875 (99%)	801 (93%)	63 (7%)	17	13
1	C	864/875 (99%)	806 (93%)	58 (7%)	20	16
1	D	864/875 (99%)	806 (93%)	58 (7%)	20	16
All	All	3456/3500 (99%)	3215 (93%)	241 (7%)	19	15

All (241) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER
1	A	76	CYS
1	A	92	MET
1	A	126	THR
1	A	128	ASN
1	A	131	GLU
1	A	135	GLN
1	A	171	PHE
1	A	181	GLU
1	A	237	ARG
1	A	245	GLN
1	A	251	ARG
1	A	262	GLN
1	A	267	VAL
1	A	299	LYS
1	A	319	ASP
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	519	SER
1	A	535	LEU
1	A	546	LEU
1	A	581	ASN
1	A	599	ARG
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	661	LYS
1	A	667	GLU

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Mol	Chain	Res	Type
1	A	680	ILE
1	A	681	GLU
1	A	685	LEU
1	A	687	GLN
1	A	704	ASN
1	A	727	SER
1	A	729	THR
1	A	735	HIS
1	A	737	ILE
1	A	745	MET
1	A	750	GLU
1	A	755	ARG
1	A	772	ASP
1	A	773	LYS
1	A	774	LYS
1	A	776	LEU
1	A	778	THR
1	A	796	SER
1	A	799	THR
1	A	817	GLN
1	A	829	THR
1	A	854	LYS
1	A	857	ARG
1	A	859	ASP
1	A	863	GLN
1	A	894	ARG
1	A	910	LEU
1	A	951	TRP
1	A	956	GLN
1	A	980	GLU
1	A	1017	GLN
1	A	1023	LYS
1	B	46	ARG
1	B	80	GLU
1	B	90	TRP
1	B	125	LEU
1	B	132	SER
1	B	135	GLN
1	B	157	ARG
1	B	178	ARG
1	B	181	GLU
1	B	237	ARG

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Mol	Chain	Res	Type
1	B	262	GLN
1	B	277	GLU
1	B	278	ILE
1	B	279	ILE
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	394	ASN
1	B	519	SER
1	B	546	LEU
1	B	600	GLN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	672	VAL
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	699	ARG
1	B	730	LEU
1	B	737	ILE
1	B	741	THR
1	B	743	SER
1	B	745	MET
1	B	754	LYS
1	B	755	ARG
1	B	766	SER
1	B	773	LYS
1	B	774	LYS
1	B	781	ARG
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	804	ASN
1	B	819	GLU
1	B	822	LEU
1	B	845	GLN
1	B	847	LYS

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Mol	Chain	Res	Type
1	B	850	PHE
1	B	855	THR
1	B	856	TYR
1	B	857	ARG
1	B	858	ILE
1	B	910	LEU
1	B	917	ARG
1	B	926	TYR
1	B	956	GLN
1	B	1022	GLN
1	B	1023	LYS
1	C	39	SER
1	C	49	GLN
1	C	52	ARG
1	C	71	GLU
1	C	76	CYS
1	C	80	GLU
1	C	90	TRP
1	C	135	GLN
1	C	157	ARG
1	C	165	SER
1	C	181	GLU
1	C	214	LEU
1	C	218	PRO
1	C	230	ARG
1	C	237	ARG
1	C	262	GLN
1	C	278	ILE
1	C	279	ILE
1	C	292	ARG
1	C	296	GLU
1	C	333	ARG
1	C	344	LEU
1	C	370	GLN
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	554	GLN
1	C	580	GLU
1	C	604	ASN
1	C	632	SER
1	C	634	GLN

