



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:02 PM GMT

PDB ID : 1DP0
Title : E. COLI BETA-GALACTOSIDASE AT 1.7 ANGSTROM
Authors : Juers, D.H.; Jacobson, R.H.; Wigley, D.; Zhang, X.J.; Huber, R.E.; Tronrud, D.E.; Matthews, B.W.
Deposited on : 1999-12-22
Resolution : 1.70 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

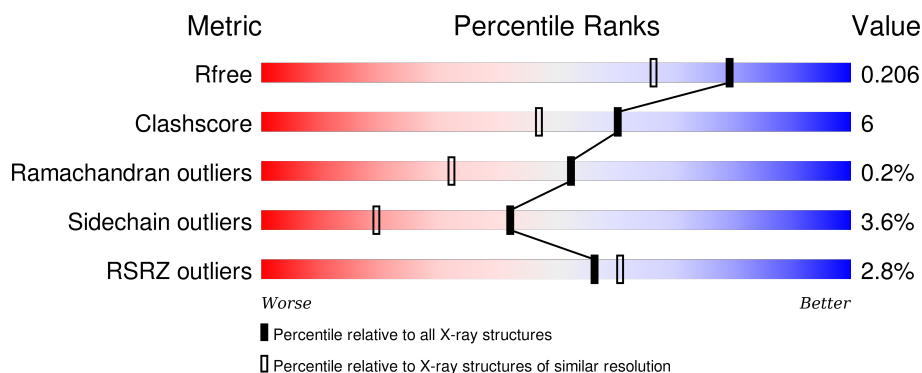
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	1023	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	B	1023	<div> <div>2%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
1	C	1023	<div> <div>3%</div> <div>75%</div> <div>20%</div> <div>..</div> </div>
1	D	1023	<div> <div>3%</div> <div>76%</div> <div>19%</div> <div>..</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
3	NA	D	3103	-	-	-	X
4	DMS	A	8406	-	-	-	X
4	DMS	A	8407	-	-	-	X
4	DMS	A	8413	-	X	-	-
4	DMS	A	8417	-	-	-	X
4	DMS	A	8420	-	-	-	X
4	DMS	A	8423	-	-	-	X
4	DMS	A	8502	-	X	-	-
4	DMS	B	8406	-	-	-	X
4	DMS	B	8407	-	X	-	X
4	DMS	B	8415	-	X	-	-
4	DMS	B	8420	-	-	-	X
4	DMS	B	8425	-	-	-	X
4	DMS	B	8502	-	-	-	X
4	DMS	B	8506	-	-	-	X
4	DMS	B	8508	-	-	-	X
4	DMS	C	8407	-	-	-	X
4	DMS	C	8410	-	-	-	X
4	DMS	C	8419	-	-	-	X
4	DMS	C	8420	-	-	-	X
4	DMS	C	8423	-	-	-	X
4	DMS	C	8425	-	-	-	X
4	DMS	C	8506	-	-	-	X
4	DMS	D	8404	-	-	-	X
4	DMS	D	8407	-	X	-	X
4	DMS	D	8408	-	-	-	X
4	DMS	D	8417	-	-	-	X
4	DMS	D	8423	-	-	-	X
4	DMS	D	8425	-	-	-	X
4	DMS	D	8701	-	X	-	-
4	DMS	D	8703	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37408 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called BETA-GALACTOSIDASE.

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

There are 32 discrepancies between the modelled and reference sequences:

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

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	4	Total Mg 4 4	0	0
2	D	4	Total Mg 4 4	0	0
2	C	5	Total Mg 5 5	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	5	Total Na 5 5	0	0
3	A	5	Total Na 5 5	0	0
3	D	5	Total Na 5 5	0	0
3	C	5	Total Na 5 5	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C₂H₆OS).



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

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

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

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

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

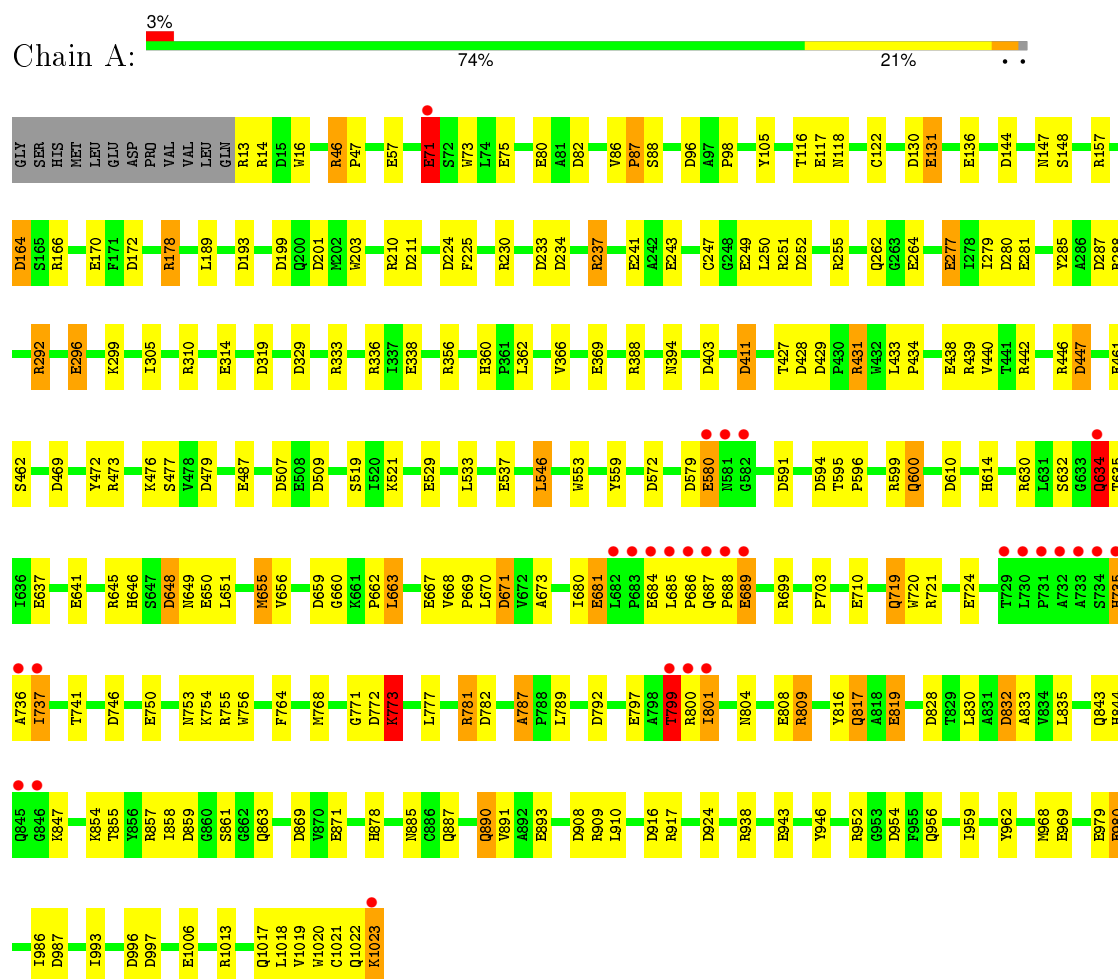
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1134	Total O 1134 1134	0	0
5	B	1104	Total O 1104 1104	0	0
5	C	1072	Total O 1072 1072	0	0
5	D	1114	Total O 1114 1114	0	0

