



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:25 PM GMT

PDB ID : 1JZ5
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH D-GALCT
OPYRANOSYL-1-ON
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.80 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

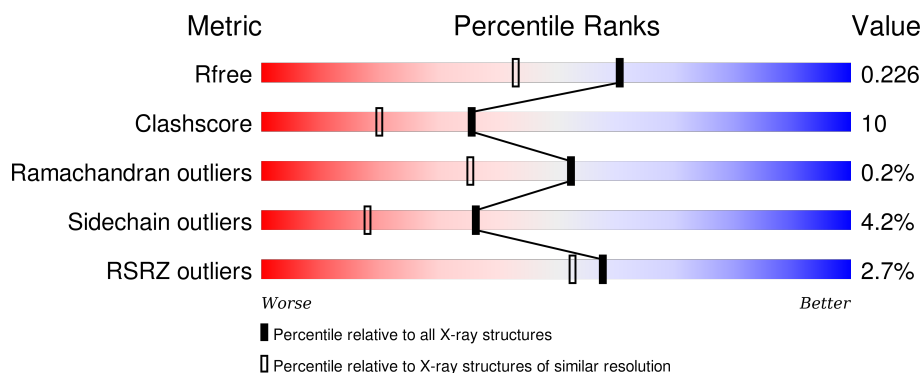
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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>2%</div> <div>68% 25% 5% •</div> </div>
1	B	1023	<div> <div>2%</div> <div>68% 26% 5% •</div> </div>
1	C	1023	<div> <div>3%</div> <div>70% 24% 5% ••</div> </div>
1	D	1023	<div> <div>3%</div> <div>70% 24% 5% •</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
5	DMS	A	8404	-	-	-	X
5	DMS	A	8406	-	-	-	X
5	DMS	A	8407	-	-	-	X
5	DMS	B	8408	-	-	-	X
5	DMS	B	8414	-	-	X	-
5	DMS	B	8417	-	-	-	X
5	DMS	B	8420	-	-	-	X
5	DMS	B	8423	-	-	-	X
5	DMS	B	8425	-	-	-	X
5	DMS	B	8502	-	-	-	X
5	DMS	B	8504	-	-	X	-
5	DMS	B	8508	-	-	-	X
5	DMS	C	8407	-	-	-	X
5	DMS	C	8420	-	-	-	X
5	DMS	C	8423	-	-	-	X
5	DMS	C	8425	-	-	-	X
5	DMS	C	8428	-	-	-	X
5	DMS	D	8403	-	-	-	X
5	DMS	D	8406	-	-	-	X
5	DMS	D	8410	-	-	-	X
5	DMS	D	8419	-	-	X	-
5	DMS	D	8423	-	-	-	X
5	DMS	D	8508	-	-	X	-
5	DMS	D	8703	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36964 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	98	11	0
			8205	5185	1455	1527	38			
1	B	1011	Total	C	N	O	S	64	11	0
			8205	5185	1455	1527	38			
1	C	1011	Total	C	N	O	S	49	11	0
			8205	5185	1455	1527	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8125	5138	1440	1509	38			

There are 32 discrepancies between the modelled and reference sequences:

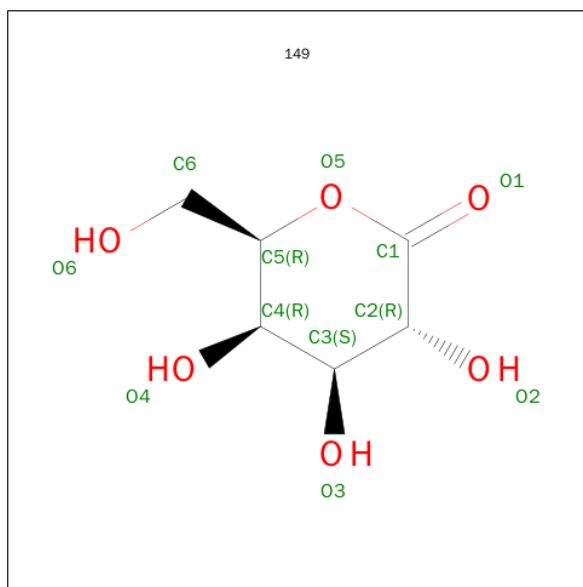
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT	? P00722
A	8	PRO	ALA	CLONING ARTIFACT	? P00722
B	1	GLY	THR	CLONING ARTIFACT	? P00722
B	2	SER	MET	CLONING ARTIFACT	? P00722
B	3	HIS	ILE	CLONING ARTIFACT	? P00722
B	4	MET	THR	CLONING ARTIFACT	? P00722
B	5	LEU	ASP	CLONING ARTIFACT	? P00722
B	6	GLU	SER	CLONING ARTIFACT	? P00722
B	7	ASP	LEU	CLONING ARTIFACT	? P00722
B	8	PRO	ALA	CLONING ARTIFACT	? P00722
C	1	GLY	THR	CLONING ARTIFACT	? P00722
C	2	SER	MET	CLONING ARTIFACT	? P00722
C	3	HIS	ILE	CLONING ARTIFACT	? P00722
C	4	MET	THR	CLONING ARTIFACT	? P00722
C	5	LEU	ASP	CLONING ARTIFACT	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	6	GLU	SER	CLONING ARTIFACT	? P00722
C	7	ASP	LEU	CLONING ARTIFACT	? P00722
C	8	PRO	ALA	CLONING ARTIFACT	? P00722
D	1	GLY	THR	CLONING ARTIFACT	? P00722
D	2	SER	MET	CLONING ARTIFACT	? P00722
D	3	HIS	ILE	CLONING ARTIFACT	? P00722
D	4	MET	THR	CLONING ARTIFACT	? P00722
D	5	LEU	ASP	CLONING ARTIFACT	? P00722
D	6	GLU	SER	CLONING ARTIFACT	? P00722
D	7	ASP	LEU	CLONING ARTIFACT	? P00722
D	8	PRO	ALA	CLONING ARTIFACT	? P00722

- Molecule 2 is SUGAR (D-GALACTONOLACTONE) (three-letter code: 149) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 12 6 6	0	0
2	B	1	Total C O 12 6 6	0	0
2	C	1	Total C O 12 6 6	0	0
2	D	1	Total C O 12 6 6	0	0

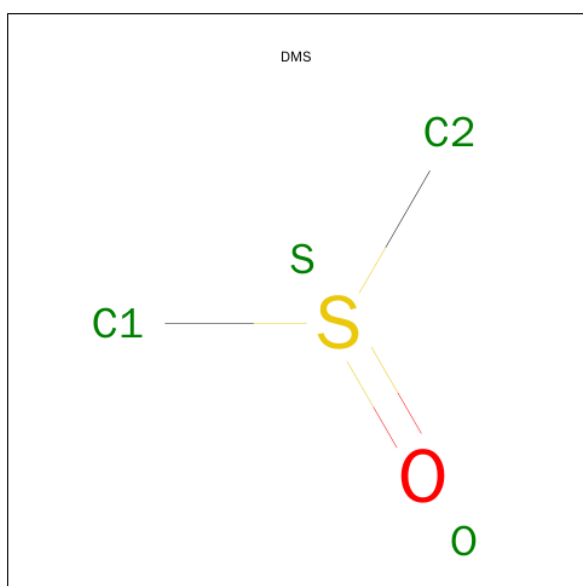
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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



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

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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	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	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	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

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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	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
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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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	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

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

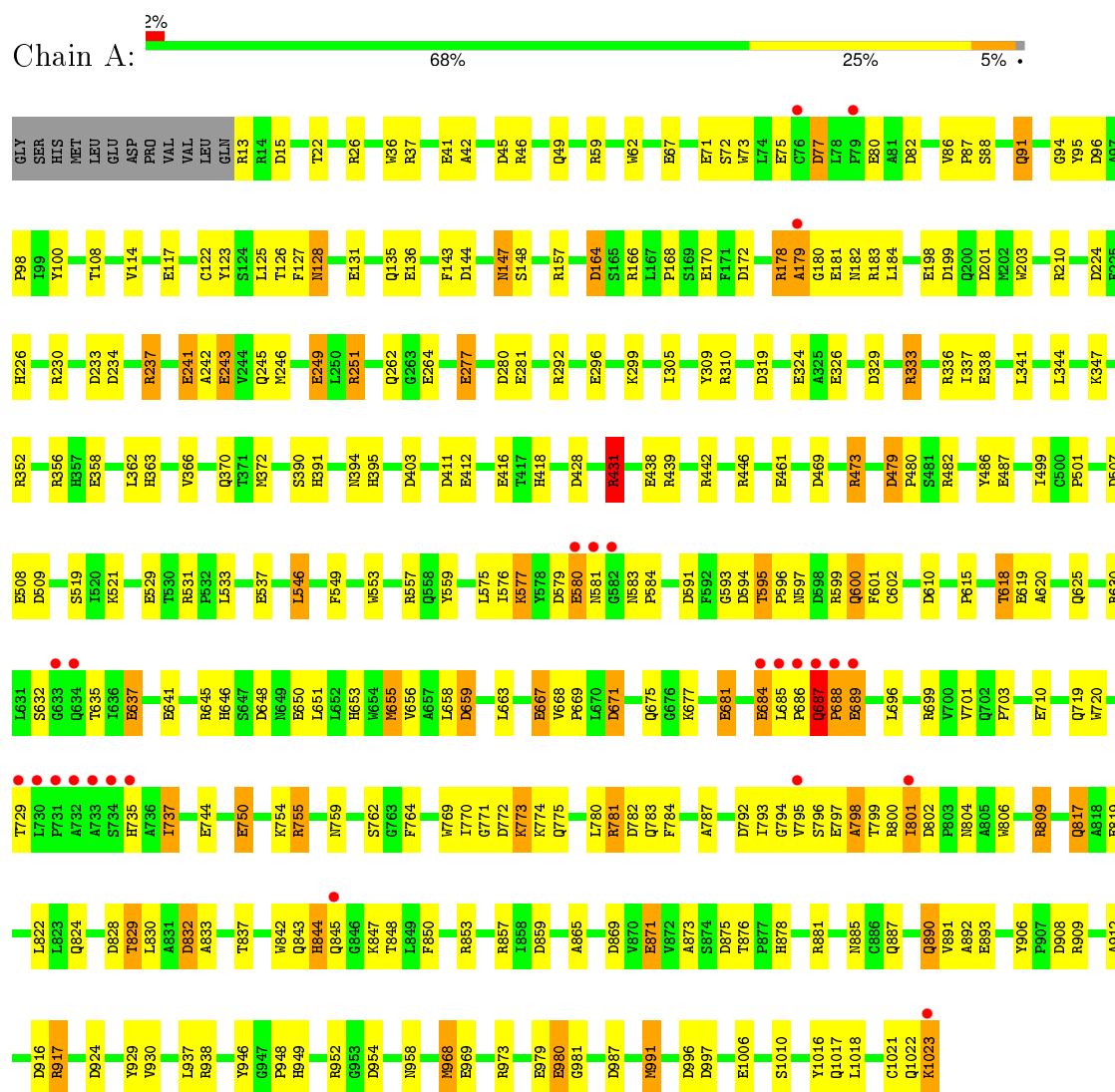
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	953	Total	O	0	0
			953	953		
6	B	937	Total	O	0	0
			937	937		
6	C	952	Total	O	0	0
			952	952		
6	D	959	Total	O	0	0
			959	959		

3 Residue-property plots

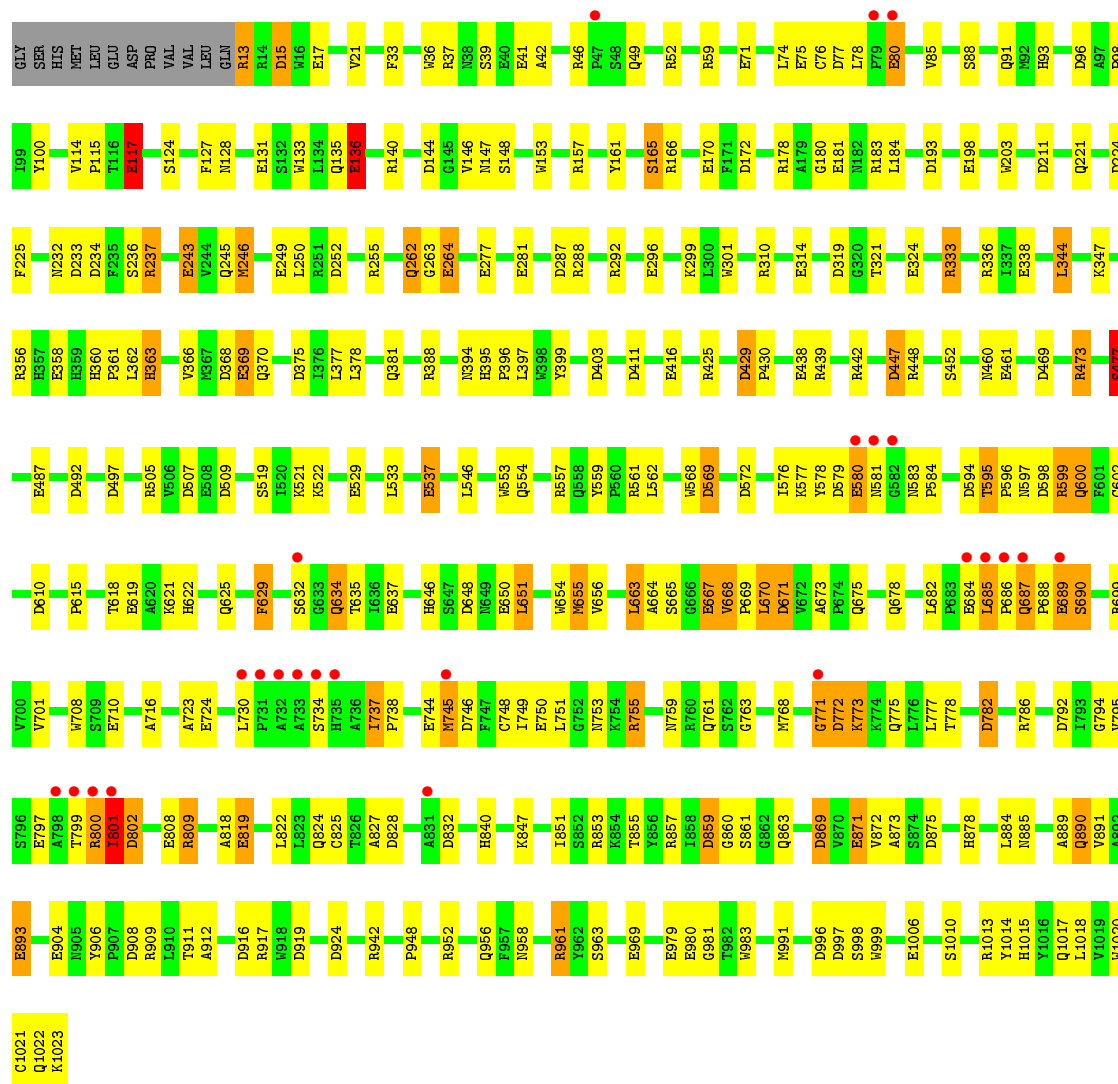
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