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Mol	Chain	Res	Type
1	C	651	LEU
1	C	655	MET
1	C	661	LYS
1	C	681	GLU
1	C	687	GLN
1	C	689	GLU
1	C	743	SER
1	C	751	LEU
1	C	759	ASN
1	C	760	ARG
1	C	761	GLN
1	C	772	ASP
1	C	773	LYS
1	C	778	THR
1	C	799	THR
1	C	800	ARG
1	C	819	GLU
1	C	822	LEU
1	C	824	GLN
1	C	828	ASP
1	C	830	LEU
1	C	893	GLU
1	C	894	ARG
1	C	917	ARG
1	C	956	GLN
1	C	986	ILE
1	C	997	ASP
1	D	48	SER
1	D	52	ARG
1	D	71	GLU
1	D	72	SER
1	D	75	GLU
1	D	76	CYS
1	D	90	TRP
1	D	130	ASP
1	D	131	GLU
1	D	157	ARG
1	D	237	ARG
1	D	249	GLU
1	D	264	GLU
1	D	277	GLU
1	D	324	GLU

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Mol	Chain	Res	Type
1	D	333	ARG
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	535	LEU
1	D	546	LEU
1	D	580	GLU
1	D	581	ASN
1	D	595	THR
1	D	630	ARG
1	D	653	HIS
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	665	SER
1	D	667	GLU
1	D	675	GLN
1	D	677	LYS
1	D	685	LEU
1	D	687	GLN
1	D	699	ARG
1	D	710	GLU
1	D	729	THR
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	745	MET
1	D	755	ARG
1	D	761	GLN
1	D	772	ASP
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	800	ARG
1	D	804	ASN
1	D	856	TYR
1	D	893	GLU
1	D	894	ARG
1	D	910	LEU
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN

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Mol	Chain	Res	Type
1	D	1022	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	262	GLN
1	A	266	GLN
1	A	510	GLN
1	A	600	GLN
1	A	624	GLN
1	A	702	GLN
1	A	761	GLN
1	A	804	ASN
1	A	817	GLN
1	A	824	GLN
1	A	863	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1022	GLN
1	B	102	ASN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	687	GLN
1	B	761	GLN
1	B	817	GLN
1	B	878	HIS
1	B	977	HIS
1	C	49	GLN
1	C	135	GLN
1	C	394	ASN
1	C	583	ASN
1	C	624	GLN
1	C	634	GLN
1	C	675	GLN
1	C	702	GLN
1	C	704	ASN
1	C	757	GLN
1	C	761	GLN
1	C	843	GLN