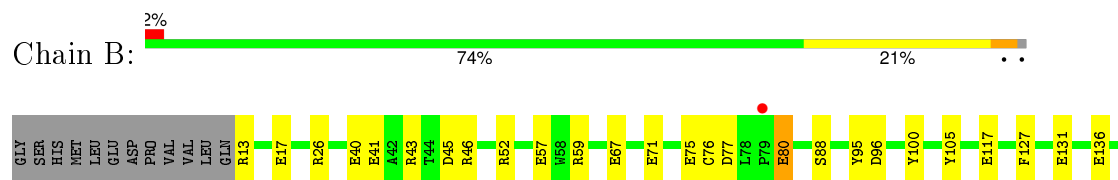
3 Residue-property plots

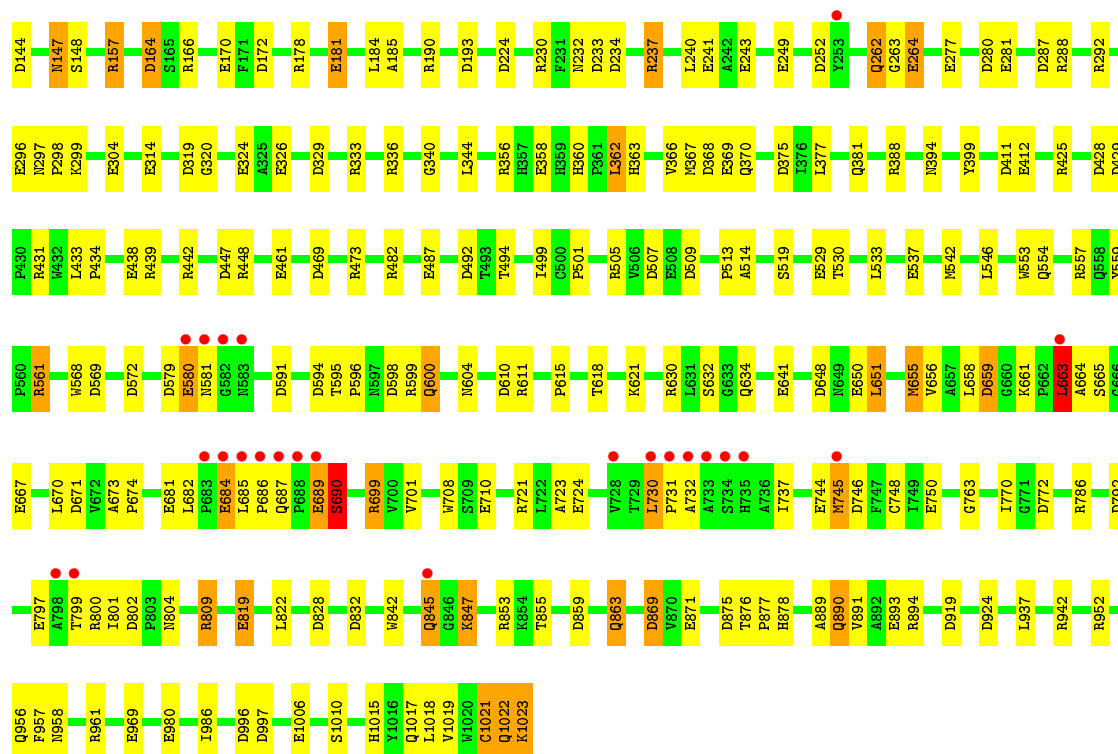
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