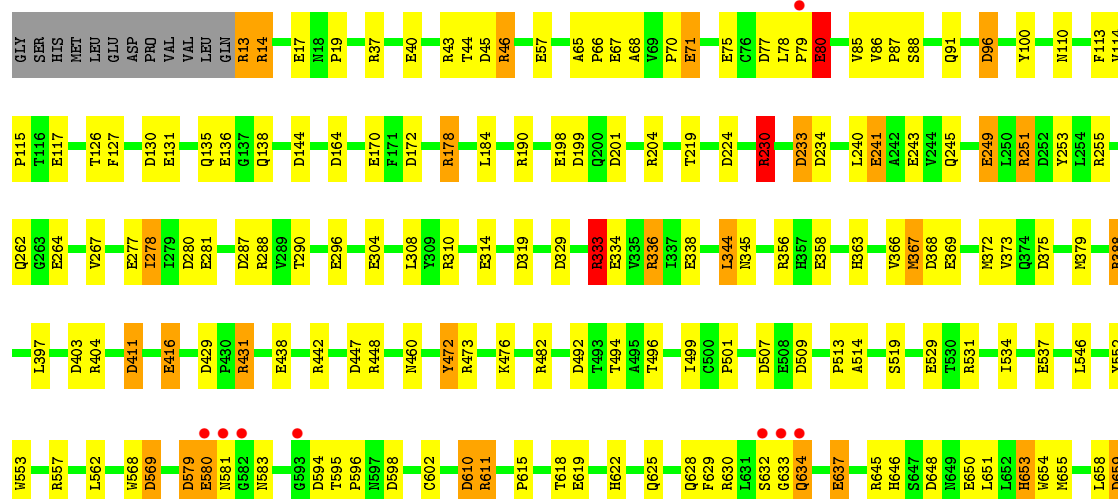


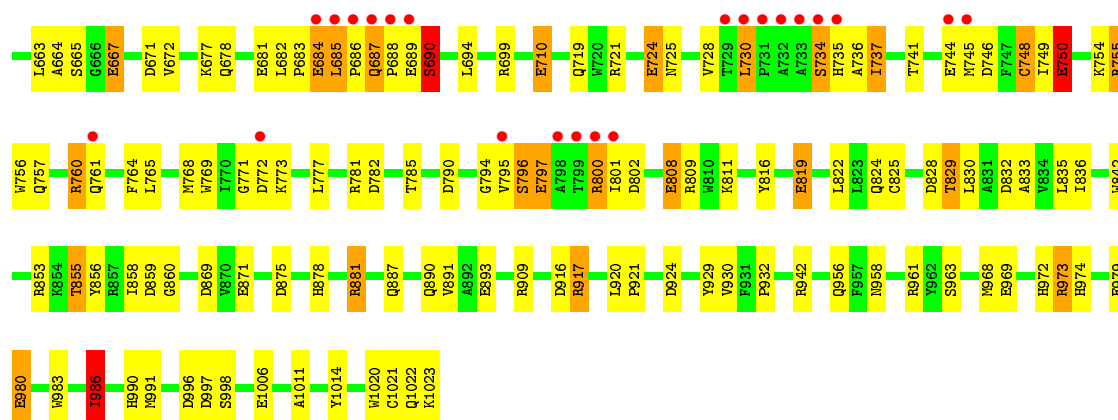
• Molecule 1: Beta-Galactosidase



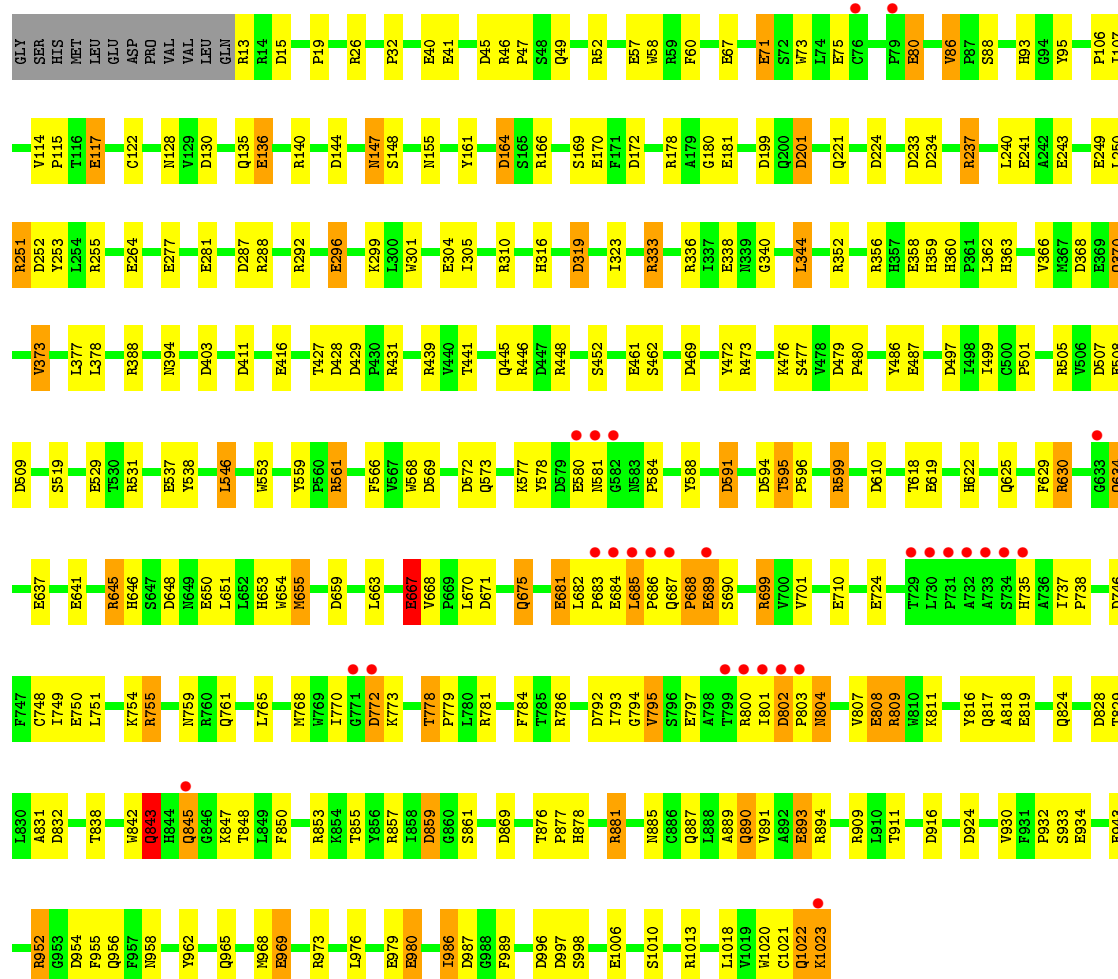


• Molecule 1: Beta-Galactosidase





• 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	149.69Å 168.02Å 201.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.80 17.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	90.4 (17.00-1.80) 90.0 (17.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 1.80Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.160 , 0.231 0.163 , 0.226	Depositor DCC
R_{free} test set	6049 reflections (1.46%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 106.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 419689 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36964	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 37.04 % 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 4.5593e-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, 149

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	1.13	46/8448 (0.5%)	1.66	159/11526 (1.4%)
1	B	1.14	46/8448 (0.5%)	1.70	177/11526 (1.5%)
1	C	1.12	45/8448 (0.5%)	1.64	148/11526 (1.3%)
1	D	1.14	43/8367 (0.5%)	1.66	164/11415 (1.4%)
All	All	1.13	180/33711 (0.5%)	1.67	648/45993 (1.4%)

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	D	1	0

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	537	GLU	CD-OE2	11.40	1.38	1.25
1	A	681	GLU	CD-OE2	10.55	1.37	1.25
1	A	710	GLU	CD-OE2	10.27	1.36	1.25
1	D	893	GLU	CD-OE2	9.79	1.36	1.25
1	D	537	GLU	CD-OE2	9.66	1.36	1.25
1	D	650	GLU	CD-OE2	9.49	1.36	1.25
1	B	580	GLU	CD-OE2	9.35	1.35	1.25
1	A	249	GLU	CD-OE2	9.33	1.35	1.25
1	D	580	GLU	CD-OE2	9.29	1.35	1.25
1	C	75	GLU	CD-OE2	9.22	1.35	1.25
1	C	893	GLU	CD-OE2	9.12	1.35	1.25
1	D	681	GLU	CD-OE2	8.94	1.35	1.25
1	D	80	GLU	CD-OE2	8.86	1.35	1.25
1	D	980	GLU	CD-OE2	8.80	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	980	GLU	CD-OE2	8.76	1.35	1.25
1	C	117	GLU	CD-OE2	8.74	1.35	1.25
1	A	684	GLU	CD-OE2	8.67	1.35	1.25
1	C	170	GLU	CD-OE2	8.61	1.35	1.25
1	D	71	GLU	CD-OE2	8.57	1.35	1.25
1	D	684	GLU	CD-OE2	8.49	1.34	1.25
1	D	117	GLU	CD-OE2	8.46	1.34	1.25
1	D	689	GLU	CD-OE2	8.35	1.34	1.25
1	C	529	GLU	CD-OE2	8.31	1.34	1.25
1	A	487	GLU	CD-OE2	8.29	1.34	1.25
1	C	249	GLU	CD-OE2	8.27	1.34	1.25
1	C	580	GLU	CD-OE2	8.24	1.34	1.25
1	C	969	GLU	CD-OE2	8.23	1.34	1.25
1	C	67	GLU	CD-OE2	8.21	1.34	1.25
1	C	684	GLU	CD-OE2	8.14	1.34	1.25
1	D	710	GLU	CD-OE2	8.09	1.34	1.25
1	D	461	GLU	CD-OE2	7.99	1.34	1.25
1	B	170	GLU	CD-OE2	7.91	1.34	1.25
1	A	689	GLU	CD-OE2	7.84	1.34	1.25
1	C	296	GLU	CD-OE2	7.83	1.34	1.25
1	B	797[A]	GLU	CD-OE2	7.80	1.34	1.25
1	B	797[B]	GLU	CD-OE2	7.80	1.34	1.25
1	D	667	GLU	CD-OE2	7.79	1.34	1.25
1	D	641	GLU	CD-OE1	-7.70	1.17	1.25
1	B	461	GLU	CD-OE2	7.68	1.34	1.25
1	B	117	GLU	CD-OE2	7.62	1.34	1.25
1	D	529	GLU	CD-OE2	7.59	1.34	1.25
1	A	264	GLU	CD-OE2	7.55	1.33	1.25
1	B	71	GLU	CD-OE2	7.54	1.33	1.25
1	C	724	GLU	CD-OE2	7.53	1.33	1.25
1	D	358	GLU	CD-OE2	7.50	1.33	1.25
1	C	80	GLU	CD-OE2	7.50	1.33	1.25
1	B	296	GLU	CD-OE2	7.41	1.33	1.25
1	A	580	GLU	CD-OE2	7.38	1.33	1.25
1	D	943	GLU	CD-OE2	7.38	1.33	1.25
1	D	170	GLU	CD-OE2	7.36	1.33	1.25
1	A	980	GLU	CD-OE2	7.35	1.33	1.25
1	A	75	GLU	CD-OE2	7.33	1.33	1.25
1	D	750	GLU	CD-OE2	7.20	1.33	1.25
1	C	71	GLU	CD-OE2	7.16	1.33	1.25
1	B	249	GLU	CD-OE2	7.15	1.33	1.25
1	B	264	GLU	CD-OE2	7.13	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	969	GLU	CD-OE2	7.10	1.33	1.25
1	A	979	GLU	CD-OE2	7.09	1.33	1.25
1	C	264	GLU	CD-OE2	7.08	1.33	1.25
1	B	871	GLU	CD-OE2	7.07	1.33	1.25
1	B	969	GLU	CD-OE2	7.06	1.33	1.25
1	B	277	GLU	CD-OE2	7.00	1.33	1.25
1	C	131	GLU	CD-OE2	6.95	1.33	1.25
1	A	893	GLU	CD-OE2	6.94	1.33	1.25
1	B	819	GLU	CD-OE2	6.91	1.33	1.25
1	A	170	GLU	CD-OE2	6.87	1.33	1.25
1	C	667	GLU	CD-OE2	6.84	1.33	1.25
1	D	979	GLU	CD-OE2	6.82	1.33	1.25
1	B	80	GLU	CD-OE2	6.82	1.33	1.25
1	B	724	GLU	CD-OE2	6.79	1.33	1.25
1	D	75	GLU	CD-OE2	6.75	1.33	1.25
1	C	650	GLU	CD-OE2	6.72	1.33	1.25
1	A	637	GLU	CD-OE2	6.71	1.33	1.25
1	C	537	GLU	CD-OE2	6.69	1.33	1.25
1	D	57	GLU	CD-OE2	6.69	1.33	1.25
1	B	710	GLU	CD-OE2	6.67	1.32	1.25
1	D	241	GLU	CD-OE2	6.66	1.32	1.25
1	C	304	GLU	CD-OE2	6.66	1.32	1.25
1	B	131	GLU	CD-OE2	6.66	1.32	1.25
1	A	80	GLU	CD-OE2	6.57	1.32	1.25
1	C	710	GLU	CD-OE2	6.53	1.32	1.25
1	B	314	GLU	CD-OE1	-6.52	1.18	1.25
1	C	871	GLU	CD-OE2	6.52	1.32	1.25
1	A	324	GLU	CD-OE2	6.50	1.32	1.25
1	D	243	GLU	CD-OE2	6.50	1.32	1.25
1	D	41	GLU	CD-OE2	6.49	1.32	1.25
1	C	819	GLU	CD-OE2	6.48	1.32	1.25
1	A	181	GLU	CD-OE2	6.48	1.32	1.25
1	B	529	GLU	CD-OE2	6.46	1.32	1.25
1	D	819	GLU	CD-OE2	6.38	1.32	1.25
1	B	684	GLU	CD-OE2	6.38	1.32	1.25
1	C	416	GLU	CD-OE1	-6.36	1.18	1.25
1	C	388	ARG	CZ-NH1	6.33	1.41	1.33
1	C	750	GLU	CD-OE2	6.25	1.32	1.25
1	A	281	GLU	CD-OE2	6.24	1.32	1.25
1	A	41	GLU	CD-OE2	6.23	1.32	1.25
1	A	277	GLU	CD-OE2	6.23	1.32	1.25
1	D	264	GLU	CD-OE2	6.23	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	296	GLU	CD-OE2	6.21	1.32	1.25
1	D	136	GLU	CD-OE2	6.19	1.32	1.25
1	C	136	GLU	CD-OE2	6.19	1.32	1.25
1	B	1006	GLU	CD-OE2	6.17	1.32	1.25
1	B	324	GLU	CD-OE2	6.17	1.32	1.25
1	B	650	GLU	CD-OE2	6.14	1.32	1.25
1	A	461	GLU	CD-OE2	6.09	1.32	1.25
1	A	326	GLU	CD-OE2	6.03	1.32	1.25
1	D	181	GLU	CD-OE2	5.99	1.32	1.25
1	D	797	GLU	CD-OE2	5.99	1.32	1.25
1	C	277	GLU	CD-OE2	5.98	1.32	1.25
1	A	358	GLU	CD-OE2	5.98	1.32	1.25
1	A	1006	GLU	CD-OE2	5.97	1.32	1.25
1	A	819	GLU	CD-OE2	5.97	1.32	1.25
1	B	369	GLU	CD-OE2	5.94	1.32	1.25
1	A	667	GLU	CD-OE2	5.94	1.32	1.25
1	B	281	GLU	CD-OE2	5.91	1.32	1.25
1	B	136	GLU	CD-OE2	5.88	1.32	1.25
1	C	808	GLU	CD-OE2	5.86	1.32	1.25
1	C	241	GLU	CD-OE2	5.86	1.32	1.25
1	D	296	GLU	CD-OE2	5.83	1.32	1.25
1	A	67	GLU	CD-OE2	5.83	1.32	1.25
1	B	41	GLU	CD-OE2	5.83	1.32	1.25
1	D	249	GLU	CD-OE2	5.81	1.32	1.25
1	C	198	GLU	CD-OE2	5.79	1.32	1.25
1	C	744	GLU	CD-OE2	5.78	1.32	1.25
1	A	641	GLU	CD-OE1	-5.77	1.19	1.25
1	B	980	GLU	CD-OE2	5.75	1.31	1.25
1	B	893	GLU	CD-OE2	5.73	1.31	1.25
1	B	667	GLU	CD-OE2	5.71	1.31	1.25
1	A	797[A]	GLU	CD-OE2	5.68	1.31	1.25
1	A	797[B]	GLU	CD-OE2	5.68	1.31	1.25
1	B	181	GLU	CD-OE2	5.67	1.31	1.25
1	D	808	GLU	CD-OE2	5.65	1.31	1.25
1	A	438	GLU	CD-OE2	5.65	1.31	1.25
1	D	969	GLU	CD-OE2	5.63	1.31	1.25
1	B	904	GLU	CD-OE2	5.62	1.31	1.25
1	B	198	GLU	CD-OE2	5.61	1.31	1.25
1	C	619	GLU	CD-OE2	5.61	1.31	1.25
1	D	338	GLU	CD-OE2	5.59	1.31	1.25
1	B	689	GLU	CD-OE2	5.59	1.31	1.25
1	D	304	GLU	CD-OE2	5.58	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	979	GLU	CD-OE2	5.54	1.31	1.25
1	C	338	GLU	CD-OE2	5.53	1.31	1.25
1	D	281	GLU	CD-OE2	5.51	1.31	1.25
1	C	416	GLU	CD-OE2	5.49	1.31	1.25
1	A	136	GLU	CD-OE2	5.47	1.31	1.25
1	B	699	ARG	CZ-NH1	5.46	1.40	1.33
1	B	358	GLU	CD-OE2	5.46	1.31	1.25
1	A	508	GLU	CD-OE2	5.42	1.31	1.25
1	A	241	GLU	CD-OE2	5.42	1.31	1.25
1	A	338	GLU	CD-OE2	5.40	1.31	1.25
1	B	750	GLU	CD-OE2	5.40	1.31	1.25
1	B	537	GLU	CD-OE2	5.39	1.31	1.25
1	D	619	GLU	CD-OE1	-5.38	1.19	1.25
1	D	724	GLU	CD-OE2	5.38	1.31	1.25
1	A	744	GLU	CD-OE2	5.37	1.31	1.25
1	B	744	GLU	CD-OE2	5.35	1.31	1.25
1	D	508	GLU	CD-OE2	5.31	1.31	1.25
1	C	17	GLU	CD-OE1	-5.30	1.19	1.25
1	A	871	GLU	CD-OE2	5.30	1.31	1.25
1	C	797[A]	GLU	CD-OE2	5.28	1.31	1.25
1	C	797[B]	GLU	CD-OE2	5.28	1.31	1.25
1	D	40	GLU	CD-OE2	5.26	1.31	1.25
1	C	314	GLU	CD-OE1	-5.25	1.19	1.25
1	B	17	GLU	CD-OE1	-5.24	1.19	1.25
1	B	75	GLU	CD-OE2	5.24	1.31	1.25
1	B	438	GLU	CD-OE2	5.22	1.31	1.25
1	B	487	GLU	CD-OE2	5.22	1.31	1.25
1	D	487	GLU	CD-OE2	5.21	1.31	1.25
1	A	650	GLU	CD-OE2	5.17	1.31	1.25
1	B	243	GLU	CD-OE2	5.17	1.31	1.25
1	B	979	GLU	CD-OE2	5.14	1.31	1.25
1	A	198	GLU	CD-OE2	5.10	1.31	1.25
1	A	412	GLU	CD-OE2	5.10	1.31	1.25
1	C	281	GLU	CD-OE2	5.09	1.31	1.25
1	C	1006	GLU	CD-OE2	5.09	1.31	1.25
1	C	57	GLU	CD-OE2	5.09	1.31	1.25
1	A	243	GLU	CD-OE1	-5.08	1.20	1.25
1	A	750	GLU	CD-OE2	5.02	1.31	1.25
1	A	529	GLU	CD-OE2	5.02	1.31	1.25
1	C	637	GLU	CD-OE2	5.01	1.31	1.25