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Mol	Chain	Res	Type
1	C	878	HIS
1	C	977	HIS
1	D	110	ASN
1	D	216	HIS
1	D	262	GLN
1	D	266	GLN
1	D	624	GLN
1	D	628	GLN
1	D	653	HIS
1	D	675	GLN
1	D	687	GLN
1	D	718	GLN
1	D	757	GLN
1	D	761	GLN
1	D	775	GLN
1	D	817	GLN
1	D	845	GLN
1	D	863	GLN
1	D	878	HIS
1	D	977	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 95 ligands modelled in this entry, 20 are monoatomic - leaving 75 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2FG	A	2001	1,4	11,11,12	0.87	0	11,15,17	2.35	2 (18%)
5	DMS	A	8401	-	3,3,3	1.31	0	3,3,3	0.34	0
5	DMS	A	8402	-	3,3,3	2.24	2 (66%)	3,3,3	0.52	0
5	DMS	A	8403	-	3,3,3	0.75	0	3,3,3	0.38	0
5	DMS	A	8404	-	3,3,3	0.73	0	3,3,3	0.35	0
5	DMS	A	8405	-	3,3,3	1.09	0	3,3,3	0.22	0
5	DMS	A	8406	-	3,3,3	0.86	0	3,3,3	0.45	0
5	DMS	A	8407	-	3,3,3	1.20	0	3,3,3	0.80	0
5	DMS	A	8408	-	3,3,3	0.50	0	3,3,3	0.30	0
5	DMS	A	8409	-	3,3,3	1.71	2 (66%)	3,3,3	0.34	0
5	DMS	A	8410	-	3,3,3	0.68	0	3,3,3	0.09	0
5	DMS	A	8411	-	3,3,3	0.42	0	3,3,3	0.86	0
5	DMS	A	8412	-	3,3,3	0.43	0	3,3,3	0.34	0
5	DMS	A	8414	-	3,3,3	1.03	0	3,3,3	0.31	0
5	DMS	A	8417	-	3,3,3	2.07	2 (66%)	3,3,3	1.18	1 (33%)
5	DMS	A	8419	-	3,3,3	0.77	0	3,3,3	0.19	0
5	DMS	A	8423	-	3,3,3	1.10	0	3,3,3	0.11	0
5	DMS	A	8501	-	3,3,3	0.31	0	3,3,3	0.26	0
5	DMS	A	8502	-	3,3,3	0.99	0	3,3,3	0.11	0
5	DMS	A	8504	-	3,3,3	1.00	0	3,3,3	0.10	0
2	2FG	B	2001	1,4	11,11,12	1.23	1 (9%)	11,15,17	2.11	3 (27%)
6	BTB	B	2002	-	12,13,13	1.31	2 (16%)	8,16,16	0.96	1 (12%)
5	DMS	B	8401	-	3,3,3	1.86	1 (33%)	3,3,3	0.28	0
5	DMS	B	8402	-	3,3,3	0.76	0	3,3,3	0.40	0
5	DMS	B	8403	-	3,3,3	1.24	0	3,3,3	0.43	0
5	DMS	B	8404	-	3,3,3	0.53	0	3,3,3	0.41	0
5	DMS	B	8405	-	3,3,3	0.96	0	3,3,3	0.12	0
5	DMS	B	8406	-	3,3,3	0.81	0	3,3,3	0.26	0
5	DMS	B	8407	-	3,3,3	1.19	0	3,3,3	1.07	0
5	DMS	B	8408	-	3,3,3	0.72	0	3,3,3	0.63	0
5	DMS	B	8409	-	3,3,3	1.42	0	3,3,3	0.11	0
5	DMS	B	8411	-	3,3,3	1.02	0	3,3,3	0.39	0
5	DMS	B	8412	-	3,3,3	1.05	0	3,3,3	0.09	0
5	DMS	B	8414	-	3,3,3	1.65	1 (33%)	3,3,3	0.61	0
5	DMS	B	8417	-	3,3,3	0.58	0	3,3,3	0.13	0
5	DMS	B	8421	-	3,3,3	0.78	0	3,3,3	0.24	0
5	DMS	B	8423	-	3,3,3	0.99	0	3,3,3	0.09	0
5	DMS	B	8425	-	3,3,3	1.13	0	3,3,3	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8502	-	3,3,3	1.40	1 (33%)	3,3,3	0.81	0
5	DMS	B	8504	-	3,3,3	0.68	0	3,3,3	0.34	0
5	DMS	B	8506	-	3,3,3	1.17	0	3,3,3	0.56	0
5	DMS	B	8508	-	3,3,3	1.83	1 (33%)	3,3,3	0.76	0
2	2FG	C	2001	1,4	11,11,12	1.17	1 (9%)	11,15,17	1.96	3 (27%)
5	DMS	C	8401	-	3,3,3	1.33	1 (33%)	3,3,3	1.07	0
5	DMS	C	8402	-	3,3,3	0.84	0	3,3,3	0.31	0
5	DMS	C	8403	-	3,3,3	0.95	0	3,3,3	0.91	0
5	DMS	C	8404	-	3,3,3	1.27	0	3,3,3	0.40	0
5	DMS	C	8405	-	3,3,3	0.85	0	3,3,3	0.14	0
5	DMS	C	8408	-	3,3,3	1.01	0	3,3,3	0.58	0
5	DMS	C	8409	-	3,3,3	1.31	0	3,3,3	0.22	0