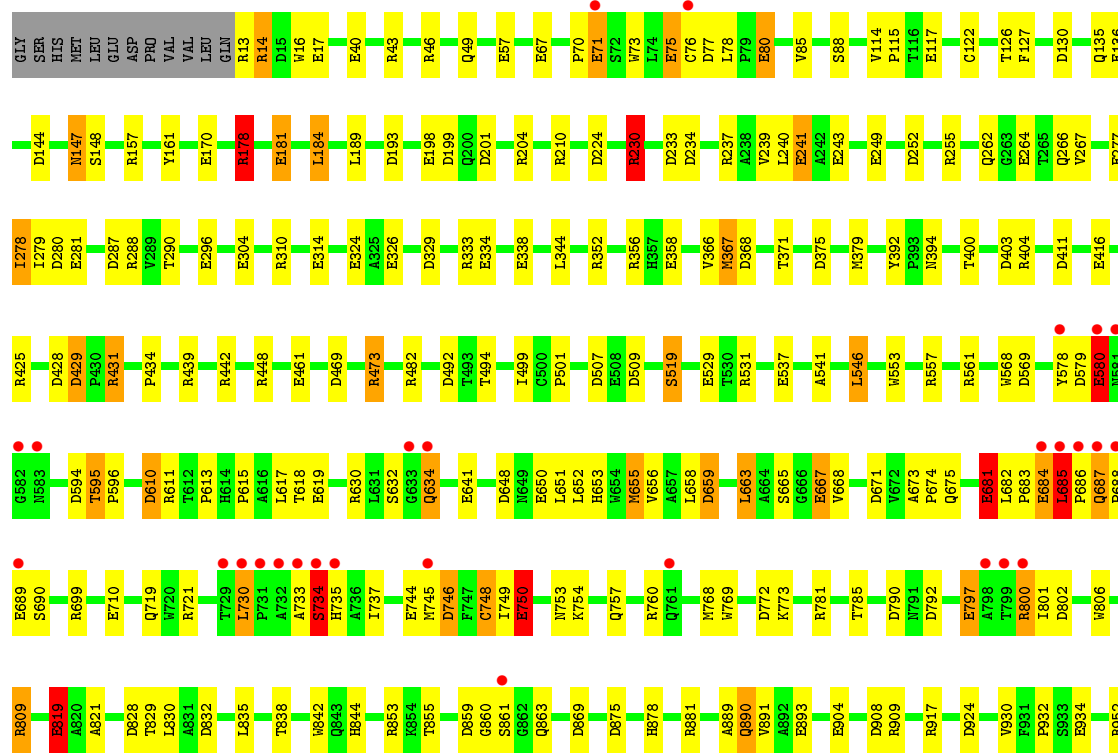


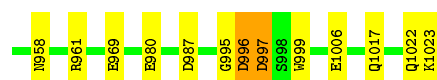
• Molecule 1: BETA-GALACTOSIDASE



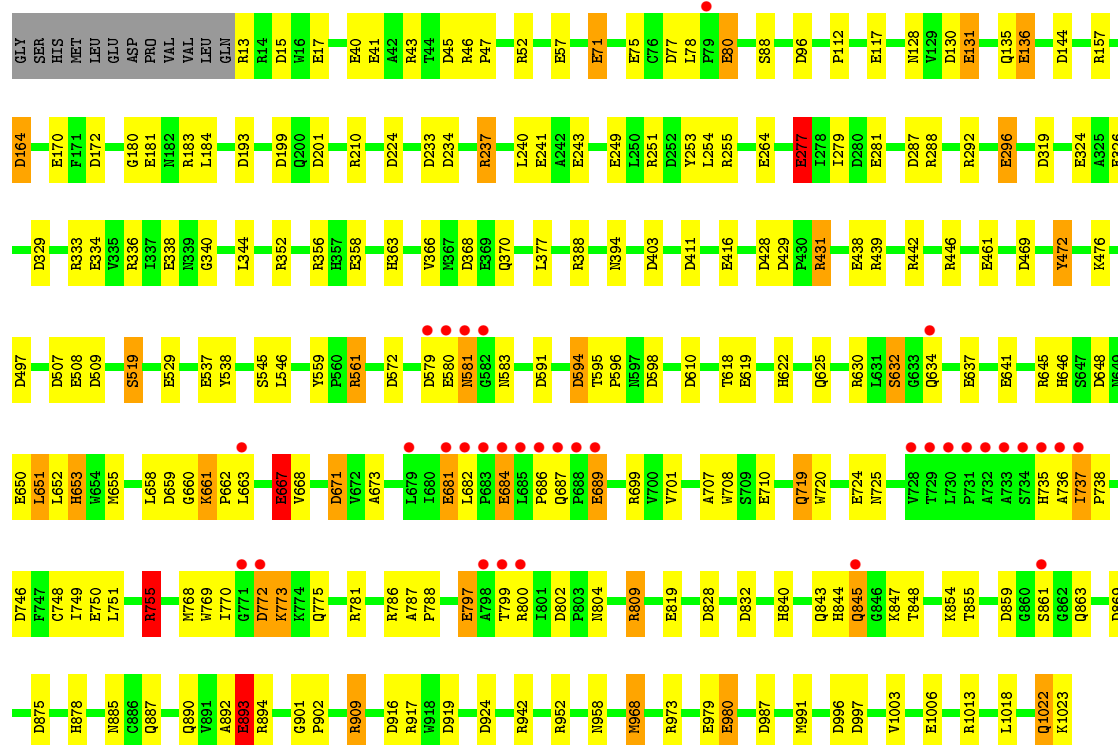
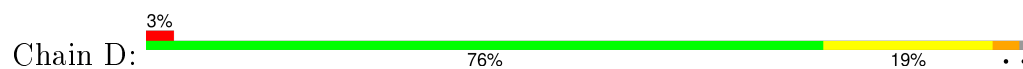


• Molecule 1: BETA-GALACTOSIDASE





• 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	149.60Å 168.38Å 200.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.70 27.49 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (15.00-1.70) 98.6 (27.49-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.70Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.157 , 0.211 0.158 , 0.206	Depositor DCC
R_{free} test set	7905 reflections (1.48%)	DCC
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 90.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 543040 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37408	wwPDB-VP
Average B, all atoms (Å ²)	21.0	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 35.66 % 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 5.6394e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	39/8367 (0.5%)	1.63	166/11415 (1.5%)
1	B	1.15	50/8367 (0.6%)	1.64	163/11415 (1.4%)
1	C	1.14	51/8367 (0.6%)	1.63	150/11415 (1.3%)
1	D	1.17	47/8367 (0.6%)	1.62	163/11415 (1.4%)
All	All	1.15	187/33468 (0.6%)	1.63	642/45660 (1.4%)