All (648) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	ARG	NE-CZ-NH1	21.57	131.08	120.30
1	B	699	ARG	NE-CZ-NH2	-16.36	112.12	120.30
1	B	442	ARG	NE-CZ-NH2	-16.07	112.27	120.30
1	C	809	ARG	NE-CZ-NH1	15.09	127.85	120.30
1	B	442	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	B	46	ARG	NE-CZ-NH2	-13.69	113.45	120.30
1	A	442	ARG	NE-CZ-NH2	-13.28	113.66	120.30
1	C	442	ARG	NE-CZ-NH2	-12.87	113.87	120.30
1	C	230	ARG	NE-CZ-NH2	-12.85	113.87	120.30
1	B	579	ASP	CB-CG-OD2	-12.34	107.20	118.30
1	A	952	ARG	NE-CZ-NH1	12.07	126.34	120.30
1	B	919	ASP	CB-CG-OD2	-12.07	107.43	118.30
1	A	403	ASP	CB-CG-OD2	-11.90	107.58	118.30
1	A	411	ASP	CB-CG-OD2	-11.73	107.75	118.30
1	A	403	ASP	CB-CG-OD1	11.53	128.68	118.30
1	A	987	ASP	CB-CG-OD1	11.50	128.65	118.30
1	D	429	ASP	CB-CG-OD2	-11.47	107.98	118.30
1	B	809	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	A	251	ARG	NE-CZ-NH1	11.30	125.95	120.30
1	A	853	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	233	ASP	CB-CG-OD2	-11.17	108.25	118.30
1	B	594	ASP	CB-CG-OD1	11.14	128.33	118.30
1	A	687	GLN	C-N-CD	-11.00	96.40	120.60
1	D	431	ARG	NE-CZ-NH1	10.85	125.73	120.30
1	D	869	ASP	CB-CG-OD1	10.84	128.06	118.30
1	B	505	ARG	NE-CZ-NH1	10.75	125.68	120.30
1	D	599	ARG	NE-CZ-NH2	-10.72	114.94	120.30
1	A	172	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	C	473	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	B	233	ASP	CB-CG-OD1	10.57	127.82	118.30
1	D	431	ARG	NE-CZ-NH2	-10.57	115.01	120.30
1	D	172	ASP	CB-CG-OD2	-10.52	108.84	118.30
1	B	648	ASP	CB-CG-OD2	-10.39	108.94	118.30
1	D	234	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	A	233	ASP	CB-CG-OD1	10.31	127.58	118.30
1	A	439	ARG	NE-CZ-NH1	10.28	125.44	120.30
1	D	1013	ARG	NE-CZ-NH2	-10.27	115.17	120.30
1	B	853	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	A	987	ASP	CB-CG-OD2	-10.26	109.07	118.30
1	C	961	ARG	NE-CZ-NH1	10.26	125.43	120.30
1	D	786	ARG	NE-CZ-NH2	-10.25	115.17	120.30
1	A	251	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	D	439	ARG	NE-CZ-NH2	-10.24	115.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	594	ASP	CB-CG-OD1	10.20	127.48	118.30
1	D	594	ASP	CB-CG-OD2	-10.13	109.19	118.30
1	B	425	ARG	NE-CZ-NH1	10.11	125.35	120.30
1	D	172	ASP	CB-CG-OD1	10.10	127.39	118.30
1	A	172	ASP	CB-CG-OD1	9.98	127.28	118.30
1	B	287	ASP	CB-CG-OD1	9.96	127.26	118.30
1	C	233	ASP	CB-CG-OD1	9.94	127.24	118.30
1	C	199	ASP	CB-CG-OD1	9.90	127.21	118.30
1	B	561	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	A	224	ASP	CB-CG-OD1	9.86	127.17	118.30
1	A	630	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	B	336	ARG	NE-CZ-NH1	9.82	125.21	120.30
1	D	472	TYR	CB-CG-CD2	-9.81	115.11	121.00
1	D	403	ASP	CB-CG-OD1	9.79	127.11	118.30
1	D	336	ARG	NE-CZ-NH1	9.77	125.18	120.30
1	B	246	MET	CG-SD-CE	-9.76	84.59	100.20
1	D	996	ASP	CB-CG-OD1	9.75	127.07	118.30
1	B	572	ASP	CB-CG-OD2	-9.74	109.53	118.30
1	B	233	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	B	368	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	B	448	ARG	NE-CZ-NH2	-9.68	115.46	120.30
1	C	579	ASP	CB-CG-OD1	9.66	126.99	118.30
1	C	507	ASP	CB-CG-OD1	9.63	126.97	118.30
1	B	492	ASP	CB-CG-OD1	9.60	126.94	118.30
1	C	43	ARG	NE-CZ-NH1	9.60	125.10	120.30
1	B	429	ASP	CB-CG-OD2	-9.52	109.73	118.30
1	B	792	ASP	CB-CG-OD1	9.49	126.85	118.30
1	D	746	ASP	CB-CG-OD2	-9.46	109.79	118.30
1	A	594	ASP	CB-CG-OD1	9.41	126.77	118.30
1	D	659	ASP	CB-CG-OD1	9.40	126.76	118.30
1	D	144	ASP	CB-CG-OD1	9.36	126.73	118.30
1	A	224	ASP	CB-CG-OD2	-9.33	109.90	118.30
1	A	280	ASP	CB-CG-OD2	-9.32	109.91	118.30
1	A	439	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	D	388	ARG	NE-CZ-NH2	-9.28	115.66	120.30
1	A	411	ASP	CB-CG-OD1	9.25	126.62	118.30
1	B	685	LEU	C-N-CD	-9.20	100.35	120.60
1	C	594	ASP	CB-CG-OD2	-9.20	110.02	118.30
1	B	828	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	A	954	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	D	509	ASP	CB-CG-OD1	9.11	126.50	118.30
1	A	591	ASP	CB-CG-OD2	-9.09	110.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	ASP	CB-CG-OD2	-9.07	110.14	118.30
1	A	356	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	B	144	ASP	CB-CG-OD2	-9.01	110.19	118.30
1	D	429	ASP	CB-CG-OD1	9.00	126.40	118.30
1	C	310	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	D	368	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	C	233	ASP	CB-CG-OD2	-8.94	110.25	118.30
1	C	224	ASP	CB-CG-OD1	8.93	126.34	118.30
1	B	594	ASP	CB-CG-OD2	-8.92	110.27	118.30
1	A	594	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	C	310	ARG	NE-CZ-NH2	-8.84	115.88	120.30
1	A	699	ARG	NE-CZ-NH1	8.79	124.69	120.30
1	B	375	ASP	CB-CG-OD1	8.68	126.11	118.30
1	D	699	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	D	996	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	D	446	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	D	287	ASP	CB-CG-OD1	8.62	126.06	118.30
1	C	201	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	D	255	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	A	479	ASP	CB-CG-OD1	8.59	126.03	118.30
1	C	579	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	B	448	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	B	809	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	C	404	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	D	869	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	B	310	ARG	NE-CZ-NH1	8.56	124.58	120.30
1	C	507	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	B	579	ASP	CB-CG-OD1	8.54	125.99	118.30
1	B	144	ASP	CB-CG-OD1	8.53	125.97	118.30
1	A	166	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	509	ASP	CB-CG-OD1	8.51	125.96	118.30
1	C	45	ASP	CB-CG-OD1	8.51	125.96	118.30
1	D	472	TYR	CB-CG-CD1	8.50	126.10	121.00
1	A	869	ASP	CB-CG-OD1	8.49	125.94	118.30
1	D	336	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	D	411	ASP	CB-CG-OD1	8.46	125.91	118.30
1	A	509	ASP	CB-CG-OD1	8.44	125.89	118.30
1	A	857	ARG	NE-CZ-NH1	8.40	124.50	120.30
1	C	996	ASP	CB-CG-OD1	8.40	125.86	118.30
1	B	469	ASP	CB-CG-OD1	8.38	125.84	118.30
1	B	853	ARG	NE-CZ-NH2	-8.37	116.11	120.30
1	B	388	ARG	NE-CZ-NH2	-8.37	116.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	591	ASP	CB-CG-OD1	8.36	125.82	118.30
1	B	439	ARG	NE-CZ-NH1	8.36	124.48	120.30
1	A	234	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	492	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	A	909	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	A	591	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	224	ASP	CB-CG-OD1	8.31	125.78	118.30
1	C	630	ARG	NE-CZ-NH2	-8.28	116.16	120.30
1	B	319	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	C	772	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	C	741	THR	CA-CB-CG2	-8.21	100.91	112.40
1	B	924	ASP	CB-CG-OD1	8.21	125.69	118.30
1	A	329	ASP	CB-CG-OD1	8.20	125.68	118.30
1	B	509	ASP	CB-CG-OD1	8.19	125.67	118.30
1	C	916	ASP	CB-CG-OD1	8.17	125.66	118.30
1	D	319	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	A	828	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	B	287	ASP	CB-CG-OD2	-8.14	110.97	118.30
1	D	578	TYR	CB-CG-CD2	-8.13	116.12	121.00
1	B	1013	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	B	172	ASP	CB-CG-OD2	-8.11	111.00	118.30
1	C	472	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	C	509	ASP	CB-CG-OD2	-8.08	111.03	118.30
1	A	997	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	B	699	ARG	CD-NE-CZ	8.06	134.89	123.60
1	D	699	ARG	NE-CZ-NH2	-8.05	116.27	120.30
1	B	140	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	809	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	579	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	B	96	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	D	997	ASP	CB-CG-OD2	-7.94	111.16	118.30
1	B	610	ASP	CB-CG-OD2	-7.88	111.20	118.30
1	C	569	ASP	CB-CG-OD1	7.84	125.36	118.30
1	B	368	ASP	CB-CG-OD1	7.83	125.34	118.30
1	C	144	ASP	CB-CG-OD1	7.80	125.33	118.30
1	A	319	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	B	832	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	469	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	772	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	C	958	ASN	N-CA-CB	7.78	124.61	110.60
1	B	869	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	C	172	ASP	CB-CG-OD2	-7.78	111.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	507	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	B	996	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	A	46	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	D	234	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	428	ASP	CB-CG-OD1	7.75	125.27	118.30
1	C	853	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	C	809	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	B	875	ASP	CB-CG-OD1	7.68	125.21	118.30
1	D	667	GLU	N-CA-CB	7.63	124.34	110.60
1	A	916	ASP	CB-CG-OD1	7.59	125.14	118.30
1	C	630	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	671	ASP	CB-CG-OD2	-7.57	111.48	118.30
1	D	572	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	368	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	C	917	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	D	786	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	164	ASP	CB-CG-OD1	7.56	125.10	118.30
1	B	507	ASP	CB-CG-OD1	7.54	125.09	118.30
1	A	469	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	B	832	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	D	659	ASP	CB-CG-OD2	-7.51	111.54	118.30
1	A	610	ASP	CB-CG-OD1	7.50	125.05	118.30
1	D	845	GLN	C-N-CA	-7.50	106.56	122.30
1	B	557	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	D	746	ASP	CB-CG-OD1	7.49	125.04	118.30
1	D	448	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	D	352	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	37	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	961	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	A	924	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	997	ASP	CB-CG-OD1	7.42	124.98	118.30
1	D	469	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	B	569	ASP	CB-CG-OD1	7.42	124.97	118.30
1	B	224	ASP	CB-CG-OD1	7.41	124.97	118.30
1	A	431	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	D	224	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	A	509	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	C	230	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	924	ASP	CB-CG-OD1	7.38	124.94	118.30
1	C	442	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	859	ASP	CB-CG-OD1	7.35	124.92	118.30
1	D	15	ASP	CB-CG-OD2	-7.35	111.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	469	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	428	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	C	611	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	786	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	D	531	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	A	755	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	B	76	CYS	CA-CB-SG	-7.28	100.90	114.00
1	B	403	ASP	CB-CG-OD2	-7.27	111.75	118.30
1	B	942	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	954	ASP	CB-CG-OD1	7.23	124.81	118.30
1	A	859	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	632	SER	N-CA-CB	7.21	121.32	110.50
1	B	310	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	37	ARG	NE-CZ-NH1	-7.21	116.69	120.30
1	B	916	ASP	CB-CG-OD1	7.21	124.78	118.30
1	D	1018	LEU	CB-CA-C	-7.21	96.51	110.20
1	C	594	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	610	ASP	CB-CG-OD1	7.18	124.77	118.30
1	B	572	ASP	CB-CG-OD1	7.17	124.76	118.30
1	D	853	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	A	531	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	853	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	D	648	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	B	1014	TYR	CB-CG-CD2	-7.10	116.74	121.00
1	A	446	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	D	166	ARG	NE-CZ-NH1	7.05	123.82	120.30
1	B	800[A]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	800[B]	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	375	ASP	CB-CG-OD2	-7.04	111.97	118.30
1	B	497	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	B	473	ARG	CD-NE-CZ	7.02	133.43	123.60
1	D	909	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	809	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	996	ASP	CB-CG-OD1	7.00	124.60	118.30
1	B	875	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	B	1013	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	869	ASP	CB-CG-OD1	6.97	124.58	118.30
1	C	856	TYR	CB-CG-CD2	-6.96	116.82	121.00
1	C	448	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	C	431	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	C	645	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	13	ARG	NE-CZ-NH2	-6.95	116.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	772	ASP	CB-CG-OD1	6.94	124.55	118.30
1	A	310	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	B	172	ASP	CB-CG-OD1	6.93	124.53	118.30
1	D	319	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	961	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	610	ASP	CB-CG-OD1	6.90	124.51	118.30
1	B	958	ASN	N-CA-CB	6.90	123.02	110.60
1	B	507	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	D	853	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	D	889	ALA	CB-CA-C	-6.89	99.77	110.10
1	B	857	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	C	610	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	A	553	TRP	CA-CB-CG	-6.84	100.70	113.70
1	A	909	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	309	TYR	CB-CG-CD2	-6.83	116.90	121.00
1	A	699	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	832	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	144	ASP	CB-CG-OD1	6.82	124.43	118.30
1	B	828	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	509	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	166	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	778	THR	CA-CB-CG2	-6.77	102.93	112.40
1	B	399	TYR	CB-CG-CD1	-6.76	116.94	121.00
1	B	802[A]	ASP	N-CA-CB	6.76	122.77	110.60
1	B	802[B]	ASP	N-CA-CB	6.76	122.77	110.60
1	B	670	LEU	CB-CA-C	-6.76	97.36	110.20
1	A	997	ASP	N-CA-CB	6.75	122.76	110.60
1	D	802	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	C	748	CYS	CA-CB-SG	-6.72	101.91	114.00
1	C	190	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	D	446	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	C	190	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	B	52	ARG	CB-CA-C	-6.70	97.01	110.40
1	A	473	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	D	630	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	B	388	ARG	NE-CZ-NH1	6.67	123.64	120.30
1	D	411	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	D	486	TYR	CB-CG-CD2	-6.63	117.02	121.00
1	A	507	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	A	782	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	A	875	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	C	403	ASP	CB-CG-OD2	-6.60	112.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	559	TYR	CB-CG-CD1	6.60	124.96	121.00
1	C	267	VAL	CA-CB-CG2	-6.58	101.02	110.90
1	C	287	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	234	ASP	CB-CG-OD1	6.58	124.22	118.30
1	C	234	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	859	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	1021	CYS	CA-CB-SG	-6.53	102.25	114.00
1	B	234	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	A	938	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	952	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	B	997	ASP	N-CA-CB	6.48	122.27	110.60
1	C	473	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	37	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	D	505	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	1018	LEU	CB-CA-C	-6.47	97.91	110.20
1	B	473	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	C	204	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	710	GLU	CB-CA-C	-6.46	97.47	110.40
1	B	356	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	C	917	ARG	CD-NE-CZ	-6.46	114.56	123.60
1	A	671	ASP	CB-CG-OD1	6.45	124.11	118.30
1	D	1013	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	D	954	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	A	82	ASP	CB-CG-OD2	-6.44	112.51	118.30
1	B	292	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	B	595	THR	CA-CB-CG2	-6.43	103.40	112.40
1	B	576	ILE	CB-CA-C	-6.42	98.75	111.60
1	A	199	ASP	CB-CG-OD1	6.42	124.08	118.30
1	D	987	ASP	CB-CG-OD1	6.42	124.07	118.30
1	A	280	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	252	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	828	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	924	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	632	SER	N-CA-CB	6.40	120.11	110.50