5	DMS	C	8411	-	3,3,3	1.06	0	3,3,3	0.42	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.14	0
5	DMS	C	8414	-	3,3,3	0.36	0	3,3,3	0.15	0
5	DMS	C	8417	-	3,3,3	0.61	0	3,3,3	0.26	0
5	DMS	C	8419	-	3,3,3	0.81	0	3,3,3	0.15	0
5	DMS	C	8421	-	3,3,3	1.29	1 (33%)	3,3,3	0.69	0
5	DMS	C	8423	-	3,3,3	1.25	0	3,3,3	0.21	0
5	DMS	C	8504	-	3,3,3	0.58	0	3,3,3	0.30	0
2	2FG	D	2001	1,4	11,11,12	1.37	2 (18%)	11,15,17	2.28	3 (27%)
6	BTB	D	2002	-	12,13,13	1.23	2 (16%)	8,16,16	0.71	0
5	DMS	D	8401	-	3,3,3	1.12	0	3,3,3	0.59	0
5	DMS	D	8402	-	3,3,3	1.84	2 (66%)	3,3,3	0.11	0
5	DMS	D	8403	-	3,3,3	1.63	1 (33%)	3,3,3	0.62	0
5	DMS	D	8405	-	3,3,3	1.18	0	3,3,3	0.09	0
5	DMS	D	8406	-	3,3,3	0.63	0	3,3,3	0.59	0
5	DMS	D	8408	-	3,3,3	0.47	0	3,3,3	0.63	0
5	DMS	D	8409	-	3,3,3	1.50	1 (33%)	3,3,3	0.13	0
5	DMS	D	8411	-	3,3,3	0.86	0	3,3,3	0.21	0
5	DMS	D	8412	-	3,3,3	1.63	1 (33%)	3,3,3	0.29	0
5	DMS	D	8414	-	3,3,3	0.32	0	3,3,3	0.40	0
5	DMS	D	8416	-	3,3,3	0.64	0	3,3,3	0.63	0
5	DMS	D	8421	-	3,3,3	0.68	0	3,3,3	0.11	0
5	DMS	D	8423	-	3,3,3	0.96	0	3,3,3	0.20	0
5	DMS	D	8427	-	3,3,3	1.16	0	3,3,3	0.78	0
5	DMS	D	8501	-	3,3,3	0.28	0	3,3,3	0.32	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2FG	A	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
5	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
2	2FG	B	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
6	BTB	B	2002	-	-	0/21/21/21	0/0/0/0
5	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8425	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8506	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
2	2FG	C	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
5	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
2	2FG	D	2001	1,4	1/1/4/5	0/2/19/22	0/1/1/1
6	BTB	D	2002	-	-	0/21/21/21	0/0/0/0
5	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8427	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8501	-	-	0/0/0/0	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2001	2FG	O5-C1	-2.80	1.39	1.43
6	D	2002	BTB	C1-C2	-2.61	1.49	1.53
6	B	2002	BTB	C1-C2	-2.50	1.50	1.53
5	A	8409	DMS	O-S	2.00	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2002	BTB	C3-C2	2.03	1.55	1.53
5	A	8402	DMS	O-S	2.13	1.64	1.50
6	B	2002	BTB	C3-C2	2.15	1.55	1.53
5	C	8421	DMS	O-S	2.15	1.64	1.50
5	A	8409	DMS	C2-S	2.17	1.92	1.75
2	B	2001	2FG	C2-C3	2.19	1.53	1.51
5	D	8402	DMS	C2-S	2.20	1.92	1.75
5	A	8417	DMS	C1-S	2.22	1.92	1.75
5	C	8401	DMS	C2-S	2.22	1.92	1.75
5	B	8502	DMS	C1-S	2.24	1.93	1.75
5	D	8402	DMS	O-S	2.27	1.65	1.50
5	D	8403	DMS	C2-S	2.41	1.94	1.75
5	D	8409	DMS	O-S	2.50	1.67	1.50
5	B	8401	DMS	C2-S	2.67	1.96	1.75
5	A	8417	DMS	C2-S	2.75	1.96	1.75
5	B	8414	DMS	C2-S	2.77	1.97	1.75
5	D	8412	DMS	C1-S	2.80	1.97	1.75
5	B	8508	DMS	C1-S	2.80	1.97	1.75
2	C	2001	2FG	C2-C3	2.85	1.54	1.51
2	D	2001	2FG	C2-C3	2.89	1.54	1.51
5	A	8402	DMS	C2-S	3.22	2.00	1.75