All (187) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	11.39	1.38	1.25
1	D	893	GLU	CD-OE2	10.72	1.37	1.25
1	D	277	GLU	CD-OE2	10.36	1.37	1.25
1	C	80	GLU	CD-OE2	9.44	1.36	1.25
1	D	650	GLU	CD-OE2	9.05	1.35	1.25
1	A	296	GLU	CD-OE2	8.88	1.35	1.25
1	D	75	GLU	CD-OE2	8.83	1.35	1.25
1	D	80	GLU	CD-OE2	8.82	1.35	1.25
1	D	684	GLU	CD-OE2	8.13	1.34	1.25
1	D	980	GLU	CD-OE2	8.09	1.34	1.25
1	A	249	GLU	CD-OE2	8.07	1.34	1.25
1	D	979	GLU	CD-OE2	8.04	1.34	1.25
1	A	243	GLU	CD-OE2	7.85	1.34	1.25
1	C	529	GLU	CD-OE2	7.75	1.34	1.25
1	A	1006	GLU	CD-OE2	7.72	1.34	1.25
1	B	650	GLU	CD-OE2	7.71	1.34	1.25
1	D	170	GLU	CD-OE2	7.69	1.34	1.25
1	B	71	GLU	CD-OE2	7.65	1.34	1.25
1	C	684	GLU	CD-OE2	7.65	1.34	1.25
1	C	296	GLU	CD-OE2	7.63	1.34	1.25
1	A	281	GLU	CD-OE2	7.62	1.34	1.25
1	B	281	GLU	CD-OE2	7.62	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	689	GLU	CD-OE2	7.62	1.34	1.25
1	B	819	GLU	CD-OE2	7.60	1.34	1.25
1	B	537	GLU	CD-OE2	7.55	1.33	1.25
1	B	710	GLU	CD-OE2	7.51	1.33	1.25
1	B	529	GLU	CD-OE2	7.51	1.33	1.25
1	A	681	GLU	CD-OE2	7.45	1.33	1.25
1	A	487	GLU	CD-OE2	7.45	1.33	1.25
1	B	684	GLU	CD-OE2	7.42	1.33	1.25
1	A	580	GLU	CD-OE2	7.33	1.33	1.25
1	C	580	GLU	CD-OE2	7.31	1.33	1.25
1	A	277	GLU	CD-OE2	7.31	1.33	1.25
1	D	681	GLU	CD-OE2	7.28	1.33	1.25
1	C	934	GLU	CD-OE2	7.28	1.33	1.25
1	C	819	GLU	CD-OE2	7.28	1.33	1.25
1	C	304	GLU	CD-OE2	7.24	1.33	1.25
1	C	281	GLU	CD-OE2	7.22	1.33	1.25
1	D	580	GLU	CD-OE2	7.19	1.33	1.25
1	D	136	GLU	CD-OE2	7.15	1.33	1.25
1	A	689	GLU	CD-OE2	7.06	1.33	1.25
1	B	487	GLU	CD-OE2	7.05	1.33	1.25
1	B	580	GLU	CD-OE2	7.05	1.33	1.25
1	B	1006	GLU	CD-OE2	7.00	1.33	1.25
1	C	744	GLU	CD-OE2	7.00	1.33	1.25
1	B	689	GLU	CD-OE2	6.99	1.33	1.25
1	C	681	GLU	CD-OE2	6.94	1.33	1.25
1	A	314	GLU	CD-OE1	-6.85	1.18	1.25
1	A	80	GLU	CD-OE2	6.82	1.33	1.25
1	D	243	GLU	CD-OE2	6.82	1.33	1.25
1	C	241	GLU	CD-OE2	6.81	1.33	1.25
1	A	969	GLU	CD-OE2	6.81	1.33	1.25
1	A	980	GLU	CD-OE2	6.80	1.33	1.25
1	A	71	GLU	CD-OE2	6.76	1.33	1.25
1	B	641	GLU	CD-OE1	-6.75	1.18	1.25
1	A	819	GLU	CD-OE2	6.72	1.33	1.25
1	D	797	GLU	CD-OE2	6.70	1.33	1.25
1	D	819	GLU	CD-OE2	6.70	1.33	1.25
1	C	71	GLU	CD-OE2	6.68	1.32	1.25
1	B	264	GLU	CD-OE2	6.67	1.32	1.25
1	B	969	GLU	CD-OE2	6.66	1.32	1.25
1	B	243	GLU	CD-OE2	6.65	1.32	1.25
1	D	17	GLU	CD-OE2	6.64	1.32	1.25
1	C	797	GLU	CD-OE2	6.61	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	75	GLU	CD-OE2	6.57	1.32	1.25
1	B	241	GLU	CD-OE2	6.57	1.32	1.25
1	B	17	GLU	CD-OE2	6.55	1.32	1.25
1	B	667	GLU	CD-OE2	6.55	1.32	1.25
1	B	181	GLU	CD-OE2	6.54	1.32	1.25
1	C	893	GLU	CD-OE2	6.54	1.32	1.25
1	C	641	GLU	CD-OE1	-6.50	1.18	1.25
1	C	416	GLU	CD-OE2	6.48	1.32	1.25
1	B	277	GLU	CD-OE2	6.40	1.32	1.25
1	C	277	GLU	CD-OE2	6.40	1.32	1.25
1	A	637	GLU	CD-OE2	6.39	1.32	1.25
1	D	249	GLU	CD-OE2	6.35	1.32	1.25
1	B	296	GLU	CD-OE2	6.35	1.32	1.25
1	B	744	GLU	CD-OE2	6.34	1.32	1.25
1	D	281	GLU	CD-OE2	6.32	1.32	1.25
1	C	324	GLU	CD-OE2	6.32	1.32	1.25
1	B	461	GLU	CD-OE2	6.30	1.32	1.25
1	C	358	GLU	CD-OE2	6.30	1.32	1.25
1	C	980	GLU	CD-OE2	6.29	1.32	1.25
1	A	131	GLU	CD-OE2	6.27	1.32	1.25
1	B	304	GLU	CD-OE2	6.27	1.32	1.25
1	B	893	GLU	CD-OE2	6.27	1.32	1.25
1	C	338	GLU	CD-OE2	6.27	1.32	1.25
1	A	170	GLU	CD-OE2	6.22	1.32	1.25
1	B	980	GLU	CD-OE2	6.21	1.32	1.25
1	A	438	GLU	CD-OE2	6.19	1.32	1.25
1	C	667	GLU	CD-OE2	6.19	1.32	1.25
1	C	67	GLU	CD-OE2	6.17	1.32	1.25
1	A	650	GLU	CD-OE2	6.17	1.32	1.25