1	C	96	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	C	648	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	C	319	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	997	ASP	N-CA-CB	6.38	122.08	110.60
1	D	253	TYR	CB-CG-CD1	-6.38	117.17	121.00
1	A	178	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	924	ASP	CB-CG-OD2	-6.37	112.57	118.30
1	C	494	THR	CA-CB-CG2	-6.37	103.49	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	336	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	659	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	634	GLN	CB-CA-C	6.34	123.07	110.40
1	D	980	GLU	C-N-CA	-6.34	108.99	122.30
1	B	477	SER	CB-CA-C	6.33	122.13	110.10
1	A	859	ASP	CB-CG-OD1	6.33	124.00	118.30
1	C	721	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	C	719	GLN	CB-CA-C	-6.32	97.76	110.40
1	A	123	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	D	958	ASN	N-CA-CB	6.30	121.95	110.60
1	C	280	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	844	HIS	CA-CB-CG	-6.30	102.89	113.60
1	B	193	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	442	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	C	373	VAL	CA-CB-CG2	-6.27	101.50	110.90
1	C	411	ASP	CB-CG-OD1	6.25	123.92	118.30
1	B	802[A]	ASP	CB-CG-OD1	6.24	123.91	118.30
1	B	802[B]	ASP	CB-CG-OD1	6.24	123.91	118.30
1	C	790	ASP	CB-CG-OD1	6.24	123.91	118.30
1	D	233	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	755	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	292	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	77	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	D	479	ASP	CB-CG-OD1	6.18	123.87	118.30
1	A	832	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C	13	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	A	991	MET	CG-SD-CE	6.17	110.08	100.20
1	C	130	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	211	ASP	CB-CG-OD1	6.17	123.85	118.30
1	B	996	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	136	GLU	CB-CA-C	-6.16	98.08	110.40
1	B	723	ALA	CB-CA-C	-6.15	100.87	110.10
1	D	403	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	B	991	MET	CG-SD-CE	6.14	110.03	100.20
1	B	319	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	108	THR	CA-CB-CG2	-6.14	103.80	112.40
1	D	356	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	795	VAL	CA-CB-CG2	-6.13	101.70	110.90
1	D	916	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	A	22	THR	CA-CB-CG2	-6.12	103.83	112.40
1	D	553	TRP	CA-CB-CG	-6.12	102.08	113.70
1	A	246	MET	CG-SD-CE	-6.11	90.42	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	857	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	C	909	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	221	GLN	N-CA-CB	-6.10	99.61	110.60
1	C	996	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	C	664	ALA	CB-CA-C	-6.08	100.97	110.10
1	B	997	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	362	LEU	CB-CA-C	-6.06	98.68	110.20
1	C	916	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	D	924	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	404	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	210	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	B	668	VAL	CB-CA-C	-6.05	99.90	111.40
1	A	352	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	96	ASP	CB-CG-OD1	6.04	123.74	118.30
1	A	333	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	C	875	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	778	THR	CA-CB-CG2	-6.03	103.96	112.40
1	D	566	PHE	CD1-CE1-CZ	-6.02	112.87	120.10
1	D	667	GLU	CA-CB-CG	6.01	126.63	113.40
1	D	792	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	321	THR	CA-CB-CG2	-6.00	104.00	112.40
1	C	255	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	952	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	B	648	ASP	CB-CG-OD1	5.99	123.69	118.30
1	D	634	GLN	N-CA-CB	5.98	121.36	110.60
1	A	632	SER	N-CA-CB	5.97	119.46	110.50
1	C	126	THR	CA-CB-CG2	-5.97	104.04	112.40
1	C	531	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	782	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	C	598	ASP	CB-CG-OD2	-5.96	112.93	118.30
1	B	46	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	C	19	PRO	N-CA-CB	5.95	110.44	103.30
1	A	958	ASN	N-CA-CB	5.95	121.31	110.60
1	D	164	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	B	919	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	1016	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	B	255	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	492	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	C	553	TRP	CA-CB-CG	-5.93	102.44	113.70
1	A	164	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	B	255	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	C	650	GLU	CG-CD-OE2	-5.92	106.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	881	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	D	610	ASP	CB-CG-OD1	5.92	123.62	118.30
1	A	782	ASP	CB-CG-OD1	5.89	123.61	118.30
1	A	929	TYR	CB-CG-CD1	-5.89	117.47	121.00
1	D	561	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	178	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	A	144	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	C	416	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	D	288	ARG	NE-CZ-NH2	-5.87	117.37	120.30
1	B	800[A]	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	800[B]	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	D	448	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	B	656	VAL	CG1-CB-CG2	-5.85	101.54	110.90
1	C	855	THR	N-CA-CB	5.84	121.41	110.30
1	D	199	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	D	199	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	486	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	B	671	ASP	CB-CG-OD1	5.83	123.54	118.30
1	D	507	ASP	CB-CG-OD1	5.82	123.53	118.30
1	A	15	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	869	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	219	THR	CA-CB-CG2	-5.80	104.28	112.40
1	C	973	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	A	13	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	C	96	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	599	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	A	82	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	363	HIS	CA-CB-CG	-5.78	103.77	113.60
1	A	201	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	832	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	746	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	486	TYR	CB-CG-CD1	5.76	124.46	121.00
1	D	1006	GLU	CG-CD-OE2	-5.76	106.77	118.30
1	D	599	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	B	859	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	429	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	569	ASP	CB-CG-OD2	-5.74	113.13	118.30
1	B	356	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	356	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	15	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	172	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	881	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	986	ILE	CG1-CB-CG2	-5.72	98.82	111.40
1	B	997	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	D	746	ASP	CB-CA-C	-5.71	98.98	110.40
1	D	251	ARG	CD-NE-CZ	5.71	131.59	123.60
1	C	832	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	802[A]	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	802[B]	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	D	828	ASP	CB-CG-OD2	-5.67	113.19	118.30
1	C	333	ARG	CG-CD-NE	5.66	123.69	111.80
1	C	178	ARG	N-CA-CB	5.66	120.79	110.60
1	C	859	ASP	CB-CG-OD2	-5.66	113.20	118.30
1	B	772	ASP	CB-CG-OD1	5.66	123.39	118.30
1	D	287	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	B	786	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	45	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	710	GLU	CB-CA-C	-5.64	99.12	110.40
1	A	769	TRP	CE3-CZ3-CH2	5.64	127.40	121.20
1	D	772	ASP	CB-CG-OD2	-5.64	113.23	118.30
1	D	45	ASP	N-CA-CB	5.63	120.73	110.60
1	B	859	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	D	686	PRO	N-CA-CB	5.60	110.02	103.30
1	A	802[A]	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	802[B]	ASP	CB-CG-OD1	5.59	123.33	118.30
1	B	809	ARG	CD-NE-CZ	5.59	131.42	123.60
1	D	439	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	579	ASP	CB-CG-OD1	5.57	123.31	118.30
1	A	431	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	C	760	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	B	221	GLN	N-CA-CB	-5.56	100.58	110.60
1	A	772	ASP	CB-CG-OD1	5.56	123.31	118.30
1	C	144	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	C	329	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	184	LEU	CB-CA-C	-5.56	99.64	110.20
1	A	648	ASP	CB-CG-OD2	-5.55	113.30	118.30
1	C	14	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	B	314	GLU	CB-CA-C	-5.55	99.30	110.40
1	A	45	ASP	CB-CG-OD1	5.55	123.29	118.30
1	D	645	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	39	SER	CA-CB-OG	-5.54	96.24	111.20
1	A	618	THR	CA-CB-CG2	-5.53	104.66	112.40
1	B	553	TRP	CA-CB-CG	-5.53	103.20	113.70
1	D	843	GLN	CA-CB-CG	-5.53	101.24	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	667	GLU	CB-CA-C	-5.52	99.35	110.40
1	C	85	VAL	CA-CB-CG2	-5.52	102.62	110.90
1	D	373	VAL	CA-CB-CG1	-5.51	102.63	110.90
1	A	546	LEU	N-CA-CB	5.51	121.41	110.40
1	B	855	THR	N-CA-CB	5.50	120.76	110.30
1	A	996	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	1018	LEU	CB-CA-C	-5.49	99.77	110.20
1	D	477	SER	CB-CA-C	-5.49	99.67	110.10
1	C	557	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	B	447	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	610	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	D	333	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	D	559	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	B	403	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	828	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	123	TYR	CB-CG-CD1	5.46	124.28	121.00
1	C	344	LEU	CA-CB-CG	-5.46	102.74	115.30
1	B	908	ASP	CB-CG-OD1	5.46	123.21	118.30
1	B	909	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	C	438	GLU	CG-CD-OE2	-5.46	107.39	118.30
1	A	37	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	D	161	TYR	N-CA-CB	-5.45	100.79	110.60
1	D	561	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	21	VAL	CG1-CB-CG2	-5.44	102.20	110.90
1	C	201	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	917	ARG	NE-CZ-NH1	-5.43	117.59	120.30
1	B	578	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	917	ARG	CD-NE-CZ	-5.42	116.01	123.60
1	B	906	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	447	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	595	THR	CA-CB-CG2	-5.40	104.83	112.40
1	C	224	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	881	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	D	538	TYR	CB-CG-CD1	-5.39	117.76	121.00
1	C	829	THR	CA-CB-CG2	-5.39	104.85	112.40
1	D	140	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	675	GLN	N-CA-CB	5.37	120.27	110.60
1	D	52	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	D	428	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	B	840	HIS	CB-CA-C	-5.36	99.67	110.40
1	C	842	TRP	CG-CD2-CE3	-5.36	129.08	133.90
1	D	67	GLU	CG-CD-OE2	-5.36	107.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	559	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	C	333	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	233	ASP	CB-CG-OD1	5.35	123.11	118.30
1	D	855	THR	N-CA-CB	5.35	120.46	110.30
1	A	908	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	497	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	482	ARG	CB-CA-C	-5.33	99.73	110.40
1	D	816	TYR	CG-CD2-CE2	5.33	125.56	121.30
1	C	725	ASN	CA-CB-CG	-5.32	101.69	113.40
1	A	91	GLN	O-C-N	-5.32	114.19	122.70
1	C	782	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	C	375	ASP	CB-CG-OD1	5.31	123.08	118.30
1	D	344	LEU	CA-CB-CG	-5.30	103.10	115.30
1	B	77	ASP	CB-CG-OD1	5.30	123.07	118.30
1	B	161	TYR	N-CA-CB	-5.30	101.06	110.60
1	D	968	MET	N-CA-CB	-5.29	101.08	110.60
1	A	781	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	179	ALA	N-CA-CB	5.29	117.50	110.10
1	C	431	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	952	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	363	HIS	CA-CB-CG	-5.28	104.63	113.60
1	D	850	PHE	CB-CA-C	-5.27	99.85	110.40
1	D	670	LEU	CB-CA-C	-5.27	100.19	110.20
1	A	828	ASP	N-CA-CB	5.27	120.08	110.60
1	D	987	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	D	252	ASP	CB-CG-OD1	5.25	123.03	118.30
1	D	832	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	684	GLU	N-CA-CB	5.25	120.05	110.60
1	D	546	LEU	N-CA-CB	5.25	120.89	110.40
1	A	771	GLY	N-CA-C	-5.24	100.00	113.10
1	C	942	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	B	818	ALA	N-CA-CB	5.23	117.42	110.10
1	C	358	GLU	N-CA-CB	-5.22	101.21	110.60
1	D	310	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	86	VAL	CA-CB-CG2	-5.20	103.09	110.90
1	D	668	VAL	CA-CB-CG2	-5.20	103.10	110.90
1	B	792	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	828	ASP	CB-CG-OD1	5.19	122.97	118.30
1	D	201	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	140	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	771	GLY	N-CA-C	-5.17	100.17	113.10
1	C	690	SER	CB-CA-C	-5.17	100.28	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	D	147	ASN	N-CA-CB	-5.16	101.32	110.60
1	D	497	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	C	482	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	314	GLU	OE1-CD-OE2	-5.15	117.12	123.30
1	B	33	PHE	CB-CA-C	-5.15	100.10	110.40
1	D	416	GLU	CG-CD-OE1	5.14	128.59	118.30
1	C	46	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	929	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	D	816	TYR	CB-CG-CD2	5.13	124.08	121.00
1	B	827	ALA	N-CA-CB	5.12	117.27	110.10
1	D	838	THR	CA-CB-CG2	-5.12	105.23	112.40
1	B	598	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	997	ASP	N-CA-CB	5.12	119.81	110.60
1	B	629	PHE	CB-CA-C	-5.11	100.18	110.40
1	D	610	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	496	THR	CA-CB-CG2	-5.11	105.25	112.40
1	A	77	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	659	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	19	PRO	N-CA-CB	5.10	109.42	103.30
1	D	890	GLN	N-CA-CB	-5.10	101.42	110.60
1	A	461	GLU	CA-CB-CG	-5.10	102.19	113.40
1	C	13	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	147	ASN	N-CA-CB	-5.08	101.46	110.60
1	B	85	VAL	CB-CA-C	-5.08	101.75	111.40
1	D	893	GLU	CB-CG-CD	5.08	127.92	114.20
1	B	801[A]	ILE	N-CA-CB	-5.07	99.14	110.80
1	B	801[B]	ILE	N-CA-CB	-5.07	99.14	110.80
1	C	138	GLN	N-CA-CB	-5.07	101.47	110.60
1	A	869	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	C	699	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	26	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	C	308	LEU	CB-CA-C	-5.05	100.59	110.20
1	C	429	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	62	TRP	CB-CG-CD2	5.05	133.16	126.60
1	C	40	GLU	CG-CD-OE1	5.05	128.39	118.30
1	A	529	GLU	CG-CD-OE1	5.04	128.39	118.30
1	C	77	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	178	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	D	130	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	577	LYS	N-CA-CB	5.04	119.67	110.60
1	A	865	ALA	CB-CA-C	-5.04	102.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	114	VAL	CA-CB-CG1	-5.03	103.35	110.90
1	B	165	SER	CB-CA-C	-5.03	100.53	110.10
1	B	15	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	C	552	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	D	655	MET	CA-CB-CG	5.03	121.85	113.30
1	A	719	GLN	CB-CA-C	-5.03	100.34	110.40
1	C	690	SER	N-CA-CB	-5.03	102.96	110.50
1	A	968	MET	CB-CA-C	-5.03	100.35	110.40
1	B	1014	TYR	CG-CD2-CE2	-5.03	117.28	121.30
1	C	869	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	A	792	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	670	LEU	C-N-CA	-5.02	109.16	121.70
1	B	911	THR	CA-CB-CG2	-5.02	105.38	112.40
1	C	68	ALA	N-CA-CB	-5.02	103.08	110.10
1	C	288	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	B	15	ASP	CB-CG-OD1	5.00	122.80	118.30
1	B	546	LEU	N-CA-CB	5.00	120.41	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	634	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	8205	0	7791	158	0
1	B	8205	0	7791	160	0
1	C	8205	0	7791	159	0
1	D	8125	0	7716	142	0
2	A	12	0	9	0	0
2	B	12	0	9	1	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	80	0	120	4	0
5	B	88	0	132	10	0
5	C	88	0	132	7	0
5	D	92	0	138	18	0
6	A	953	0	0	22	0
6	B	937	0	0	25	1
6	C	952	0	0	15	0
6	D	959	0	0	23	1
All	All	36964	0	31647	623	1