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	2FG	O5-C1-C2	-6.79	101.51	111.78
2	D	2001	2FG	O5-C1-C2	-6.15	102.48	111.78
2	B	2001	2FG	O5-C1-C2	-4.88	104.40	111.78
2	C	2001	2FG	O5-C1-C2	-4.16	105.49	111.78
2	C	2001	2FG	C6-C5-C4	-2.77	106.19	113.02
2	A	2001	2FG	O5-C5-C6	-2.59	101.74	107.35
6	B	2002	BTB	O4-C4-C2	-2.18	105.87	111.12
2	B	2001	2FG	C3-C4-C5	-2.05	106.63	110.20
5	A	8417	DMS	C2-S-C1	2.01	108.85	98.46
2	D	2001	2FG	F2-C2-C3	2.26	112.72	107.41
2	D	2001	2FG	O3-C3-C2	2.87	113.67	109.03
2	C	2001	2FG	C1-O5-C5	3.01	116.07	112.25
2	B	2001	2FG	O3-C3-C2	3.52	114.72	109.03

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2001	2FG	C1
2	A	2001	2FG	C1
2	B	2001	2FG	C1
2	C	2001	2FG	C1

There are no torsion outliers.

There are no ring outliers.

29 monomers are involved in 81 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	2FG	1	0
5	A	8402	DMS	3	0
5	A	8404	DMS	1	0
5	A	8406	DMS	5	0
5	A	8407	DMS	2	0
5	A	8410	DMS	1	0
5	A	8412	DMS	3	0
5	A	8414	DMS	4	0
5	A	8419	DMS	3	0
5	A	8501	DMS	2	0
5	A	8504	DMS	2	0
6	B	2002	BTB	7	0
5	B	8409	DMS	2	0
5	B	8411	DMS	2	0
5	B	8412	DMS	2	0
5	B	8417	DMS	4	0
5	B	8425	DMS	2	0
5	B	8502	DMS	1	0
5	B	8504	DMS	8	0
5	B	8506	DMS	5	0
5	C	8404	DMS	1	0
5	C	8412	DMS	2	0
5	C	8417	DMS	1	0
5	C	8419	DMS	2	0
5	C	8421	DMS	5	0
6	D	2002	BTB	6	0
5	D	8403	DMS	1	0
5	D	8411	DMS	1	0
5	D	8427	DMS	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.30	32 (3%)	51	60	14, 27, 61, 100	0
1	B	1011/1023 (98%)	-0.24	28 (2%)	56	64	15, 28, 64, 100	0
1	C	1011/1023 (98%)	-0.24	33 (3%)	50	59	14, 28, 62, 100	0
1	D	1011/1023 (98%)	-0.33	33 (3%)	50	59	12, 27, 62, 99	0
All	All	4044/4092 (98%)	-0.28	126 (3%)	52	61	12, 28, 63, 100	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	798	ALA	9.8
1	A	732	ALA	8.1
1	C	732	ALA	7.8
1	C	799	THR	7.7
1	A	735	HIS	7.7
1	B	799	THR	7.3
1	C	798	ALA	7.0
1	B	796	SER	6.9
1	D	735	HIS	6.8
1	D	798	ALA	6.6
1	A	801	ILE	6.3
1	C	800	ARG	6.3
1	D	799	THR	6.0
1	C	733	ALA	6.0
1	D	801	ILE	5.7
1	B	801	ILE	5.7
1	C	801	ILE	5.6
1	A	798	ALA	5.3
1	A	799	THR	5.2
1	C	795	VAL	5.1
1	A	685	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
1	D	733	ALA	4.9
1	C	731	PRO	4.8