1	A	117	GLU	CD-OE2	6.15	1.32	1.25
1	B	80	GLU	CD-OE2	6.14	1.32	1.25
1	C	689	GLU	CD-OE2	6.14	1.32	1.25
1	C	710	GLU	CD-OE2	6.14	1.32	1.25
1	D	750	GLU	CD-OE2	6.14	1.32	1.25
1	C	170	GLU	CD-OE2	6.12	1.32	1.25
1	D	529	GLU	CD-OE2	6.11	1.32	1.25
1	C	619	GLU	CD-OE2	6.09	1.32	1.25
1	D	264	GLU	CD-OE2	6.09	1.32	1.25
1	A	979	GLU	CD-OE2	6.08	1.32	1.25
1	C	334	GLU	CD-OE2	6.08	1.32	1.25
1	C	1006	GLU	CD-OE2	6.07	1.32	1.25
1	A	529	GLU	CD-OE2	6.07	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	264	GLU	CD-OE2	6.04	1.32	1.25
1	D	619	GLU	CD-OE2	6.03	1.32	1.25
1	A	943	GLU	CD-OE2	6.03	1.32	1.25
1	A	893	GLU	CD-OE2	6.01	1.32	1.25
1	B	724	GLU	CD-OE2	6.00	1.32	1.25
1	A	641	GLU	CD-OE1	-6.00	1.19	1.25
1	B	358	GLU	CD-OE2	6.00	1.32	1.25
1	D	667	GLU	CD-OE2	6.00	1.32	1.25
1	C	136	GLU	CD-OE2	5.97	1.32	1.25
1	B	117	GLU	CD-OE2	5.96	1.32	1.25
1	C	969	GLU	CD-OE2	5.95	1.32	1.25
1	D	117	GLU	CD-OE2	5.93	1.32	1.25
1	C	243	GLU	CD-OE1	-5.91	1.19	1.25
1	D	241	GLU	CD-OE2	5.90	1.32	1.25
1	C	461	GLU	CD-OE2	5.88	1.32	1.25
1	D	637	GLU	CD-OE2	5.85	1.32	1.25
1	D	334	GLU	CD-OE2	5.85	1.32	1.25
1	B	871	GLU	CD-OE2	5.84	1.32	1.25
1	D	710	GLU	CD-OE2	5.82	1.32	1.25
1	D	296	GLU	CD-OE2	5.81	1.32	1.25
1	B	461	GLU	CD-OE1	-5.79	1.19	1.25
1	A	710	GLU	CD-OE2	5.76	1.31	1.25
1	D	40	GLU	CD-OE2	5.76	1.31	1.25
1	B	75	GLU	CD-OE2	5.76	1.31	1.25
1	B	131	GLU	CD-OE2	5.76	1.31	1.25
1	D	461	GLU	CD-OE2	5.76	1.31	1.25
1	C	314	GLU	CD-OE1	-5.75	1.19	1.25
1	D	438	GLU	CD-OE2	5.74	1.31	1.25
1	D	181	GLU	CD-OE2	5.73	1.31	1.25
1	C	750	GLU	CD-OE2	5.69	1.31	1.25
1	B	249	GLU	CD-OE2	5.69	1.31	1.25
1	B	57	GLU	CD-OE2	5.68	1.31	1.25
1	A	57	GLU	CD-OE2	5.67	1.31	1.25
1	C	198	GLU	CD-OE2	5.63	1.31	1.25
1	D	641	GLU	CD-OE2	5.63	1.31	1.25
1	B	750	GLU	CD-OE1	-5.62	1.19	1.25
1	A	667	GLU	CD-OE2	5.60	1.31	1.25
1	B	170	GLU	CD-OE2	5.58	1.31	1.25
1	D	1006	GLU	CD-OE2	5.56	1.31	1.25
1	B	369	GLU	CD-OE2	5.56	1.31	1.25
1	A	75	GLU	CD-OE2	5.55	1.31	1.25
1	A	750	GLU	CD-OE2	5.54	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	508	GLU	CD-OE2	5.54	1.31	1.25
1	A	136	GLU	CD-OE2	5.51	1.31	1.25
1	B	314	GLU	CD-OE1	-5.50	1.19	1.25
1	D	358	GLU	CD-OE2	5.50	1.31	1.25
1	B	326	GLU	CD-OE2	5.49	1.31	1.25
1	C	537	GLU	CD-OE2	5.48	1.31	1.25
1	A	461	GLU	CD-OE2	5.47	1.31	1.25
1	C	809	ARG	NE-CZ	5.45	1.40	1.33
1	C	40	GLU	CD-OE2	5.45	1.31	1.25
1	C	482	ARG	CZ-NH1	5.44	1.40	1.33
1	C	326	GLU	CD-OE2	5.42	1.31	1.25
1	D	338	GLU	CD-OE2	5.40	1.31	1.25
1	C	249	GLU	CD-OE2	5.39	1.31	1.25
1	D	131	GLU	CD-OE2	5.39	1.31	1.25
1	C	181	GLU	CD-OE2	5.38	1.31	1.25
1	D	41	GLU	CD-OE1	-5.38	1.19	1.25
1	C	117	GLU	CD-OE2	5.37	1.31	1.25
1	B	412	GLU	CD-OE2	5.35	1.31	1.25
1	B	324	GLU	CD-OE2	5.33	1.31	1.25
1	C	650	GLU	CD-OE2	5.25	1.31	1.25
1	A	442	ARG	CZ-NH1	5.25	1.39	1.33
1	D	537	GLU	CD-OE2	5.21	1.31	1.25
1	B	41	GLU	CD-OE2	5.21	1.31	1.25
1	D	57	GLU	CD-OE1	-5.19	1.20	1.25
1	B	681	GLU	CD-OE2	5.18	1.31	1.25
1	C	904	GLU	CD-OE2	5.17	1.31	1.25
1	A	537	GLU	CD-OE2	5.17	1.31	1.25
1	C	264	GLU	CD-OE2	5.16	1.31	1.25
1	C	17	GLU	CD-OE2	5.12	1.31	1.25
1	A	461	GLU	CD-OE1	-5.12	1.20	1.25
1	C	57	GLU	CD-OE2	5.09	1.31	1.25
1	D	41	GLU	CD-OE2	5.07	1.31	1.25
1	A	338	GLU	CD-OE2	5.06	1.31	1.25
1	D	724	GLU	CD-OE2	5.06	1.31	1.25
1	B	40	GLU	CD-OE2	5.05	1.31	1.25
1	B	67	GLU	CD-OE1	-5.03	1.20	1.25
1	B	136	GLU	CD-OE2	5.03	1.31	1.25
1	B	243	GLU	CD-OE1	-5.02	1.20	1.25
1	D	326	GLU	CD-OE2	5.01	1.31	1.25