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 10.

All (623) 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:H	1:C:634:GLN:NE2	1.37	1.22
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.20	1.06
1:C:634:GLN:N	1:C:634:GLN:HE21	1.57	1.01
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.82	0.94
1:B:13:ARG:HG3	1:C:13:ARG:CZ	1.98	0.93
1:A:128:ASN:HD21	1:A:180:GLY:HA2	1.36	0.91
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.34	0.91
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.55	0.87
1:A:655:MET:HE2	1:A:656:VAL:N	1.91	0.86
1:A:237:ARG:HH11	1:A:237:ARG:CB	1.90	0.84
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.60	0.83
1:C:765:LEU:HD21	1:C:768:MET:CE	2.10	0.82
1:D:804:ASN:CG	1:D:809:ARG:HH21	1.83	0.82
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.92	0.82
1:D:622:HIS:O	1:D:625:GLN:HG3	1.79	0.82
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.16	0.81
1:B:878:HIS:HD2	6:B:8687:HOH:O	1.65	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:GLN:H	1:C:634:GLN:HE21	0.80	0.80
1:B:801[A]:ILE:HG22	1:B:802[A]:ASP:H	1.47	0.80
1:B:13:ARG:HG3	1:C:13:ARG:NH1	1.97	0.80
1:A:653:HIS:CD2	1:A:667:GLU:HG3	2.17	0.79
1:B:473:ARG:NH2	1:B:477:SER:HB2	1.98	0.79
1:D:682:LEU:HB3	1:D:683:PRO:HD2	1.65	0.78
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.82	0.78
1:C:653:HIS:ND1	1:C:667:GLU:HG2	1.98	0.78
1:D:651:LEU:HD12	1:D:651:LEU:O	1.84	0.77
1:C:634:GLN:N	1:C:634:GLN:NE2	2.21	0.77
1:C:781:ARG:HH11	1:C:781:ARG:HG2	1.48	0.77
1:A:262:GLN:HG3	6:A:9518:HOH:O	1.85	0.77
1:B:1017:GLN:HB2	6:B:9454:HOH:O	1.86	0.76
1:B:651:LEU:O	1:B:651:LEU:HD23	1.84	0.76
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.18	0.76
1:A:887:GLN:NE2	1:A:980:GLU:O	2.17	0.76
1:B:668:VAL:HG12	1:B:669:PRO:O	1.85	0.76
1:B:737:ILE:HD11	6:B:9453:HOH:O	1.84	0.75
1:D:847:LYS:HG3	1:D:848:THR:N	2.01	0.75
1:D:128:ASN:HB3	1:D:180:GLY:O	1.88	0.73
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.00	0.73
1:D:779:PRO:HG2	1:D:781:ARG:NH2	2.04	0.73
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.89	0.73
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.70	0.73
1:C:690:SER:HB2	6:C:9321:HOH:O	1.87	0.73
1:C:651:LEU:C	1:C:651:LEU:HD12	2.10	0.72
1:C:754:LYS:HE3	1:C:1022:GLN:OE1	1.90	0.71
1:A:890:GLN:OE1	1:A:948:PRO:HD3	1.90	0.71
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.26	0.71
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.74	0.71
1:A:128:ASN:ND2	1:A:180:GLY:HA2	2.05	0.71
1:A:754:LYS:NZ	6:A:9425:HOH:O	2.23	0.71
1:B:600:GLN:H	1:B:600:GLN:HE21	1.36	0.71
1:C:44:THR:OG1	1:C:46:ARG:HD3	1.91	0.70
1:D:277:GLU:H	1:D:277:GLU:CD	1.95	0.70
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.25	0.70
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.55	0.70
1:C:724:GLU:O	1:D:847:LYS:NZ	2.24	0.70
1:C:230:ARG:CG	1:C:230:ARG:HH11	2.05	0.69
1:C:748:CYS:C	1:C:749:ILE:HD12	2.12	0.69
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.03	0.69
5:D:8508:DMS:H12	6:D:8857:HOH:O	1.93	0.69
1:A:635:THR:OG1	1:A:681:GLU:HG3	1.92	0.69
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.75	0.69
1:C:230:ARG:HB3	6:C:9470:HOH:O	1.92	0.69
5:D:8503:DMS:H21	6:D:9153:HOH:O	1.92	0.69
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.05	0.68
1:C:243:GLU:OE2	1:C:245:GLN:NE2	2.27	0.68
1:B:236:SER:C	1:B:237:ARG:HG2	2.09	0.68
1:A:655:MET:HE2	1:A:656:VAL:H	1.58	0.68
1:C:794[B]:GLY:HA2	6:C:8944:HOH:O	1.94	0.68
1:D:651:LEU:HD12	1:D:651:LEU:C	2.14	0.68
1:C:800[A]:ARG:NE	1:C:800[A]:ARG:HA	2.09	0.68
1:D:480:PRO:HG2	6:D:9614:HOH:O	1.92	0.68
1:C:749:ILE:HD12	1:C:749:ILE:N	2.06	0.68
1:A:794[B]:GLY:HA2	6:A:8919:HOH:O	1.92	0.68
1:A:157:ARG:HD3	6:A:9380:HOH:O	1.93	0.68
1:D:890:GLN:HG3	1:D:891:VAL:N	2.09	0.68
1:D:653:HIS:NE2	1:D:667:GLU:OE2	2.27	0.68
1:A:737:ILE:O	1:A:737:ILE:HD13	1.95	0.67
1:A:770:ILE:HD12	1:A:775:GLN:NE2	2.09	0.67
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.76	0.67
1:A:600:GLN:H	1:A:600:GLN:HE21	1.43	0.67
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.28	0.67
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.25	0.67
1:A:179:ALA:HB3	6:A:9338:HOH:O	1.94	0.67
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.06	0.66
1:D:237:ARG:NH1	6:D:9255:HOH:O	2.28	0.66
1:C:651:LEU:O	1:C:651:LEU:HD12	1.95	0.66
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.10	0.66
1:A:473:ARG:NH1	6:A:9253:HOH:O	2.22	0.66
1:C:625:GLN:NE2	6:C:8826:HOH:O	2.27	0.66
1:B:771:GLY:HA3	6:B:9446:HOH:O	1.95	0.66
1:D:682:LEU:CB	1:D:683:PRO:HD2	2.26	0.66
1:D:749:ILE:N	1:D:749:ILE:HD12	2.10	0.66
1:A:794[B]:GLY:O	6:A:8843:HOH:O	2.13	0.66
1:D:155:ASN:HB3	1:D:178:ARG:NH1	2.11	0.66
1:A:832:ASP:OD1	1:A:832:ASP:N	2.29	0.66
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.10	0.66
1:D:893:GLU:O	1:D:893:GLU:HG3	1.96	0.66
1:A:703:PRO:HG2	5:A:8425:DMS:C1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:ALA:HA	1:A:968:MET:HG3	1.78	0.65
1:D:634:GLN:NE2	1:D:682:LEU:O	2.28	0.65
1:B:671:ASP:N	1:B:678:GLN:OE1	2.19	0.65
1:A:277:GLU:H	1:A:277:GLU:CD	1.98	0.65
1:A:581:ASN:HB2	1:A:583:ASN:ND2	2.11	0.65
1:B:753:ASN:HB2	1:B:771:GLY:HA2	1.79	0.64
1:A:804[B]:ASN:OD1	1:A:809:ARG:NH2	2.30	0.64
1:C:230:ARG:HG2	1:C:230:ARG:HH11	1.61	0.64
1:D:595:THR:HA	1:D:596:PRO:C	2.16	0.64
1:D:49:GLN:HB3	5:D:8703:DMS:O	1.98	0.64
1:C:637:GLU:OE2	1:C:677:LYS:NZ	2.26	0.64
1:C:671:ASP:N	1:C:678:GLN:OE1	2.22	0.64
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.28	0.64
1:B:615:PRO:O	1:B:618:THR:HG22	1.98	0.64
1:A:615:PRO:O	1:A:618:THR:HG22	1.97	0.64
1:D:817:GLN:OE1	6:D:9154:HOH:O	2.14	0.64
1:A:781:ARG:HG2	1:A:781:ARG:NH1	2.13	0.64
1:A:1022:GLN:NE2	1:A:1023:LYS:O	2.26	0.63
1:A:686:PRO:HB2	1:A:688:PRO:HD3	1.80	0.63
1:B:183:ARG:HH11	1:B:183:ARG:HG2	1.64	0.63
1:A:817:GLN:N	1:A:817:GLN:NE2	2.46	0.63
1:B:893:GLU:HG3	6:B:9472:HOH:O	1.97	0.63
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.33	0.63
1:B:13:ARG:HG3	1:C:13:ARG:NH2	2.14	0.63
1:D:292:ARG:HH12	5:D:8412:DMS:H21	1.64	0.62
1:D:804:ASN:OD1	1:D:809:ARG:NH2	2.31	0.62
1:A:651:LEU:HD12	1:A:651:LEU:C	2.19	0.62
1:C:781:ARG:NH1	1:C:781:ARG:HG2	2.13	0.62
1:D:859:ASP:OD1	1:D:861:SER:N	2.29	0.62
1:D:117:GLU:HB2	6:D:9142:HOH:O	1.99	0.62
1:C:730:LEU:HD23	1:C:730:LEU:N	2.15	0.62
1:C:890:GLN:HG3	1:C:891:VAL:N	2.13	0.62
1:D:250:LEU:O	1:D:251:ARG:HG2	2.00	0.62
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.29	0.62
1:C:800[A]:ARG:CZ	1:C:800[A]:ARG:HA	2.29	0.62
1:A:873:ALA:O	1:A:876:THR:HG22	1.99	0.62
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.65	0.62
1:C:878:HIS:HD2	6:C:8698:HOH:O	1.82	0.62
5:D:8423:DMS:H13	6:D:9269:HOH:O	1.99	0.62
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.35	0.61
1:C:628:GLN:NE2	5:C:8402:DMS:O	2.27	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:734:SER:HB3	1:B:860:GLY:HA3	1.82	0.61
1:D:770:ILE:HD13	1:D:1022:GLN:OE1	1.99	0.61
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.13	0.61
1:C:615:PRO:O	1:C:618:THR:HG22	2.00	0.61
1:D:962:TYR:CE1	5:D:8508:DMS:H13	2.35	0.61
1:D:817:GLN:OE1	6:D:9079:HOH:O	2.16	0.61
1:B:777:LEU:HG	1:B:889:ALA:HA	1.81	0.61
1:D:878:HIS:HD2	6:D:8820:HOH:O	1.84	0.61
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.81	0.60
1:A:703:PRO:HG2	5:A:8425:DMS:H11	1.83	0.60
1:A:781:ARG:HG2	1:A:781:ARG:HH11	1.66	0.60
1:D:629:PHE:O	1:D:630:ARG:HD3	2.01	0.60
1:B:651:LEU:C	1:B:651:LEU:HD23	2.22	0.60
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.37	0.60
1:D:651:LEU:HD11	1:D:701:VAL:HB	1.82	0.60
1:C:797[A]:GLU:HB3	1:C:800[A]:ARG:H	1.67	0.60
1:A:625:GLN:NE2	6:A:8801:HOH:O	2.24	0.60
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.37	0.60
1:A:230:ARG:NH1	1:A:241:GLU:OE2	2.35	0.59
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.82	0.59
1:B:890:GLN:HG3	1:B:891:VAL:N	2.17	0.59
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.83	0.59
1:B:801[A]:ILE:HG23	1:B:808:GLU:CD	2.22	0.59
1:B:1022:GLN:HG3	1:B:1023:LYS:O	2.02	0.59
1:C:796[A]:SER:OG	1:C:802[A]:ASP:N	2.29	0.59
1:A:770:ILE:HD12	1:A:775:GLN:CD	2.23	0.59
1:D:135:GLN:C	1:D:136:GLU:HG2	2.22	0.59
1:A:595:THR:HA	1:A:596:PRO:C	2.23	0.59
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.38	0.59
1:C:251:ARG:HH11	1:C:251:ARG:HB3	1.67	0.59
1:C:356:ARG:HD2	1:C:379:MET:CE	2.33	0.59
1:D:818:ALA:HB1	1:D:842:TRP:HB3	1.84	0.59
1:B:381:GLN:O	1:B:621:LYS:HE3	2.03	0.59
1:D:976:LEU:HB2	5:D:8423:DMS:H11	1.84	0.58
1:B:49:GLN:HB3	6:B:9403:HOH:O	2.02	0.58
1:D:32:PRO:HB2	5:D:8404:DMS:H12	1.85	0.58
1:D:675:GLN:HG3	6:D:9517:HOH:O	2.01	0.58
1:B:595:THR:HA	1:B:596:PRO:C	2.24	0.58
6:B:9330:HOH:O	5:C:8420:DMS:H21	2.03	0.58
1:D:989:PHE:HA	6:D:9457:HOH:O	2.04	0.58
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.39	0.58
1:A:597:ASN:OD1	1:A:599:ARG:HD3	2.04	0.58
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.86	0.58
1:D:618:THR:HG21	6:D:9056:HOH:O	2.04	0.58
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.19	0.57
1:B:668:VAL:HG12	1:B:669:PRO:N	2.17	0.57
1:B:93:HIS:CD2	5:B:8414:DMS:H23	2.39	0.57
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.84	0.57
1:A:521:LYS:HE2	6:A:9019:HOH:O	2.03	0.57
1:B:768:MET:SD	1:B:775:GLN:HG3	2.44	0.57
1:B:634:GLN:HG3	1:B:682:LEU:O	2.04	0.57
1:B:369:GLU:HB2	1:B:397:LEU:CD2	2.35	0.57
1:A:593:GLY:O	1:A:595:THR:HG22	2.05	0.57
1:D:754:LYS:NZ	6:D:9565:HOH:O	2.38	0.57
1:D:795:VAL:HG11	1:D:800:ARG:O	2.05	0.57
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.74	0.56
1:C:802[A]:ASP:O	1:C:808:GLU:HG3	2.05	0.56
1:A:49:GLN:N	6:A:9254:HOH:O	2.26	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.06	0.56
1:D:363:HIS:HD2	6:D:9297:HOH:O	1.88	0.56
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.06	0.56
1:B:157:ARG:HD3	6:B:9385:HOH:O	2.05	0.56
1:B:800[A]:ARG:O	1:B:801[A]:ILE:O	2.24	0.56
1:C:278:ILE:N	1:C:278:ILE:HD13	2.21	0.56
1:C:88:SER:HA	1:C:366:VAL:HG21	1.88	0.55
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.18	0.55
1:A:131:GLU:O	1:A:135:GLN:HG2	2.06	0.55
1:A:804[B]:ASN:CG	1:A:809:ARG:NH2	2.59	0.55
1:C:356:ARG:HD2	1:C:379:MET:HE3	1.89	0.55
1:A:127:PHE:CD2	1:A:127:PHE:N	2.74	0.55
1:D:646:HIS:ND1	6:D:9524:HOH:O	2.33	0.55
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.74	0.55
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.71	0.55
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.37	0.55
1:A:370:GLN:HB2	6:A:9087:HOH:O	2.06	0.55
1:D:887:GLN:NE2	1:D:980:GLU:O	2.36	0.55
1:A:750:GLU:HG3	1:A:755:ARG:HG2	1.88	0.55
1:B:669:PRO:HB3	6:B:9407:HOH:O	2.06	0.55
1:B:597:ASN:OD1	1:B:599:ARG:HD3	2.07	0.54
1:A:817:GLN:N	1:A:817:GLN:HE21	2.04	0.54
1:A:249:GLU:OE2	1:A:251:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ILE:HA	5:D:8419:DMS:H23	1.90	0.54
1:C:771:GLY:HA2	6:C:9478:HOH:O	2.06	0.54
1:B:654:TRP:O	1:B:665:SER:HB2	2.06	0.54
1:A:601:PHE:CZ	1:A:796[B]:SER:HB2	2.43	0.54
1:B:347:LYS:HE3	6:B:8873:HOH:O	2.07	0.54
1:B:78:LEU:HD23	6:B:9092:HOH:O	2.06	0.54
1:B:759:ASN:OD1	1:B:761:GLN:N	2.37	0.54
1:D:584:PRO:HD2	6:D:9415:HOH:O	2.05	0.54
1:A:363:HIS:HA	6:A:9154:HOH:O	2.07	0.54
1:D:360:HIS:HE1	1:D:362:LEU:HG	1.73	0.54
1:D:911:THR:HA	6:D:9328:HOH:O	2.08	0.53
1:C:800[A]:ARG:NH1	1:C:800[A]:ARG:HB3	2.23	0.53
1:B:809:ARG:HD2	6:B:9200:HOH:O	2.07	0.53
1:B:745:MET:SD	1:B:745:MET:N	2.77	0.53
1:A:890:GLN:HG3	1:A:891:VAL:N	2.23	0.53
1:D:807:VAL:HG13	1:D:808:GLU:N	2.24	0.53
1:C:801[A]:ILE:HG23	1:C:808:GLU:CD	2.29	0.53
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.90	0.53
1:D:737:ILE:HD12	1:D:831:ALA:O	2.07	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.77	0.53
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.43	0.53
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.43	0.53
1:C:534:ILE:HB	6:C:9175:HOH:O	2.08	0.53
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.72	0.53
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.91	0.53
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.52
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.44	0.52
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.40	0.52
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.90	0.52
1:A:637:GLU:OE2	1:A:677:LYS:HE3	2.10	0.52
1:D:893:GLU:HG2	1:D:894:ARG:HD2	1.91	0.52
1:C:737:ILE:HG13	1:C:737:ILE:O	2.06	0.52
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.39	0.52
1:B:521:LYS:HE2	6:B:9035:HOH:O	2.08	0.52
1:C:646:HIS:HB3	6:C:9414:HOH:O	2.08	0.52
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.45	0.52
1:D:893:GLU:HG3	6:D:9241:HOH:O	2.08	0.52
1:C:251:ARG:NH1	1:C:253:TYR:CE2	2.78	0.52
1:B:773:LYS:HD2	1:B:773:LYS:N	2.21	0.52
1:B:262:GLN:HE21	1:B:263:GLY:N	2.07	0.52
1:B:473:ARG:CZ	1:B:477:SER:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.40	0.51
1:B:15:ASP:OD2	6:B:8788:HOH:O	2.19	0.51
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.08	0.51
1:D:441:THR:O	1:D:445:GLN:HG3	2.09	0.51
1:C:65:ALA:HB1	1:C:66:PRO:HD2	1.91	0.51
1:D:106:PRO:C	5:D:8419:DMS:H22	2.31	0.51
1:A:891:VAL:HG23	1:A:981:GLY:HA2	1.93	0.51
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.54	0.51
1:B:135:GLN:HG3	1:B:136:GLU:HG2	1.93	0.51
1:B:655:MET:HG2	6:B:9494:HOH:O	2.11	0.51
1:C:240:LEU:HD23	1:C:240:LEU:C	2.31	0.51
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.92	0.51
1:B:599:ARG:NH1	6:B:9488:HOH:O	2.44	0.51
1:C:794[A]:GLY:HA2	1:C:998:SER:O	2.11	0.51
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.44	0.51
1:B:363:HIS:HD2	6:B:9170:HOH:O	1.93	0.51
1:D:778:THR:HG23	1:D:781:ARG:HH12	1.74	0.51
1:A:737:ILE:HD13	1:A:737:ILE:C	2.32	0.51
1:C:930:VAL:O	1:C:932:PRO:HD3	2.11	0.51
1:A:843:GLN:HG2	1:A:848:THR:HA	1.93	0.50
1:B:245:GLN:HG2	1:B:288:ARG:CG	2.37	0.50
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.45	0.50
1:B:262:GLN:HE21	1:B:262:GLN:C	2.15	0.50
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.47	0.50
1:C:367:MET:HB3	1:C:372:MET:HE3	1.94	0.50
1:B:625:GLN:HG2	1:B:716:ALA:CB	2.41	0.50
1:C:654:TRP:O	1:C:665:SER:HB2	2.12	0.50
1:B:822:LEU:HD21	1:B:825:CYS:HB2	1.93	0.50
1:D:843:GLN:HB3	1:D:847:LYS:O	2.11	0.50
1:A:804[B]:ASN:CG	1:A:809:ARG:HH21	2.15	0.50
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.12	0.50
1:D:299:LYS:NZ	6:D:9389:HOH:O	2.43	0.50
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.92	0.50
1:C:654:TRP:CZ3	1:C:665:SER:HA	2.47	0.50
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.46	0.50
1:B:93:HIS:NE2	5:B:8414:DMS:H22	2.26	0.49
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.47	0.49
1:C:829:THR:HG22	1:C:830:LEU:O	2.12	0.49
1:D:748:CYS:C	1:D:749:ILE:HD12	2.32	0.49
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.95	0.49
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.28	0.49
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.95	0.49
1:B:133:TRP:CD1	5:B:8504:DMS:C1	2.96	0.49
1:A:658:LEU:O	1:A:659:ASP:C	2.50	0.49
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.42	0.49