1	C	685	LEU	4.8
1	C	580	GLU	4.7
1	B	689	GLU	4.7
1	B	797	GLU	4.6
1	A	800	ARG	4.6
1	D	689	GLU	4.6
1	A	733	ALA	4.5
1	C	745	MET	4.4
1	D	687	GLN	4.3
1	D	581	ASN	4.3
1	D	732	ALA	4.3
1	D	800	ARG	4.2
1	D	730	LEU	4.2
1	B	800	ARG	4.2
1	A	730	LEU	3.9
1	C	761	GLN	3.9
1	B	795	VAL	3.9
1	A	686	PRO	3.9
1	A	687	GLN	3.9
1	C	686	PRO	3.8
1	A	797	GLU	3.8
1	C	730	LEU	3.7
1	D	734	SER	3.7
1	C	797	GLU	3.6
1	C	687	GLN	3.6
1	C	735	HIS	3.6
1	B	135	GLN	3.6
1	B	731	PRO	3.6
1	A	581	ASN	3.6
1	B	730	LEU	3.6
1	A	580	GLU	3.5
1	B	686	PRO	3.4
1	C	581	ASN	3.4
1	A	795	VAL	3.4
1	A	731	PRO	3.3
1	C	684	GLU	3.3
1	A	734	SER	3.3
1	B	685	LEU	3.3
1	A	796	SER	3.3
1	B	745	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	689	GLU	3.2
1	A	729	THR	3.2
1	D	580	GLU	3.2
1	B	733	ALA	3.2
1	B	688	PRO	3.2
1	B	729	THR	3.1
1	D	686	PRO	3.1
1	A	582	GLY	3.0
1	A	737	ILE	3.0
1	B	732	ALA	3.0
1	C	729	THR	2.9
1	D	797	GLU	2.9
1	B	79	PRO	2.9
1	D	685	LEU	2.8
1	B	687	GLN	2.8
1	D	688	PRO	2.8
1	D	81	ALA	2.8
1	A	736	ALA	2.7
1	C	803	PRO	2.7
1	D	796	SER	2.7
1	C	802	ASP	2.6
1	A	684	GLU	2.6
1	D	582	GLY	2.6
1	D	179	ALA	2.6
1	A	180	GLY	2.6
1	B	684	GLU	2.6
1	A	583	ASN	2.5
1	D	729	THR	2.5
1	D	831	ALA	2.5
1	C	76	CYS	2.5
1	C	734	SER	2.5
1	D	684	GLU	2.4
1	C	831	ALA	2.4
1	D	634	GLN	2.4
1	B	581	ASN	2.3
1	B	735	HIS	2.3
1	B	76	CYS	2.3
1	C	690	SER	2.3
1	C	634	GLN	2.3
1	C	689	GLU	2.3
1	A	188	VAL	2.2
1	B	146	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	71	GLU	2.2
1	B	690	SER	2.2
1	B	188	VAL	2.2
1	D	681	GLU	2.2
1	A	146	VAL	2.2
1	D	583	ASN	2.1
1	C	149	ALA	2.1
1	D	736	ALA	2.1
1	D	690	SER	2.1
1	A	579	ASP	2.1
1	C	513	PRO	2.1
1	A	534	ILE	2.1
1	D	772	ASP	2.1
1	D	679	LEU	2.1
1	A	738	PRO	2.1
1	B	136	GLU	2.1
1	C	688	PRO	2.1
1	C	583	ASN	2.1
1	D	79	PRO	2.0
1	C	146	VAL	2.0
1	D	752	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	DMS	B	8508	4/4	0.69	0.24	9.59	41,70,84,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	D	8423	4/4	0.90	0.16	9.46	40,91,100,100	0
5	DMS	D	8408	4/4	0.98	0.19	5.68	28,52,55,88	0
5	DMS	A	8419	4/4	0.93	0.23	5.67	54,61,62,77	0
5	DMS	B	8407	4/4	0.76	0.21	5.18	26,40,100,100	0
5	DMS	A	8412	4/4	0.95	0.22	5.06	31,40,69,100	0
5	DMS	C	8419	4/4	0.89	0.30	4.97	43,81,100,100	0