All (642) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	NE-CZ-NH1	28.53	134.56	120.30
1	B	699	ARG	NE-CZ-NH1	17.58	129.09	120.30
1	D	781	ARG	NE-CZ-NH1	16.66	128.63	120.30
1	B	699	ARG	NE-CZ-NH2	-16.65	111.97	120.30
1	C	442	ARG	NE-CZ-NH2	-16.61	112.00	120.30
1	D	172	ASP	CB-CG-OD2	-14.03	105.67	118.30
1	D	439	ARG	NE-CZ-NH2	-13.80	113.40	120.30
1	D	431	ARG	NE-CZ-NH2	-13.66	113.47	120.30
1	B	442	ARG	NE-CZ-NH1	13.16	126.88	120.30
1	A	431	ARG	NE-CZ-NH2	-13.06	113.77	120.30
1	B	442	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	234	ASP	CB-CG-OD2	-12.33	107.20	118.30
1	A	442	ARG	NE-CZ-NH2	-11.71	114.45	120.30
1	C	199	ASP	CB-CG-OD1	11.65	128.79	118.30
1	A	166	ARG	NE-CZ-NH2	-11.60	114.50	120.30
1	A	224	ASP	CB-CG-OD1	11.39	128.55	118.30
1	C	809	ARG	NE-CZ-NH2	-11.38	114.61	120.30
1	C	233	ASP	CB-CG-OD1	11.17	128.35	118.30
1	A	599	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	A	610	ASP	CB-CG-OD1	11.06	128.25	118.30
1	B	853	ARG	NE-CZ-NH1	11.04	125.82	120.30
1	D	429	ASP	CB-CG-OD2	-11.01	108.39	118.30
1	A	388	ARG	NE-CZ-NH2	-10.88	114.86	120.30
1	A	755	ARG	NE-CZ-NH1	10.84	125.72	120.30
1	B	252	ASP	CB-CG-OD2	-10.66	108.71	118.30
1	D	859	ASP	CB-CG-OD2	-10.64	108.72	118.30
1	A	442	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	C	224	ASP	CB-CG-OD1	10.47	127.73	118.30
1	D	224	ASP	CB-CG-OD1	10.45	127.70	118.30
1	C	473	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	B	336	ARG	NE-CZ-NH1	10.41	125.50	120.30
1	A	336	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	997	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	B	648	ASP	CB-CG-OD2	-10.32	109.01	118.30
1	C	43	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	D	439	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	A	234	ASP	CB-CG-OD1	10.22	127.50	118.30
1	D	446	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	D	429	ASP	CB-CG-OD1	10.20	127.48	118.30
1	A	233	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	B	368	ASP	CB-CG-OD1	10.06	127.35	118.30
1	C	425	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	A	659	ASP	CB-CG-OD2	-9.82	109.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	442	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	C	178	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	B	611	ARG	NE-CZ-NH1	9.62	125.11	120.30
1	B	671	ASP	CB-CG-OD2	-9.57	109.69	118.30
1	B	557	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	B	469	ASP	CB-CG-OD1	9.55	126.90	118.30
1	C	230	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	D	561	ARG	NE-CZ-NH2	-9.45	115.57	120.30
1	D	561	ARG	NE-CZ-NH1	9.37	124.99	120.30
1	B	557	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	B	505	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	B	233	ASP	CB-CG-OD1	9.32	126.69	118.30
1	D	859	ASP	CB-CG-OD1	9.30	126.67	118.30
1	A	233	ASP	CB-CG-OD1	9.28	126.65	118.30
1	C	659	ASP	CB-CG-OD2	-9.21	110.01	118.30
1	D	699	ARG	NE-CZ-NH1	9.18	124.89	120.30
1	D	388	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	C	721	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	C	659	ASP	CB-CG-OD1	9.13	126.51	118.30
1	B	13	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	A	255	ARG	NE-CZ-NH1	9.07	124.84	120.30
1	C	579	ASP	CB-CG-OD2	-9.03	110.17	118.30
1	B	45	ASP	CB-CG-OD1	9.00	126.40	118.30
1	D	446	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	D	172	ASP	CB-CG-OD1	8.90	126.31	118.30
1	A	987	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	B	368	ASP	CB-CG-OD2	-8.89	110.30	118.30
1	C	809	ARG	CD-NE-CZ	8.87	136.02	123.60
1	A	144	ASP	CB-CG-OD1	8.86	126.28	118.30
1	B	996	ASP	CB-CG-OD1	8.83	126.25	118.30
1	A	431	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	C	909	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	B	319	ASP	CB-CG-OD1	8.81	126.23	118.30
1	C	233	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	C	875	ASP	CB-CG-OD1	8.80	126.22	118.30
1	B	594	ASP	CB-CG-OD2	-8.80	110.38	118.30
1	A	130	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	B	26	ARG	NE-CZ-NH1	-8.76	115.92	120.30
1	B	832	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	B	802	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	648	ASP	CB-CG-OD1	8.68	126.11	118.30
1	C	869	ASP	CB-CG-OD1	8.68	126.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	ASP	CB-CG-OD1	8.65	126.08	118.30
1	D	996	ASP	CB-CG-OD2	-8.63	110.53	118.30
1	A	594	ASP	CB-CG-OD1	8.62	126.06	118.30
1	B	772	ASP	CB-CG-OD2	-8.61	110.55	118.30
1	B	428	ASP	CB-CG-OD1	8.60	126.03	118.30
1	B	869	ASP	CB-CG-OD1	8.56	126.00	118.30
1	D	579	ASP	CB-CG-OD2	-8.54	110.61	118.30
1	B	853	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	492	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	D	469	ASP	CB-CG-OD1	8.49	125.94	118.30
1	B	473	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	B	594	ASP	CB-CG-OD1	8.46	125.92	118.30
1	B	166	ARG	NE-CZ-NH2	-8.45	116.07	120.30
1	D	746	ASP	CB-CG-OD1	8.44	125.90	118.30
1	B	388	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	C	473	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	A	14	ARG	NE-CZ-NH1	-8.34	116.13	120.30
1	D	800	ARG	NE-CZ-NH1	8.32	124.46	120.30
1	D	403	ASP	CB-CG-OD1	8.26	125.74	118.30
1	A	356	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	A	859	ASP	CB-CG-OD2	-8.25	110.88	118.30
1	D	255	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	509	ASP	CB-CG-OD1	8.23	125.71	118.30
1	D	630	ARG	NE-CZ-NH2	-8.23	116.18	120.30
1	C	996	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	439	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	634	GLN	N-CA-CB	8.20	125.36	110.60
1	A	800	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	D	802	ASP	CB-CG-OD2	-8.20	110.92	118.30
1	D	630	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	875	ASP	CB-CG-OD1	8.17	125.65	118.30
1	D	287	ASP	CB-CG-OD1	8.16	125.64	118.30
1	B	671	ASP	CB-CG-OD1	8.15	125.63	118.30
1	A	428	ASP	CB-CG-OD1	8.13	125.61	118.30
1	C	561	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	746	ASP	CB-CG-OD2	-8.10	111.01	118.30
1	D	193	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	A	292	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	828	ASP	CB-CG-OD2	-8.06	111.04	118.30
1	B	832	ASP	CB-CG-OD1	8.06	125.56	118.30
1	D	234	ASP	CB-CG-OD2	-8.03	111.08	118.30
1	A	210	ARG	NE-CZ-NH2	-8.03	116.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	446	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	D	15	ASP	CB-CG-OD2	-7.97	111.13	118.30
1	D	996	ASP	CB-CG-OD1	7.95	125.45	118.30
1	B	579	ASP	CB-CG-OD1	7.93	125.44	118.30
1	D	368	ASP	CB-CG-OD2	-7.93	111.16	118.30
1	B	319	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	439	ARG	NE-CZ-NH2	-7.91	116.35	120.30
1	C	448	ARG	NE-CZ-NH2	-7.89	116.36	120.30
1	A	987	ASP	CB-CG-OD1	7.86	125.38	118.30
1	B	996	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	C	809	ARG	NH1-CZ-NH2	-7.81	110.81	119.40
1	D	987	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	610	ASP	CB-CG-OD2	-7.79	111.28	118.30
1	D	828	ASP	CB-CG-OD2	-7.77	111.31	118.30
1	D	659	ASP	CB-CG-OD1	7.77	125.29	118.30
1	C	961	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	D	952	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	52	ARG	NE-CZ-NH1	7.73	124.16	120.30
1	B	1018	LEU	CB-CA-C	-7.72	95.52	110.20
1	C	802	ASP	CB-CG-OD1	7.72	125.25	118.30
1	D	659	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	C	368	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	C	255	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	D	699	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	997	ASP	CB-CG-OD1	7.66	125.19	118.30