1:C:251:ARG:NH1	1:C:253:TYR:HE2	2.10	0.49
1:D:793:ILE:HG22	1:D:795:VAL:HG22	1.94	0.49
1:B:146:VAL:O	1:B:165:SER:HA	2.13	0.49
1:C:824:GLN:CG	1:C:825:CYS:N	2.76	0.49
1:B:737:ILE:HD12	1:B:738:PRO:HD2	1.94	0.49
1:B:646:HIS:CE1	1:B:673:ALA:CA	2.96	0.49
1:A:347:LYS:HE3	6:A:9480:HOH:O	2.12	0.49
1:B:687:GLN:CB	1:B:688:PRO:HD2	2.42	0.49
1:D:804:ASN:HD21	1:D:809:ARG:NH2	2.11	0.49
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.75	0.49
1:A:599:ARG:HB3	1:A:600:GLN:HE21	1.78	0.49
1:A:581:ASN:HB2	1:A:583:ASN:HD21	1.77	0.49
1:C:728:VAL:O	1:C:730:LEU:HD23	2.13	0.49
1:B:824:GLN:HG2	1:B:825:CYS:N	2.27	0.49
1:D:340:GLY:O	1:D:561:ARG:HG2	2.13	0.49
1:A:646:HIS:ND1	6:A:9371:HOH:O	2.18	0.49
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.94	0.49
1:A:793:ILE:HG22	1:A:795[B]:VAL:HG22	1.94	0.49
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.94	0.48
1:A:128:ASN:ND2	1:A:180:GLY:CA	2.74	0.48
1:C:785:THR:O	1:C:881:ARG:HD2	2.11	0.48
1:C:431:ARG:HD2	6:C:9089:HOH:O	2.12	0.48
1:D:32:PRO:HB2	5:D:8404:DMS:C1	2.43	0.48
1:B:629:PHE:HA	1:B:637:GLU:O	2.14	0.48
1:C:595:THR:HA	1:C:596:PRO:C	2.34	0.48
1:A:337:ILE:HA	1:A:341:LEU:O	2.14	0.48
1:C:629:PHE:HA	1:C:637:GLU:O	2.14	0.48
1:C:114:VAL:HB	1:C:115:PRO:HD2	1.96	0.48
1:B:961:ARG:NE	1:B:981:GLY:O	2.44	0.48
1:D:955:PHE:CD1	1:D:986:ILE:HD13	2.49	0.48
1:D:250:LEU:C	1:D:251:ARG:HG2	2.33	0.47
1:C:887:GLN:NE2	1:C:980:GLU:O	2.45	0.47
1:B:246:MET:CE	1:B:250:LEU:HD23	2.44	0.47
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.96	0.47
1:B:675:GLN:HA	1:B:675:GLN:OE1	2.14	0.47
1:C:757:GLN:NE2	6:C:9453:HOH:O	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:687:GLN:N	1:A:688:PRO:CD	2.75	0.47
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.42	0.47
1:C:734:SER:CB	1:C:860:GLY:HA3	2.43	0.47
1:B:738:PRO:HB3	1:B:751:LEU:HB2	1.96	0.47
1:C:811:LYS:HB3	1:C:811:LYS:HE2	1.82	0.47
1:D:107:ILE:CA	5:D:8419:DMS:C2	2.93	0.47
1:D:147:ASN:HA	1:D:148:SER:HA	1.76	0.47
1:C:622:HIS:CE1	5:C:8402:DMS:C1	2.97	0.47
1:B:98:PRO:HB2	1:B:203:TRP:CE3	2.49	0.47
1:B:338:GLU:HG2	6:B:9297:HOH:O	2.14	0.47
1:C:833:ALA:HB1	1:C:858:ILE:O	2.15	0.47
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.44	0.47
1:B:773:LYS:CD	1:B:773:LYS:N	2.76	0.47
1:C:796[A]:SER:OG	1:C:808:GLU:OE2	2.32	0.47
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.67	0.47
1:C:986:ILE:HD13	1:C:986:ILE:HG23	1.35	0.47
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.50	0.47
1:A:653:HIS:CD2	1:A:667:GLU:CG	2.96	0.47
1:B:773:LYS:HD2	1:B:773:LYS:HA	1.59	0.46
1:B:74:LEU:HD22	1:B:153:TRP:CD2	2.51	0.46
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.97	0.46
1:B:117:GLU:HB2	6:B:9018:HOH:O	2.15	0.46
1:C:230:ARG:HD3	6:C:9470:HOH:O	2.14	0.46
1:B:93:HIS:CD2	5:B:8414:DMS:C2	2.99	0.46
1:C:416:GLU:HA	1:C:460:ASN:O	2.14	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.15	0.46
1:C:369:GLU:HB2	1:C:397:LEU:CD2	2.45	0.46
1:D:107:ILE:C	5:D:8419:DMS:H21	2.36	0.46
1:C:822:LEU:HD11	1:C:824:GLN:O	2.14	0.46
1:B:768:MET:HG3	6:B:9511:HOH:O	2.15	0.46
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.51	0.46
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.46	0.46
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.65	0.46
1:C:114:VAL:HB	1:C:115:PRO:CD	2.46	0.46
1:B:689:GLU:O	1:B:690:SER:OG	2.22	0.46
1:B:801[A]:ILE:HG23	1:B:808:GLU:OE1	2.15	0.46
1:C:749:ILE:N	1:C:749:ILE:CD1	2.78	0.46
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.51	0.46
1:B:533:LEU:HD23	1:B:533:LEU:C	2.36	0.46
1:B:768:MET:O	1:B:775:GLN:HG2	2.16	0.46
1:D:800:ARG:NH2	6:D:9637:HOH:O	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.51	0.46
1:C:651:LEU:CD1	1:C:651:LEU:C	2.83	0.46
1:C:689:GLU:O	1:C:690:SER:HB3	2.15	0.46
1:D:986:ILE:HD13	1:D:986:ILE:HG23	1.44	0.46
1:B:338:GLU:OE2	6:B:9297:HOH:O	2.20	0.46
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.51	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.16	0.45
1:A:663:LEU:HB3	1:A:686:PRO:HG3	1.97	0.45
1:C:356:ARG:HH22	1:C:367:MET:HE2	1.81	0.45
1:D:930:VAL:O	1:D:932:PRO:HD3	2.17	0.45
1:D:965:GLN:O	1:D:969:GLU:HG3	2.15	0.45
1:A:230:ARG:HH11	1:A:241:GLU:HG3	1.82	0.45
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.51	0.45
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.35	0.45
1:B:802[A]:ASP:C	1:B:802[A]:ASP:OD1	2.55	0.45
1:B:416:GLU:HA	1:B:460:ASN:O	2.16	0.45
1:D:654:TRP:CH2	1:D:685:LEU:HD21	2.51	0.45
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.35	0.45
1:D:843:GLN:HA	1:D:847:LYS:O	2.17	0.45
1:A:127:PHE:O	1:A:182:ASN:N	2.39	0.45
1:D:807:VAL:CG1	1:D:808:GLU:N	2.80	0.45
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.13	0.45
1:C:990:HIS:HD2	1:C:991:MET:O	2.00	0.45
1:C:230:ARG:HG2	1:C:230:ARG:NH1	2.30	0.45
1:C:278:ILE:N	1:C:278:ILE:CD1	2.80	0.45
5:B:8420:DMS:H11	6:C:9196:HOH:O	2.16	0.45
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.52	0.45
1:A:822:LEU:HD11	1:A:824:GLN:O	2.17	0.45
1:C:816:TYR:CE2	1:C:968:MET:CE	3.00	0.45
1:D:629:PHE:HA	1:D:637:GLU:O	2.17	0.45
1:C:233:ASP:HA	5:C:8417:DMS:S	2.57	0.45
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.83	0.45
1:D:427:THR:HG21	1:D:462:SER:HB3	1.99	0.45
1:A:663:LEU:CD1	1:A:686:PRO:HG3	2.46	0.45
1:A:49:GLN:HG2	6:A:9254:HOH:O	2.17	0.45
1:C:986:ILE:HG21	1:C:986:ILE:HD12	1.54	0.45
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.32	0.45
1:C:633:GLY:HA3	1:C:634:GLN:HE21	1.81	0.45
1:A:817:GLN:NE2	6:A:8937:HOH:O	2.49	0.45
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.16	0.45
1:C:824:GLN:HG2	1:C:825:CYS:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.98	0.44
1:D:93:HIS:HB3	1:D:95:TYR:CE1	2.51	0.44
1:C:755:ARG:HG3	1:C:756:TRP:N	2.32	0.44
1:B:646:HIS:CE1	1:B:673:ALA:HB2	2.53	0.44
1:A:178:ARG:HD2	6:A:9400:HOH:O	2.15	0.44
1:C:579:ASP:OD1	1:C:583:ASN:N	2.32	0.44
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.47	0.44
1:A:781:ARG:NH1	6:A:9290:HOH:O	2.49	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.44
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.99	0.44
1:B:795[A]:VAL:HG13	1:B:999:TRP:CB	2.48	0.44
1:A:533:LEU:C	1:A:533:LEU:HD23	2.38	0.44
1:A:829:THR:O	1:A:829:THR:HG22	2.17	0.44
1:A:128:ASN:HD21	1:A:180:GLY:CA	2.17	0.44
1:D:749:ILE:N	1:D:749:ILE:CD1	2.80	0.44
1:A:804[B]:ASN:ND2	1:A:809:ARG:NH2	2.65	0.44
1:B:93:HIS:NE2	5:B:8414:DMS:C2	2.81	0.44
1:D:360:HIS:CE1	1:D:362:LEU:HG	2.52	0.44
1:C:734:SER:HB2	1:C:860:GLY:HA3	2.00	0.44
1:B:299:LYS:HE2	6:B:9258:HOH:O	2.17	0.44
1:D:738:PRO:HB3	1:D:751:LEU:HB2	1.99	0.44
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.99	0.44
1:B:183:ARG:NH1	1:B:183:ARG:HG2	2.31	0.44
1:C:816:TYR:CE2	1:C:968:MET:HE3	2.51	0.44
1:D:88:SER:HA	1:D:366:VAL:HG21	2.00	0.44
1:B:668:VAL:CG1	1:B:669:PRO:N	2.79	0.44
1:B:262:GLN:NE2	1:B:263:GLY:N	2.66	0.44
1:C:658:LEU:HB2	1:C:694:LEU:HD23	1.99	0.44
1:A:576:ILE:HA	1:A:576:ILE:HD13	1.81	0.44
1:C:890:GLN:HG3	1:C:891:VAL:H	1.83	0.44
1:A:619:GLU:HA	1:A:912:ALA:HB2	2.00	0.44
1:A:850:PHE:HA	1:A:871:GLU:O	2.17	0.44
1:A:687:GLN:N	1:A:688:PRO:HD3	2.33	0.44
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.53	0.44
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.53	0.44
1:B:537:GLU:OE1	2:B:2001:149:O2	2.35	0.44
1:A:801[B]:ILE:N	1:A:801[B]:ILE:HD12	2.32	0.44
1:D:804:ASN:HA	1:D:809:ARG:HE	1.83	0.44
1:D:60:PHE:HA	1:D:122:CYS:O	2.17	0.44
1:A:557:ARG:HD2	1:A:557:ARG:HH11	1.65	0.43
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.15	0.43
1:B:755:ARG:O	1:B:768:MET:HG2	2.18	0.43
1:B:687:GLN:CB	1:B:688:PRO:CD	2.95	0.43
1:D:26:ARG:HD2	1:D:169:SER:HA	1.98	0.43
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.99	0.43
1:B:301:TRP:CH2	1:B:452:SER:HA	2.53	0.43
1:A:577:LYS:O	1:A:584:PRO:HA	2.18	0.43
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.18	0.43
1:B:243:GLU:OE2	1:B:245:GLN:NE2	2.46	0.43
1:C:46:ARG:HG2	6:C:9454:HOH:O	2.18	0.43
1:A:390:SER:HA	1:A:391:HIS:HA	1.85	0.43
1:D:370:GLN:HB2	6:D:9233:HOH:O	2.18	0.43
1:C:730:LEU:CD2	1:C:730:LEU:H	2.19	0.43
1:A:784:PHE:HA	1:A:881:ARG:O	2.19	0.43
1:D:58:TRP:CD1	1:D:86:VAL:HB	2.54	0.43
1:C:356:ARG:NH2	1:C:367:MET:CE	2.81	0.43
1:C:745:MET:HA	1:C:761:GLN:HE22	1.84	0.43
1:A:759:ASN:HB3	1:A:762:SER:OG	2.18	0.43
1:B:651:LEU:HD21	1:B:701:VAL:HB	2.00	0.43
1:D:107:ILE:CA	5:D:8419:DMS:H23	2.49	0.43
1:D:933:SER:O	1:D:934:GLU:C	2.57	0.43
1:C:513:PRO:O	1:C:514:ALA:HB3	2.19	0.43
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.19	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.66	0.43
1:A:599:ARG:HG2	1:A:798[B]:ALA:HB2	2.00	0.43
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.18	0.43
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.81	0.43
1:C:835:LEU:O	1:C:836:ILE:HD13	2.18	0.43
1:B:595:THR:O	1:B:595:THR:HG23	2.18	0.43
1:A:126:THR:HA	1:A:182:ASN:O	2.19	0.43
1:D:373:VAL:O	1:D:377:LEU:HG	2.18	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.19	0.43
1:C:356:ARG:NH2	1:C:367:MET:HE1	2.34	0.43
1:B:794[A]:GLY:HA2	1:B:998:SER:O	2.19	0.43
1:D:962:TYR:CE1	5:D:8508:DMS:C1	3.00	0.43
1:B:622:HIS:CE1	5:B:8402:DMS:H11	2.54	0.43
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.53	0.43
1:D:651:LEU:CD1	1:D:651:LEU:C	2.87	0.42
1:A:701:VAL:O	1:A:703:PRO:HD3	2.18	0.42
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.36	0.42
1:B:333:ARG:HG3	1:B:344:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ARG:HB2	1:B:124:SER:OG	2.19	0.42
1:C:653:HIS:CE1	1:C:667:GLU:CG	3.01	0.42
1:A:824:GLN:NE2	1:A:837:THR:HG22	2.34	0.42
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.54	0.42
1:C:334:GLU:OE1	1:C:336:ARG:HD3	2.19	0.42
1:C:13:ARG:O	1:C:14:ARG:C	2.57	0.42
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.54	0.42
1:B:133:TRP:CD1	5:B:8504:DMS:H11	2.54	0.42
1:D:654:TRP:CZ3	1:D:685:LEU:HD21	2.54	0.42
1:D:765:LEU:HD21	1:D:768:MET:SD	2.60	0.42
1:D:588:TYR:O	1:D:591:ASP:HB2	2.19	0.42
1:B:748:CYS:C	1:B:749:ILE:HD12	2.40	0.42
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.42
1:C:749:ILE:O	1:C:755:ARG:HA	2.20	0.42
1:A:663:LEU:CD1	1:A:686:PRO:CG	2.97	0.42
1:A:703:PRO:HG2	5:A:8425:DMS:H13	1.98	0.42
1:D:859:ASP:OD1	1:D:861:SER:OG	2.24	0.42
1:C:499:ILE:HG22	1:C:501:PRO:HD3	2.00	0.42
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.54	0.42
1:B:663:LEU:HA	1:B:663:LEU:HD22	1.68	0.42
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.20	0.42
1:D:618:THR:HG23	6:D:9069:HOH:O	2.19	0.42
1:D:759:ASN:OD1	1:D:761:GLN:N	2.52	0.42
5:C:8410:DMS:H12	6:C:9211:HOH:O	2.20	0.42
1:C:333:ARG:HA	1:C:345:ASN:OD1	2.20	0.42
1:D:784:PHE:HA	1:D:881:ARG:O	2.20	0.42
1:C:562:LEU:HA	1:C:562:LEU:HD23	1.78	0.42
1:D:301:TRP:CH2	1:D:452:SER:HA	2.54	0.42
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.55	0.42
1:C:658:LEU:O	1:C:659:ASP:C	2.56	0.42
1:A:127:PHE:N	1:A:182:ASN:O	2.45	0.42
1:C:687:GLN:HG3	1:C:688:PRO:HD2	2.01	0.42
1:B:655:MET:HE2	1:B:664:ALA:O	2.20	0.42
1:C:734:SER:HB3	1:C:860:GLY:C	2.40	0.42
1:B:872:VAL:O	1:B:873:ALA:C	2.57	0.42
1:C:86:VAL:HG13	1:C:87:PRO:HA	2.01	0.42
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.54	0.42
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.01	0.42
1:C:356:ARG:HH22	1:C:367:MET:CE	2.33	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.02	0.42
1:C:835:LEU:HD11	1:C:855:THR:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.55	0.42
1:D:952:ARG:NH1	1:D:952:ARG:HB2	2.35	0.42
1:C:388:ARG:HH11	1:C:388:ARG:HD3	1.73	0.41
1:C:777:LEU:HD23	1:C:777:LEU:HA	1.74	0.41
1:B:599:ARG:HB3	1:B:600:GLN:HE21	1.85	0.41
1:C:800[A]:ARG:CZ	1:C:800[A]:ARG:CB	2.98	0.41
1:A:780:LEU:C	1:A:781:ARG:HG3	2.41	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.41
1:A:781:ARG:HH11	1:A:781:ARG:CG	2.29	0.41
1:A:128:ASN:ND2	1:A:180:GLY:C	2.73	0.41
5:C:8402:DMS:H21	6:C:9405:HOH:O	2.20	0.41
1:B:646:HIS:CE1	1:B:673:ALA:CB	3.03	0.41
1:D:359:HIS:CD2	1:D:573:GLN:HA	2.55	0.41
1:A:59:ARG:HG3	1:A:77:ASP:OD1	2.20	0.41
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.47	0.41
1:C:734:SER:C	1:C:736:ALA:H	2.23	0.41
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.21	0.41
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.55	0.41
1:C:808:GLU:OE1	1:C:811:LYS:NZ	2.49	0.41
1:C:835:LEU:C	1:C:836:ILE:HD13	2.41	0.41
1:D:843:GLN:CA	1:D:847:LYS:O	2.68	0.41
1:C:890:GLN:CG	1:C:891:VAL:N	2.83	0.41
1:B:655:MET:O	1:B:655:MET:HG3	2.20	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.02	0.41
1:A:431:ARG:HG3	6:A:9315:HOH:O	2.20	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:A:88:SER:HA	1:A:366:VAL:HG21	2.02	0.41
1:B:183:ARG:HG2	6:B:8918:HOH:O	2.21	0.41
1:C:251:ARG:HH12	1:C:253:TYR:HE2	1.68	0.41
1:A:143:PHE:O	1:A:168:PRO:HA	2.21	0.41
1:B:654:TRP:CE3	1:B:665:SER:HA	2.56	0.41
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.51	0.41
1:A:843:GLN:HA	1:A:847:LYS:O	2.20	0.41
1:B:133:TRP:NE1	5:B:8504:DMS:H12	2.36	0.41
1:D:688:PRO:C	1:D:690:SER:H	2.23	0.41
5:A:8405:DMS:O	6:A:9240:HOH:O	2.22	0.41
1:A:774:LYS:HB2	1:A:774:LYS:HE2	1.81	0.41
1:B:685:LEU:O	1:B:686:PRO:C	2.59	0.41
1:A:237:ARG:NH1	1:A:237:ARG:CG	2.82	0.41
1:A:262:GLN:NE2	1:A:299:LYS:CD	2.84	0.41
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:O	1:A:242:ALA:HA	2.21	0.41
1:A:773:LYS:HB2	1:A:773:LYS:HE2	1.85	0.41
1:A:71:GLU:O	1:A:72:SER:C	2.58	0.41
1:B:851:ILE:HB	1:B:871:GLU:HB2	2.03	0.40
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.55	0.40
1:A:479:ASP:HA	1:A:480:PRO:HD2	1.94	0.40
1:D:962:TYR:CZ	5:D:8508:DMS:C1	3.05	0.40
1:A:686:PRO:C	1:A:688:PRO:HD3	2.41	0.40
1:A:809:ARG:HD3	6:A:9187:HOH:O	2.21	0.40
1:C:110:ASN:O	1:C:113:PHE:HB2	2.22	0.40
1:C:746:ASP:HA	1:C:760:ARG:HG3	2.03	0.40
1:C:972:HIS:HB3	1:C:974:HIS:ND1	2.36	0.40
1:D:378:LEU:HG	6:D:9268:HOH:O	2.21	0.40
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.57	0.40
1:C:800[A]:ARG:CA	1:C:800[A]:ARG:CZ	2.97	0.40
1:D:808:GLU:OE2	1:D:811:LYS:NZ	2.46	0.40
1:D:794:GLY:HA2	1:D:998:SER:O	2.21	0.40
1:A:94:GLY:O	1:A:95:TYR:C	2.59	0.40
1:C:750:GLU:OE2	1:C:755:ARG:HD3	2.20	0.40
1:C:249:GLU:CD	1:C:251:ARG:HD3	2.41	0.40
6:B:9189:HOH:O	5:C:8420:DMS:H11	2.22	0.40
1:B:782:ASP:HA	1:B:884:LEU:HD23	2.03	0.40
1:C:411:ASP:OD2	1:C:447:ASP:OD2	2.40	0.40
1:B:232:ASN:HD21	1:B:237:ARG:HG3	1.80	0.40
1:D:973:ARG:O	5:D:8423:DMS:H11	2.22	0.40
1:B:91:GLN:HG2	1:B:98:PRO:CA	2.50	0.40
1:D:577:LYS:O	1:D:584:PRO:HA	2.22	0.40
1:B:655:MET:HB3	6:B:9494:HOH:O	2.21	0.40
1:A:842:TRP:C	1:A:843:GLN:HG3	2.40	0.40
1:B:749:ILE:HD12	1:B:749:ILE:N	2.37	0.40
1:A:36:TRP:CD2	1:A:42:ALA:HA	2.57	0.40
1:B:562:LEU:HA	1:B:562:LEU:HD23	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:9538:HOH:O	6:D:9651:HOH:O[2_454]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	1020/1023 (100%)	980 (96%)	35 (3%)	5 (0%)	34	17
1	B	1020/1023 (100%)	985 (97%)	34 (3%)	1 (0%)	56	38
1	C	1020/1023 (100%)	980 (96%)	38 (4%)	2 (0%)	52	35
1	D	1009/1023 (99%)	971 (96%)	35 (4%)	3 (0%)	46	29
All	All	4069/4092 (99%)	3916 (96%)	142 (4%)	11 (0%)	52	29