5	DMS	B	8423	4/4	0.95	0.20	4.34	59,81,83,100	0
5	DMS	A	8406	4/4	0.95	0.16	4.12	41,54,65,100	0
5	DMS	A	8402	4/4	0.96	0.13	4.11	24,49,63,100	0
5	DMS	A	8423	4/4	0.90	0.15	3.91	65,80,99,100	0
5	DMS	A	8502	4/4	0.94	0.17	3.65	35,83,93,100	0
5	DMS	A	8407	4/4	0.79	0.19	3.48	41,44,100,100	0
5	DMS	C	8404	4/4	0.88	0.13	3.39	22,47,56,100	0
5	DMS	B	8502	4/4	0.90	0.16	3.35	38,65,97,100	0
5	DMS	C	8403	4/4	0.99	0.14	3.19	33,35,40,41	0
3	MG	B	3002	1/1	0.96	0.11	2.98	27,27,27,27	0
6	BTB	B	2002	14/14	0.93	0.15	2.96	12,53,100,100	0
5	DMS	B	8425	4/4	0.80	0.23	2.94	65,81,100,100	0
5	DMS	B	8405	4/4	0.97	0.13	2.64	29,48,83,100	0
5	DMS	D	8406	4/4	0.95	0.13	2.60	29,61,81,100	0
5	DMS	A	8504	4/4	0.97	0.15	2.56	55,69,100,100	0
5	DMS	B	8411	4/4	0.98	0.15	2.55	35,40,41,50	0
5	DMS	B	8406	4/4	0.94	0.18	2.51	67,84,100,100	0
5	DMS	A	8403	4/4	0.98	0.14	2.23	21,37,52,98	0
6	BTB	D	2002	14/14	0.92	0.16	2.08	23,49,100,100	0
5	DMS	A	8417	4/4	0.80	0.20	2.03	44,45,60,100	0
5	DMS	C	8423	4/4	0.74	0.14	1.87	38,49,66,90	0
4	NA	C	3103	1/1	0.96	0.19	1.80	48,48,48,48	0
5	DMS	A	8404	4/4	0.87	0.15	1.46	24,30,52,100	0
5	DMS	D	8402	4/4	0.97	0.12	1.44	24,44,46,100	0
5	DMS	B	8417	4/4	0.94	0.20	1.25	37,100,100,100	0
5	DMS	A	8401	4/4	0.99	0.11	1.20	23,24,26,27	0
3	MG	D	3002	1/1	1.00	0.11	1.15	26,26,26,26	0
5	DMS	D	8405	4/4	0.97	0.09	1.09	25,38,56,79	0
5	DMS	D	8401	4/4	0.99	0.11	1.00	21,23,30,34	0
5	DMS	A	8408	4/4	0.98	0.11	0.79	40,50,100,100	0
5	DMS	B	8402	4/4	0.96	0.10	0.68	35,39,52,74	0
5	DMS	C	8412	4/4	0.97	0.15	0.60	29,31,58,80	0
5	DMS	B	8412	4/4	0.97	0.13	0.49	34,50,86,100	0
5	DMS	C	8401	4/4	0.99	0.10	0.48	18,25,29,36	0
4	NA	D	3102	1/1	0.93	0.12	0.42	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8401	4/4	0.99	0.10	0.39	21,26,29,38	0
5	DMS	B	8408	4/4	0.97	0.10	0.37	30,62,100,100	0
5	DMS	B	8404	4/4	0.95	0.10	0.36	23,45,47,96	0
5	DMS	C	8408	4/4	0.96	0.10	0.36	21,53,78,100	0
5	DMS	A	8501	4/4	0.89	0.14	0.26	46,49,91,100	0
2	2FG	D	2001	11/12	0.98	0.11	0.25	18,23,24,26	0
2	2FG	A	2001	11/12	0.98	0.10	0.22	14,22,28,29	0
5	DMS	C	8411	4/4	0.96	0.12	0.22	42,47,52,56	0
5	DMS	A	8405	4/4	0.96	0.10	0.21	35,37,65,100	0