1	A	178	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	172	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	A	917	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	D	559	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	D	288	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	469	ASP	CB-CG-OD2	-7.55	111.50	118.30
1	A	288	ARG	NE-CZ-NH2	-7.55	116.53	120.30
1	B	356	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	D	45	ASP	CB-CG-OD1	7.52	125.07	118.30
1	D	193	ASP	CB-CG-OD1	7.52	125.06	118.30
1	A	816	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	B	288	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	610	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	D	832	ASP	CB-CG-OD2	-7.47	111.57	118.30
1	A	447	ASP	CB-CG-OD1	7.46	125.01	118.30
1	D	144	ASP	CB-CG-OD1	7.45	125.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	448	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	288	ARG	NE-CZ-NH2	-7.43	116.59	120.30
1	A	356	ARG	NE-CZ-NH2	-7.41	116.59	120.30
1	D	469	ASP	CB-CG-OD2	-7.41	111.63	118.30
1	A	924	ASP	CB-CG-OD1	7.40	124.96	118.30
1	D	781	ARG	CD-NE-CZ	7.40	133.96	123.60
1	B	859	ASP	CB-CG-OD2	-7.38	111.65	118.30
1	C	828	ASP	CB-CG-OD2	-7.36	111.68	118.30
1	C	204	ARG	NE-CZ-NH1	7.35	123.98	120.30
1	D	772	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	917	ARG	NE-CZ-NH2	7.35	123.97	120.30
1	A	251	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	C	234	ASP	CB-CG-OD1	7.34	124.91	118.30
1	D	632	SER	N-CA-CB	7.34	121.51	110.50
1	D	403	ASP	CB-CG-OD2	-7.33	111.70	118.30
1	D	802	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	916	ASP	CB-CG-OD1	7.31	124.88	118.30
1	A	469	ASP	CB-CG-OD1	7.28	124.85	118.30
1	C	579	ASP	CB-CG-OD1	7.28	124.85	118.30
1	D	157	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	B	599	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	B	224	ASP	CB-CG-OD1	7.24	124.81	118.30
1	C	648	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	D	356	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	A	172	ASP	CB-CG-OD1	7.21	124.79	118.30
1	B	144	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	431	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	204	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	431	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	C	610	ASP	CB-CG-OD1	7.16	124.74	118.30
1	B	356	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	559	TYR	CB-CG-CD2	-7.13	116.72	121.00
1	A	285	TYR	CD1-CE1-CZ	-7.12	113.39	119.80
1	A	857	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	869	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	648	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	630	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	B	792	ASP	CB-CG-OD1	7.11	124.69	118.30
1	D	591	ASP	CB-CG-OD1	7.11	124.69	118.30
1	B	45	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	352	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	D	472	TYR	CB-CG-CD2	-7.10	116.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	610	ASP	CB-CG-OD2	-7.08	111.92	118.30
1	B	77	ASP	CB-CG-OD1	7.08	124.67	118.30
1	D	352	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	B	172	ASP	CB-CG-OD1	7.07	124.66	118.30
1	B	919	ASP	CB-CG-OD1	7.07	124.66	118.30
1	C	144	ASP	CB-CG-OD1	7.07	124.66	118.30
1	D	610	ASP	CB-CG-OD1	7.06	124.65	118.30
1	B	958	ASN	N-CA-CB	7.06	123.30	110.60
1	C	429	ASP	CB-CG-OD1	7.05	124.64	118.30
1	D	594	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	411	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	126	THR	CA-CB-CG2	-7.04	102.55	112.40
1	C	890	GLN	N-CA-CB	-7.02	97.96	110.60
1	A	719	GLN	CB-CA-C	-7.01	96.38	110.40
1	A	755	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	A	166	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	B	237	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	B	579	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	336	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	632	SER	N-CA-CB	6.97	120.95	110.50
1	B	952	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	95	TYR	CB-CG-CD1	-6.95	116.83	121.00
1	B	193	ASP	CB-CG-OD1	6.95	124.55	118.30
1	C	859	ASP	CB-CG-OD1	6.93	124.54	118.30
1	D	579	ASP	CB-CG-OD1	6.93	124.53	118.30
1	B	77	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	292	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	B	429	ASP	CB-CG-OD2	-6.90	112.09	118.30
1	B	505	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	D	869	ASP	CB-CG-OD1	6.89	124.50	118.30
1	D	909	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	329	ASP	CB-CG-OD1	6.88	124.49	118.30
1	B	425	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	D	428	ASP	CB-CG-OD1	6.86	124.47	118.30
1	C	924	ASP	CB-CG-OD1	6.85	124.47	118.30
1	B	439	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	B	572	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	561	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	201	ASP	CB-CG-OD2	-6.84	112.14	118.30
1	A	1021	CYS	CA-CB-SG	-6.83	101.72	114.00
1	B	828	ASP	CB-CG-OD2	-6.82	112.16	118.30
1	B	659	ASP	CB-CG-OD1	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	786	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	645	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	A	952	ARG	NE-CZ-NH1	6.81	123.71	120.30
1	C	509	ASP	CB-CG-OD1	6.80	124.42	118.30
1	C	917	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	C	429	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	164	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	201	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	B	507	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	D	251	ARG	CD-NE-CZ	6.77	133.07	123.60
1	C	43	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	919	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	A	832	ASP	N-CA-CB	-6.75	98.46	110.60
1	D	572	ASP	CB-CG-OD1	6.75	124.37	118.30
1	A	310	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	363	HIS	CA-CB-CG	-6.73	102.17	113.60
1	D	919	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	659	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	909	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	C	404	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	477	SER	N-CA-CB	6.71	120.56	110.50
1	B	287	ASP	CB-CG-OD1	6.70	124.33	118.30
1	C	772	ASP	CB-CG-OD2	-6.70	112.28	118.30
1	D	319	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	859	ASP	CB-CG-OD2	-6.68	112.28	118.30
1	B	828	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	721	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	85	VAL	CA-CB-CG2	-6.67	100.89	110.90
1	A	869	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	287	ASP	CB-CG-OD1	6.66	124.30	118.30
1	B	507	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	611	ARG	NE-CZ-NH2	-6.64	116.98	120.30
1	A	130	ASP	CB-CG-OD1	6.64	124.27	118.30
1	A	224	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	D	329	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	A	509	ASP	CB-CG-OD2	-6.62	112.34	118.30
1	D	924	ASP	CB-CG-OD1	6.62	124.26	118.30
1	D	13	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	B	961	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	80	GLU	OE1-CD-OE2	6.60	131.22	123.30