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	C	690	SER
1	D	688	PRO
1	A	688	PRO
1	A	164	ASP
1	D	164	ASP
1	D	201	ASP
1	A	798[A]	ALA
1	A	798[B]	ALA
1	C	164	ASP
1	A	687	GLN

5.3.2 Protein sidechains [i](#)

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	873/875 (100%)	838 (96%)	35 (4%)	38	20
1	B	873/875 (100%)	833 (95%)	40 (5%)	33	15
1	C	873/875 (100%)	830 (95%)	43 (5%)	31	13
1	D	864/875 (99%)	828 (96%)	36 (4%)	36	18
All	All	3483/3500 (100%)	3329 (96%)	154 (4%)	36	17

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	GLU
1	A	128	ASN
1	A	237	ARG
1	A	333	ARG
1	A	344	LEU
1	A	394	ASN
1	A	431	ARG
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	655	MET
1	A	671	ASP
1	A	675	GLN
1	A	684	GLU
1	A	687	GLN
1	A	689	GLU
1	A	729	THR
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799[A]	THR
1	A	799[B]	THR
1	A	800[A]	ARG
1	A	800[B]	ARG
1	A	801[A]	ILE
1	A	801[B]	ILE
1	A	817	GLN
1	A	829	THR
1	A	885	ASN
1	A	890	GLN
1	A	917	ARG

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Mol	Chain	Res	Type
1	A	1017	GLN
1	A	1023	LYS
1	B	13	ARG
1	B	80	GLU
1	B	117	GLU
1	B	136	GLU
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	394	ASN
1	B	477	SER
1	B	519	SER
1	B	554	GLN
1	B	580	GLU
1	B	581	ASN
1	B	600	GLN
1	B	634	GLN
1	B	635	THR
1	B	651	LEU
1	B	655	MET
1	B	663	LEU
1	B	667	GLU
1	B	687	GLN
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	755	ARG
1	B	773	LYS
1	B	799[A]	THR
1	B	799[B]	THR
1	B	801[A]	ILE
1	B	801[B]	ILE
1	B	819	GLU
1	B	847	LYS
1	B	885	ASN
1	B	890	GLN
1	B	917	ARG
1	B	956	GLN

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Mol	Chain	Res	Type
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	367	MET
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	710	GLU
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	750	GLU
1	C	755	ARG
1	C	773	LYS
1	C	795[A]	VAL
1	C	795[B]	VAL
1	C	796[A]	SER
1	C	796[B]	SER
1	C	800[A]	ARG
1	C	800[B]	ARG
1	C	819	GLU
1	C	917	ARG
1	C	956	GLN
1	C	986	ILE

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Mol	Chain	Res	Type
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	80	GLU
1	D	237	ARG
1	D	319	ASP
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	599	ARG
1	D	655	MET
1	D	663	LEU
1	D	667	GLU
1	D	681	GLU
1	D	685	LEU
1	D	687	GLN
1	D	689	GLU
1	D	699	ARG
1	D	735	HIS
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	801	ILE
1	D	804	ASN
1	D	824	GLN
1	D	829	THR
1	D	843	GLN
1	D	845	GLN
1	D	885	ASN
1	D	956	GLN
1	D	986	ILE
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	ASN