5	DMS	D	8412	4/4	0.98	0.13	0.20	26,44,50,100	0
5	DMS	D	8501	4/4	0.95	0.12	0.19	32,52,88,100	0
5	DMS	C	8417	4/4	0.95	0.15	0.16	43,51,92,100	0
4	NA	C	3102	1/1	0.98	0.10	0.07	23,23,23,23	0
2	2FG	B	2001	11/12	0.98	0.10	-0.00	17,24,29,29	0
5	DMS	B	8504	4/4	0.95	0.14	-0.10	43,79,90,100	0
5	DMS	D	8403	4/4	0.99	0.08	-0.12	30,33,36,37	0
2	2FG	C	2001	11/12	0.98	0.10	-0.19	19,23,26,26	0
5	DMS	C	8405	4/4	0.97	0.08	-0.27	39,42,52,97	0
5	DMS	C	8402	4/4	0.98	0.09	-0.33	19,27,40,49	0
5	DMS	A	8411	4/4	0.98	0.09	-0.37	40,42,43,51	0
5	DMS	B	8403	4/4	0.99	0.10	-0.68	21,32,32,53	0
4	NA	A	3102	1/1	0.98	0.09	-0.70	31,31,31,31	0
4	NA	B	3103	1/1	0.96	0.08	-1.07	40,40,40,40	0
4	NA	A	3103	1/1	0.97	0.08	-1.26	42,42,42,42	0
4	NA	B	3102	1/1	0.98	0.04	-1.57	20,20,20,20	0
4	NA	D	3103	1/1	0.97	0.07	-1.66	39,39,39,39	0
4	NA	C	3101	1/1	0.98	0.08	-1.73	19,19,19,19	0
3	MG	C	3002	1/1	0.95	0.04	-1.88	26,26,26,26	0
3	MG	B	3001	1/1	0.99	0.06	-1.99	21,21,21,21	0
4	NA	B	3101	1/1	1.00	0.08	-2.30	19,19,19,19	0
4	NA	D	3101	1/1	1.00	0.07	-2.44	21,21,21,21	0
3	MG	A	3002	1/1	0.98	0.04	-2.47	27,27,27,27	0
3	MG	A	3001	1/1	0.96	0.05	-2.67	26,26,26,26	0
3	MG	C	3001	1/1	0.99	0.04	-3.29	23,23,23,23	0
3	MG	D	3001	1/1	0.99	0.03	-3.76	19,19,19,19	0
4	NA	A	3101	1/1	0.99	0.04	-4.58	21,21,21,21	0
5	DMS	B	8409	4/4	0.88	0.20	-	34,48,100,100	0
5	DMS	D	8409	4/4	0.92	0.13	-	38,41,72,100	0
5	DMS	B	8421	4/4	0.94	0.16	-	39,46,73,100	0
5	DMS	B	8414	4/4	0.94	0.07	-	34,37,53,100	0
5	DMS	D	8411	4/4	0.98	0.11	-	44,53,66,100	0
5	DMS	A	8409	4/4	0.93	0.09	-	33,36,40,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	C	8409	4/4	0.93	0.12	-	46,57,75,75	0
5	DMS	D	8421	4/4	0.92	0.16	-	47,80,81,100	0
5	DMS	C	8414	4/4	0.96	0.12	-	31,48,89,100	0
5	DMS	C	8421	4/4	0.88	0.18	-	44,48,73,100	0
5	DMS	A	8410	4/4	0.92	0.30	-	44,82,100,100	0
5	DMS	C	8504	4/4	0.97	0.08	-	42,65,81,81	0
5	DMS	D	8414	4/4	0.97	0.17	-	30,60,62,81	0
5	DMS	D	8416	4/4	0.94	0.20	-	47,57,62,100	0
5	DMS	D	8427	4/4	0.73	0.34	-	63,100,100,100	0
5	DMS	A	8414	4/4	0.94	0.18	-	26,74,75,100	0
5	DMS	B	8506	4/4	0.92	0.11	-	20,33,57,90	0

6.5 Other polymers [i](#)

There are no such residues in this entry.