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Mol	Chain	Res	Type
1	A	262	GLN
1	A	583	ASN
1	A	600	GLN
1	A	653	HIS
1	A	675	GLN
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	757	GLN
1	B	878	HIS
1	B	977	HIS
1	C	163	GLN
1	C	363	HIS
1	C	624	GLN
1	C	634	GLN
1	C	761	GLN
1	C	824	GLN
1	C	878	HIS
1	D	135	GLN
1	D	363	HIS
1	D	581	ASN
1	D	624	GLN
1	D	628	GLN
1	D	757	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 118 ligands modelled in this entry, 27 are monoatomic - leaving 91 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	149	A	2001	4	11,12,12	2.19	2 (18%)	13,17,17	1.98	3 (23%)
5	DMS	A	8401	-	3,3,3	0.79	0	3,3,3	0.48	0
5	DMS	A	8402	-	3,3,3	1.46	0	3,3,3	0.62	0
5	DMS	A	8403	-	3,3,3	1.86	2 (66%)	3,3,3	1.01	0
5	DMS	A	8404	-	3,3,3	1.81	1 (33%)	3,3,3	0.44	0
5	DMS	A	8405	-	3,3,3	0.57	0	3,3,3	0.62	0
5	DMS	A	8406	-	3,3,3	0.96	0	3,3,3	0.38	0
5	DMS	A	8407	-	3,3,3	1.35	0	3,3,3	0.32	0
5	DMS	A	8408	-	3,3,3	0.38	0	3,3,3	0.44	0
5	DMS	A	8409	-	3,3,3	2.69	1 (33%)	3,3,3	0.19	0
5	DMS	A	8411	-	3,3,3	1.04	0	3,3,3	0.79	0
5	DMS	A	8412	-	3,3,3	1.32	0	3,3,3	0.29	0
5	DMS	A	8414	-	3,3,3	1.27	0	3,3,3	0.30	0
5	DMS	A	8416	-	3,3,3	0.82	0	3,3,3	0.86	0
5	DMS	A	8419	-	3,3,3	1.04	0	3,3,3	0.18	0
5	DMS	A	8421	-	3,3,3	0.90	0	3,3,3	0.82	0
5	DMS	A	8425	4	3,3,3	1.54	1 (33%)	3,3,3	0.18	0
5	DMS	A	8501	-	3,3,3	1.02	0	3,3,3	0.32	0
5	DMS	A	8503	-	3,3,3	1.32	0	3,3,3	0.39	0
5	DMS	A	8504	-	3,3,3	0.67	0	3,3,3	0.40	0
5	DMS	A	8602	-	3,3,3	0.43	0	3,3,3	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	149	B	2001	4	11,12,12	2.34	1 (9%)	13,17,17	1.16	0
5	DMS	B	8401	-	3,3,3	0.87	0	3,3,3	0.55	0
5	DMS	B	8402	-	3,3,3	1.33	1 (33%)	3,3,3	0.20	0
5	DMS	B	8403	-	3,3,3	1.64	1 (33%)	3,3,3	0.24	0
5	DMS	B	8404	-	3,3,3	0.77	0	3,3,3	0.08	0
5	DMS	B	8405	-	3,3,3	1.33	0	3,3,3	0.40	0
5	DMS	B	8406	-	3,3,3	0.76	0	3,3,3	0.31	0
5	DMS	B	8408	-	3,3,3	0.28	0	3,3,3	0.48	0
5	DMS	B	8409	-	3,3,3	1.73	1 (33%)	3,3,3	1.12	0
5	DMS	B	8410	-	3,3,3	1.22	0	3,3,3	0.27	0
5	DMS	B	8411	-	3,3,3	0.29	0	3,3,3	0.58	0
5	DMS	B	8412	-	3,3,3	1.22	0	3,3,3	0.49	0
5	DMS	B	8414	-	3,3,3	0.61	0	3,3,3	0.30	0
5	DMS	B	8416	-	3,3,3	0.80	0	3,3,3	0.25	0
5	DMS	B	8417	-	3,3,3	1.15	0	3,3,3	0.59	0
5	DMS	B	8420	-	3,3,3	0.58	0	3,3,3	0.83	0
5	DMS	B	8421	-	3,3,3	0.71	0	3,3,3	0.06	0
5	DMS	B	8423	-	3,3,3	0.80	0	3,3,3	0.32	0
5	DMS	B	8425	4	3,3,3	2.70	1 (33%)	3,3,3	0.61	0
5	DMS	B	8502	-	3,3,3	1.44	1 (33%)	3,3,3	0.86	0
5	DMS	B	8504	-	3,3,3	1.19	1 (33%)	3,3,3	0.33	0
5	DMS	B	8508	-	3,3,3	1.39	0	3,3,3	0.19	0
5	DMS	B	8601	-	3,3,3	0.84	0	3,3,3	0.60	0
2	149	C	2001	4	11,12,12	1.66	2 (18%)	13,17,17	1.96	5 (38%)
5	DMS	C	8401	-	3,3,3	1.15	0	3,3,3	0.04	0
5	DMS	C	8402	-	3,3,3	2.10	1 (33%)	3,3,3	0.44	0
5	DMS	C	8403	-	3,3,3	1.60	0	3,3,3	0.55	0
5	DMS	C	8404	-	3,3,3	1.65	1 (33%)	3,3,3	0.60	0
5	DMS	C	8405	-	3,3,3	1.52	1 (33%)	3,3,3	0.50	0
5	DMS	C	8407	-	3,3,3	1.58	1 (33%)	3,3,3	0.52	0
5	DMS	C	8408	-	3,3,3	0.96	0	3,3,3	0.38	0
5	DMS	C	8409	-	3,3,3	0.67	0	3,3,3	0.71	0
5	DMS	C	8410	-	3,3,3	0.92	0	3,3,3	0.38	0
5	DMS	C	8411	-	3,3,3	1.11	0	3,3,3	0.10	0
5	DMS	C	8412	-	3,3,3	0.90	0	3,3,3	0.50	0
5	DMS	C	8414	-	3,3,3	1.82	1 (33%)	3,3,3	0.64	0
5	DMS	C	8415	-	3,3,3	1.76	1 (33%)	3,3,3	0.27	0
5	DMS	C	8416	-	3,3,3	1.23	1 (33%)	3,3,3	0.34	0
5	DMS	C	8417	-	3,3,3	0.70	0	3,3,3	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8420	-	3,3,3	1.21	1 (33%)	3,3,3	0.70	0
5	DMS	C	8421	-	3,3,3	0.65	0	3,3,3	0.13	0
5	DMS	C	8423	-	3,3,3	0.93	0	3,3,3	0.37	0
5	DMS	C	8425	4	3,3,3	0.92	0	3,3,3	0.51	0
5	DMS	C	8428	-	3,3,3	0.77	0	3,3,3	0.28	0
5	DMS	C	8501	-	3,3,3	0.84	0	3,3,3	0.22	0
5	DMS	C	8601	-	3,3,3	1.10	0	3,3,3	1.05	0
2	149	D	2001	4	11,12,12	1.96	2 (18%)	13,17,17	2.00	5 (38%)
5	DMS	D	8401	-	3,3,3	0.90	0	3,3,3	0.28	0
5	DMS	D	8402	-	3,3,3	0.70	0	3,3,3	0.67	0
5	DMS	D	8403	-	3,3,3	1.71	1 (33%)	3,3,3	0.32	0
5	DMS	D	8404	-	3,3,3	1.00	0	3,3,3	0.19	0
5	DMS	D	8405	-	3,3,3	0.38	0	3,3,3	1.21	0
5	DMS	D	8406	-	3,3,3	0.69	0	3,3,3	0.72	0
5	DMS	D	8408	-	3,3,3	1.50	1 (33%)	3,3,3	0.35	0
5	DMS	D	8409	-	3,3,3	1.47	0	3,3,3	0.47	0
5	DMS	D	8410	-	3,3,3	1.67	0	3,3,3	0.50	0
5	DMS	D	8411	-	3,3,3	0.71	0	3,3,3	0.37	0
5	DMS	D	8412	-	3,3,3	1.00	0	3,3,3	0.42	0
5	DMS	D	8414	-	3,3,3	0.66	0	3,3,3	0.31	0
5	DMS	D	8416	-	3,3,3	0.52	0	3,3,3	0.42	0
5	DMS	D	8417	-	3,3,3	0.79	0	3,3,3	0.13	0
5	DMS	D	8419	-	3,3,3	1.69	1 (33%)	3,3,3	0.44	0
5	DMS	D	8421	-	3,3,3	0.79	0	3,3,3	0.41	0
5	DMS	D	8423	-	3,3,3	0.63	0	3,3,3	0.24	0
5	DMS	D	8501	-	3,3,3	0.60	0	3,3,3	0.38	0
5	DMS	D	8503	-	3,3,3	0.51	0	3,3,3	0.29	0
5	DMS	D	8508	-	3,3,3	1.57	1 (33%)	3,3,3	0.11	0
5	DMS	D	8701	-	3,3,3	2.16	2 (66%)	3,3,3	0.60	0
5	DMS	D	8703	-	3,3,3	1.72	1 (33%)	3,3,3	0.26	0
5	DMS	D	8705	-	3,3,3	0.87	0	3,3,3	0.19	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	149	A	2001	4	-	0/2/22/22	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	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	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
5	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
2	149	B	2001	4	-	0/2/22/22	0/1/1/1
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	8408	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8410	-	-	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	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8420	-	-	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	4	-	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	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
2	149	C	2001	4	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	8407	-	-	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	8410	-	-	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	8415	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8420	-	-	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	8425	4	-	0/0/0/0	0/0/0/0
5	DMS	C	8428	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
2	149	D	2001	4	-	0/2/22/22	0/1/1/1
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	8404	-	-	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	8410	-	-	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	8417	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8419	-	-	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	8501	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8503	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
5	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8419	DMS	C2-S	-2.81	1.54	1.75
2	D	2001	149	O5-C5	-2.79	1.42	1.46
5	C	8414	DMS	O-S	-2.75	1.31	1.50
5	B	8504	DMS	C2-S	-2.03	1.60	1.75
5	C	8416	DMS	C2-S	2.02	1.91	1.75
5	C	8420	DMS	O-S	2.04	1.64	1.50
5	B	8402	DMS	C2-S	2.06	1.91	1.75
5	C	8407	DMS	C2-S	2.14	1.92	1.75
5	C	8405	DMS	O-S	2.15	1.65	1.50
5	D	8701	DMS	C1-S	2.18	1.92	1.75
5	A	8403	DMS	O-S	2.18	1.65	1.50
5	B	8502	DMS	O-S	2.27	1.65	1.50
5	A	8425	DMS	O-S	2.30	1.66	1.50
5	D	8701	DMS	O-S	2.32	1.66	1.50
5	A	8403	DMS	C2-S	2.37	1.94	1.75
5	D	8403	DMS	C2-S	2.44	1.94	1.75
5	C	8415	DMS	C1-S	2.45	1.94	1.75
5	B	8403	DMS	C2-S	2.53	1.95	1.75
2	C	2001	149	C3-C2	2.56	1.56	1.53
5	D	8408	DMS	C1-S	2.57	1.95	1.75
5	D	8508	DMS	O-S	2.60	1.68	1.50
5	C	8404	DMS	C2-S	2.61	1.95	1.75
5	A	8404	DMS	C2-S	2.67	1.96	1.75
5	D	8703	DMS	C1-S	2.80	1.97	1.75
5	B	8409	DMS	O-S	2.92	1.70	1.50
5	C	8402	DMS	C2-S	3.02	1.99	1.75
2	C	2001	149	O5-C1	3.51	1.39	1.34
2	A	2001	149	O2-C2	3.99	1.49	1.42
5	A	8409	DMS	O-S	4.25	1.79	1.50
5	B	8425	DMS	O-S	4.59	1.81	1.50
2	A	2001	149	O5-C1	5.17	1.42	1.34
2	D	2001	149	O5-C1	5.40	1.42	1.34
2	B	2001	149	O5-C1	6.83	1.44	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	149	C3-C4-C5	-4.86	101.73	110.20
2	D	2001	149	C3-C4-C5	-3.91	103.38	110.20
2	C	2001	149	O4-C4-C5	-3.81	99.14	109.24
2	C	2001	149	O3-C3-C4	-2.68	104.30	110.34
2	C	2001	149	C4-C3-C2	-2.56	107.61	110.73
2	D	2001	149	O3-C3-C4	-2.53	104.64	110.34
2	A	2001	149	O3-C3-C2	-2.53	104.93	109.49
2	D	2001	149	C4-C3-C2	-2.17	108.08	110.73
2	C	2001	149	C5-O5-C1	2.03	125.58	119.31
2	A	2001	149	O5-C1-O1	2.52	122.28	118.51
2	D	2001	149	O2-C2-C3	2.59	115.21	109.95
2	C	2001	149	O5-C5-C4	2.60	114.67	109.76
2	D	2001	149	O4-C4-C5	3.09	117.43	109.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8405	DMS	1	0
5	A	8425	DMS	3	0
2	B	2001	149	1	0
5	B	8402	DMS	1	0
5	B	8414	DMS	4	0
5	B	8420	DMS	1	0
5	B	8504	DMS	4	0
5	C	8402	DMS	3	0
5	C	8410	DMS	1	0
5	C	8417	DMS	1	0
5	C	8420	DMS	2	0
5	D	8404	DMS	2	0
5	D	8412	DMS	2	0
5	D	8419	DMS	5	0
5	D	8423	DMS	3	0
5	D	8503	DMS	1	0
5	D	8508	DMS	4	0
5	D	8703	DMS	1	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	1009/1023 (98%)	-0.40	25 (2%) 61 56	11, 23, 51, 90	9 (0%)
1	B	1011/1023 (98%)	-0.38	25 (2%) 61 56	13, 23, 49, 90	8 (0%)
1	C	1011/1023 (98%)	-0.40	30 (2%) 54 48	14, 22, 52, 89	6 (0%)
1	D	1011/1023 (98%)	-0.39	28 (2%) 56 51	13, 23, 52, 94	0
All	All	4042/4092 (98%)	-0.39	108 (2%) 58 53	11, 23, 52, 94	23 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	8.0
1	C	732	ALA	7.6
1	A	686	PRO	7.5
1	D	732	ALA	7.4
1	C	730	LEU	7.3
1	D	735	HIS	7.3
1	C	731	PRO	7.1
1	D	801	ILE	7.0
1	B	730	LEU	6.7
1	B	799[A]	THR	6.1
1	C	800[A]	ARG	6.0
1	A	731	PRO	6.0
1	D	800	ARG	5.6
1	B	689	GLU	5.6
1	A	732	ALA	5.6
1	B	731	PRO	5.4
1	B	733	ALA	5.4
1	A	801[A]	ILE	5.1
1	B	732	ALA	5.0
1	A	733	ALA	4.9
1	D	686	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
1	D	689	GLU	4.7
1	C	735	HIS	4.5
1	C	799[A]	THR	4.4
1	D	730	LEU	4.4
1	C	580	GLU	4.3
1	D	1023	LYS	4.3
1	A	689	GLU	4.2
1	D	731	PRO	4.2
1	D	733	ALA	4.1
1	D	799	THR	4.0
1	A	79	PRO	4.0
1	A	730	LEU	4.0
1	B	581	ASN	3.9
1	C	745	MET	3.9
1	C	733	ALA	3.9
1	B	745	MET	3.8
1	D	79	PRO	3.8
1	D	734	SER	3.8
1	B	686	PRO	3.8
1	C	801[A]	ILE	3.7
1	A	580	GLU	3.7
1	D	581	ASN	3.6
1	B	798[A]	ALA	3.5
1	C	689	GLU	3.5
1	A	795[A]	VAL	3.5
1	C	761	GLN	3.4
1	D	685	LEU	3.4
1	B	580	GLU	3.3
1	D	580	GLU	3.3
1	C	581	ASN	3.2
1	C	633	GLY	3.2
1	A	1023	LYS	3.2
1	A	729	THR	3.1
1	D	684	GLU	3.1
1	B	685	LEU	3.1
1	D	772	ASP	3.1
1	B	79	PRO	3.1
1	B	687	GLN	3.0
1	A	687	GLN	3.0
1	B	800[A]	ARG	3.0
1	B	684	GLU	2.9
1	C	729	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	772	ASP	2.9
1	C	582	GLY	2.9
1	A	685	LEU	2.9
1	D	845	GLN	2.9
1	C	798[A]	ALA	2.8
1	D	729	THR	2.8
1	C	634	GLN	2.8
1	A	734	SER	2.8
1	A	688	PRO	2.8
1	A	634	GLN	2.7
1	D	771	GLY	2.6
1	A	582	GLY	2.5
1	B	734	SER	2.5
1	D	582	GLY	2.5
1	D	633	GLY	2.5
1	D	76	CYS	2.5
1	C	687	GLN	2.5
1	D	803	PRO	2.5
1	C	686	PRO	2.4
1	C	795[A]	VAL	2.4
1	C	632	SER	2.3
1	B	582	GLY	2.3
1	B	831	ALA	2.3
1	D	687	GLN	2.3
1	A	633	GLY	2.3
1	A	76	CYS	2.2
1	C	79	PRO	2.2
1	A	179	ALA	2.2
1	D	802	ASP	2.2
1	B	632	SER	2.2
1	A	684	GLU	2.2
1	C	734	SER	2.2
1	A	581	ASN	2.2
1	B	735	HIS	2.2
1	C	684	GLU	2.2
1	B	80	GLU	2.1
1	C	744	GLU	2.1
1	B	771	GLY	2.1
1	C	688	PRO	2.1
1	B	47	PRO	2.1
1	D	683	PRO	2.1
1	C	685	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	845	GLN	2.1
1	C	593	GLY	2.0
1	B	801[A]	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	C	8420	4/4	0.94	0.14	13.93	48,49,57,96	0
5	DMS	D	8703	4/4	0.88	0.23	11.35	28,62,66,100	0
5	DMS	A	8407	4/4	0.78	0.18	7.41	32,46,85,100	0
5	DMS	C	8407	4/4	0.89	0.15	5.57	29,37,51,72	0
5	DMS	B	8420	4/4	0.92	0.11	5.56	35,42,50,100	0
5	DMS	B	8508	4/4	0.90	0.17	5.54	41,54,84,84	0
5	DMS	D	8410	4/4	0.95	0.17	5.25	47,58,100,100	0
5	DMS	A	8406	4/4	0.95	0.10	5.24	26,37,56,62	0
5	DMS	C	8425	4/4	0.95	0.19	4.98	37,57,68,100	0
5	DMS	B	8408	4/4	0.97	0.14	4.58	35,38,40,45	0
5	DMS	B	8423	4/4	0.95	0.18	4.29	42,61,69,100	0
5	DMS	D	8403	4/4	0.98	0.11	4.22	26,38,40,52	0
5	DMS	D	8406	4/4	0.97	0.13	3.80	29,34,37,57	0
5	DMS	C	8423	4/4	0.95	0.13	3.27	35,64,64,100	0
5	DMS	A	8404	4/4	0.94	0.10	2.98	26,32,43,45	0
5	DMS	C	8428	4/4	0.98	0.26	2.96	10,19,20,29	4
5	DMS	B	8502	4/4	0.95	0.12	2.76	36,42,48,51	0
5	DMS	D	8423	4/4	0.92	0.15	2.72	48,53,78,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8425	4/4	0.95	0.14	2.10	24,31,42,49	0
5	DMS	B	8417	4/4	0.97	0.11	2.06	31,32,68,100	0
5	DMS	C	8411	4/4	0.99	0.12	1.97	33,35,36,91	0
5	DMS	D	8404	4/4	0.97	0.10	1.94	39,39,54,63	0
5	DMS	D	8417	4/4	0.93	0.14	1.81	30,32,35,100	0
5	DMS	C	8403	4/4	0.99	0.12	1.79	25,26,27,33	0
5	DMS	A	8401	4/4	0.99	0.10	1.55	16,16,18,22	0
5	DMS	A	8504	4/4	0.99	0.10	1.51	32,45,52,100	0
5	DMS	A	8403	4/4	0.98	0.08	1.50	24,28,34,35	0
5	DMS	C	8410	4/4	0.97	0.12	1.47	39,62,82,100	0
5	DMS	B	8405	4/4	0.98	0.10	1.41	35,35,36,41	0
5	DMS	A	8425	4/4	0.95	0.17	1.16	34,43,49,89	0
4	NA	B	3104	1/1	0.98	0.13	1.11	33,33,33,33	0
5	DMS	D	8419	4/4	0.94	0.11	0.99	42,45,63,78	0
5	DMS	C	8417	4/4	0.95	0.10	0.99	33,36,57,63	0
5	DMS	D	8705	4/4	0.96	0.13	0.99	33,46,55,58	0
5	DMS	B	8401	4/4	0.99	0.08	0.92	17,18,25,33	0
2	149	B	2001	12/12	0.98	0.08	0.89	16,20,24,33	0
2	149	A	2001	12/12	0.98	0.07	0.85	16,19,26,28	0
5	DMS	A	8412	4/4	0.97	0.09	0.75	39,43,43,100	0
5	DMS	A	8408	4/4	0.98	0.09	0.70	26,39,45,100	0
5	DMS	C	8501	4/4	0.98	0.08	0.66	26,39,40,53	0
5	DMS	D	8701	4/4	0.98	0.08	0.60	21,25,32,50	0
5	DMS	B	8403	4/4	0.99	0.08	0.50	25,29,35,37	0
5	DMS	D	8408	4/4	0.98	0.11	0.37	30,37,40,44	0
5	DMS	A	8419	4/4	0.96	0.11	0.35	40,49,58,79	0
4	NA	D	3103	1/1	0.97	0.10	0.33	38,38,38,38	0
5	DMS	D	8405	4/4	0.99	0.08	0.06	26,30,41,43	0
5	DMS	B	8402	4/4	0.98	0.08	0.06	17,26,33,37	0
4	NA	A	3104	1/1	0.98	0.09	0.04	30,30,30,30	0
5	DMS	C	8402	4/4	0.98	0.07	-0.01	17,30,34,43	0
5	DMS	A	8501	4/4	0.97	0.08	-0.04	23,33,41,43	0
5	DMS	C	8408	4/4	0.97	0.08	-0.09	26,37,46,52	0
5	DMS	D	8412	4/4	0.98	0.08	-0.09	35,37,41,100	0
5	DMS	C	8412	4/4	0.99	0.08	-0.10	31,35,41,100	0
5	DMS	C	8405	4/4	0.99	0.07	-0.11	26,27,34,35	0
5	DMS	B	8406	4/4	0.98	0.10	-0.12	40,43,56,59	0
5	DMS	C	8401	4/4	0.99	0.06	-0.17	15,22,22,24	0
5	DMS	A	8405	4/4	0.99	0.07	-0.17	26,30,34,46	0
4	NA	C	3103	1/1	0.99	0.09	-0.30	36,36,36,36	0
2	149	C	2001	12/12	0.98	0.07	-0.44	17,20,26,26	0
2	149	D	2001	12/12	0.98	0.06	-0.46	12,16,21,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	B	8404	4/4	0.97	0.06	-0.49	26,28,36,40	0
5	DMS	B	8504	4/4	0.97	0.07	-0.59	26,46,64,82	0
5	DMS	B	8412	4/4	0.98	0.06	-0.61	29,30,35,38	0
5	DMS	D	8501	4/4	0.97	0.07	-0.65	40,45,46,55	0
5	DMS	D	8401	4/4	0.99	0.06	-0.68	15,21,22,23	0
4	NA	C	3104	1/1	0.98	0.07	-0.76	31,31,31,31	0
5	DMS	D	8411	4/4	0.99	0.07	-0.79	32,32,37,97	0
5	DMS	D	8402	4/4	0.98	0.06	-0.89	18,37,39,40	0
5	DMS	C	8404	4/4	0.98	0.06	-0.89	22,25,25,34	0
4	NA	C	3101	1/1	1.00	0.06	-0.92	19,19,19,19	0
3	MG	C	3002	1/1	0.99	0.05	-1.06	18,18,18,18	0
4	NA	A	3101	1/1	0.99	0.05	-1.06	22,22,22,22	0
5	DMS	B	8411	4/4	0.99	0.06	-1.08	37,37,37,79	0
5	DMS	A	8402	4/4	0.99	0.05	-1.09	22,36,36,52	0
4	NA	D	3102	1/1	0.99	0.05	-1.20	19,19,19,19	0
4	NA	D	3104	1/1	0.96	0.06	-1.20	37,37,37,37	0
4	NA	B	3101	1/1	0.99	0.06	-1.32	21,21,21,21	0
4	NA	D	3101	1/1	1.00	0.05	-1.42	21,21,21,21	0
3	MG	B	3002	1/1	0.99	0.06	-1.70	22,22,22,22	0
4	NA	B	3103	1/1	0.99	0.05	-2.07	29,29,29,29	0
5	DMS	A	8411	4/4	0.98	0.06	-2.08	25,34,38,59	0
4	NA	C	3102	1/1	0.99	0.04	-2.21	19,19,19,19	0
4	NA	A	3102	1/1	1.00	0.04	-2.22	17,17,17,17	0
4	NA	A	3103	1/1	0.99	0.05	-2.36	34,34,34,34	0
3	MG	A	3002	1/1	0.99	0.04	-2.37	22,22,22,22	0
4	NA	B	3102	1/1	1.00	0.04	-2.45	20,20,20,20	0
3	MG	D	3002	1/1	1.00	0.04	-2.62	20,20,20,20	0
3	MG	B	3001	1/1	0.99	0.04	-2.82	18,18,18,18	0
3	MG	C	3001	1/1	1.00	0.03	-2.85	18,18,18,18	0
3	MG	A	3001	1/1	0.99	0.04	-3.26	23,23,23,23	0
3	MG	D	3001	1/1	0.99	0.04	-3.53	23,23,23,23	0
5	DMS	A	8602	4/4	0.97	0.24	-	50,51,100,100	0
5	DMS	C	8415	4/4	0.96	0.13	-	27,32,55,59	0
5	DMS	D	8416	4/4	0.96	0.17	-	32,42,47,79	0
3	MG	D	3005	1/1	0.96	0.08	-	38,38,38,38	0
5	DMS	D	8421	4/4	0.98	0.17	-	44,49,60,100	0
5	DMS	C	8421	4/4	0.98	0.14	-	41,65,100,100	0
5	DMS	B	8421	4/4	0.97	0.11	-	44,57,59,87	0
5	DMS	A	8414	4/4	0.96	0.10	-	35,40,65,100	0
5	DMS	A	8421	4/4	0.96	0.26	-	61,66,87,100	0
3	MG	B	3003	1/1	0.80	0.14	-	53,53,53,53	0
5	DMS	C	8409	4/4	0.96	0.14	-	30,40,52,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	DMS	D	8414	4/4	0.96	0.15	-	36,58,70,100	0
5	DMS	A	8503	4/4	0.95	0.22	-	35,51,100,100	0
5	DMS	D	8508	4/4	0.97	0.11	-	47,58,68,100	0
5	DMS	A	8416	4/4	0.98	0.26	-	23,69,70,100	0
5	DMS	B	8414	4/4	0.97	0.20	-	39,55,61,100	0
5	DMS	C	8601	4/4	0.98	0.13	-	37,45,50,57	0
5	DMS	B	8410	4/4	0.95	0.11	-	43,50,63,100	0
5	DMS	A	8409	4/4	0.95	0.12	-	30,34,43,51	0
5	DMS	D	8409	4/4	0.97	0.10	-	31,31,42,47	0
3	MG	A	3005	1/1	0.97	0.06	-	45,45,45,45	0
5	DMS	B	8416	4/4	0.98	0.14	-	38,42,47,50	0
5	DMS	B	8601	4/4	0.96	0.12	-	40,47,61,100	0
5	DMS	B	8409	4/4	0.96	0.13	-	29,33,37,43	0
5	DMS	C	8416	4/4	0.85	0.24	-	47,66,73,96	0
5	DMS	D	8503	4/4	0.94	0.23	-	36,66,84,90	0
5	DMS	C	8414	4/4	0.99	0.10	-	28,31,53,70	0

6.5 Other polymers

There are no such residues in this entry.