1	A	572	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	B	632	SER	N-CA-CB	6.60	120.40	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	869	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	201	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	559	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	A	741	THR	CA-CB-CG2	-6.59	103.18	112.40
1	A	659	ASP	CB-CG-OD1	6.58	124.22	118.30
1	A	507	ASP	CB-CG-OD1	6.58	124.22	118.30
1	B	610	ASP	CB-CG-OD1	6.55	124.20	118.30
1	A	247	CYS	CA-CB-SG	-6.53	102.25	114.00
1	C	924	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	B	43	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	230	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	B	598	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	802	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	859	ASP	CB-CG-OD1	6.48	124.14	118.30
1	C	280	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	908	ASP	CB-CG-OD1	6.47	124.12	118.30
1	D	980	GLU	C-N-CA	-6.46	108.72	122.30
1	A	746	ASP	CB-CG-OD1	6.46	124.11	118.30
1	C	961	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	B	721	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	809	ARG	NE-CZ-NH2	6.45	123.52	120.30
1	A	689	GLU	CB-CA-C	6.44	123.29	110.40
1	D	572	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	D	755	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	A	201	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	917	ARG	CD-NE-CZ	-6.37	114.68	123.60
1	D	507	ASP	CB-CG-OD2	-6.37	112.56	118.30
1	A	792	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	368	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	388	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	782	ASP	CB-CG-OD2	-6.34	112.60	118.30
1	A	82	ASP	CB-CG-OD1	6.33	124.00	118.30
1	B	233	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	D	671	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	356	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	919	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	211	ASP	CB-CG-OD1	6.32	123.98	118.30
1	D	130	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	D	411	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	C	46	ARG	NE-CZ-NH1	-6.31	117.15	120.30
1	A	46	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	439	ARG	NE-CZ-NH2	-6.28	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	ILE	CA-CB-CG1	-6.28	99.07	111.00
1	B	942	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	648	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	924	ASP	CB-CG-OD2	-6.27	112.66	118.30
1	A	630	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	B	411	ASP	CB-CG-OD1	6.27	123.94	118.30
1	A	403	ASP	CB-CG-OD1	6.27	123.94	118.30
1	D	942	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	287	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	B	230	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	746	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	C	733	ALA	N-CA-CB	6.24	118.84	110.10
1	C	746	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	1019	VAL	CA-CB-CG2	-6.22	101.56	110.90
1	D	594	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	234	ASP	CB-CG-OD1	6.22	123.90	118.30
1	D	845	GLN	C-N-CA	-6.18	109.31	122.30
1	C	748	CYS	CA-CB-SG	-6.18	102.87	114.00
1	B	809	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	D	411	ASP	CB-CG-OD1	6.17	123.85	118.30
1	D	509	ASP	CB-CG-OD1	6.17	123.85	118.30
1	C	494	THR	CA-CB-CG2	-6.14	103.80	112.40
1	D	781	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	828	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	375	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	772	ASP	CB-CG-OD1	6.13	123.82	118.30
1	C	136	GLU	CB-CA-C	-6.13	98.14	110.40
1	A	479	ASP	CB-CG-OD1	6.12	123.80	118.30
1	C	77	ASP	CB-CG-OD1	6.11	123.80	118.30
1	C	199	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	310	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	A	857	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	C	76	CYS	N-CA-CB	-6.08	99.66	110.60
1	B	59	ARG	NE-CZ-NH1	-6.07	117.27	120.30
1	B	492	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	C	958	ASN	N-CA-CB	6.06	121.51	110.60
1	B	367	MET	CG-SD-CE	6.06	109.89	100.20
1	C	428	ASP	CB-CG-OD1	6.06	123.75	118.30
1	D	719	GLN	CB-CA-C	-6.06	98.29	110.40
1	C	201	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	507	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	D	917	ARG	CD-NE-CZ	-6.05	115.13	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	288	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	B	431	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	B	559	TYR	CD1-CE1-CZ	-6.02	114.38	119.80
1	A	630	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	671	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	792	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	D	15	ASP	CB-CG-OD1	6.01	123.71	118.30
1	B	157	ARG	NE-CZ-NH2	6.00	123.30	120.30
1	A	230	ARG	NE-CZ-NH2	-5.99	117.30	120.30
1	D	255	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	787	ALA	N-CA-CB	-5.99	101.72	110.10
1	D	997	ASP	N-CA-CB	5.98	121.37	110.60
1	A	594	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	553	TRP	CA-CB-CG	-5.97	102.35	113.70
1	A	614	HIS	CA-CB-CG	5.97	123.75	113.60
1	D	96	ASP	N-CA-CB	5.97	121.35	110.60
1	B	429	ASP	CB-CG-OD1	5.96	123.67	118.30
1	D	809	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	D	832	ASP	CB-CG-OD1	5.95	123.66	118.30
1	D	52	ARG	CB-CA-C	-5.95	98.50	110.40
1	C	80	GLU	CG-CD-OE2	-5.95	106.40	118.30
1	C	996	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	C	130	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	80	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	C	288	ARG	NE-CZ-NH1	5.92	123.26	120.30
1	D	800	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	908	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	425	ARG	NE-CZ-NH2	-5.89	117.36	120.30
1	C	821	ALA	N-CA-CB	5.89	118.35	110.10
1	C	671	ASP	CB-CG-OD1	5.88	123.59	118.30
1	C	531	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	553	TRP	CA-CB-CG	-5.87	102.55	113.70
1	C	809	ARG	CG-CD-NE	5.85	124.08	111.80
1	A	938	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	B	147	ASN	N-CA-CB	-5.84	100.09	110.60
1	D	1018	LEU	CB-CA-C	-5.84	99.11	110.20
1	C	719	GLN	CB-CA-C	-5.83	98.73	110.40
1	D	1013	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	B	96	ASP	CB-CG-OD2	-5.82	113.06	118.30
1	C	439	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	986	ILE	CB-CG1-CD1	-5.81	97.64	113.90
1	D	497	ASP	CB-CG-OD1	5.81	123.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	630	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	842	TRP	CA-CB-CG	-5.80	102.67	113.70
1	A	782	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	404	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	D	13	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	96	ASP	N-CA-CB	5.80	121.04	110.60
1	B	800	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	572	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	519	SER	N-CA-CB	-5.79	101.82	110.50
1	D	671	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	96	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	771	GLY	C-N-CA	-5.77	107.27	121.70
1	C	541	ALA	N-CA-CB	-5.77	102.02	110.10
1	D	598	ASP	CB-CG-OD1	5.77	123.49	118.30
1	B	105	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	C	280	ASP	CB-CG-OD1	5.76	123.49	118.30
1	B	723	ALA	CB-CA-C	-5.76	101.47	110.10
1	C	557	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	431	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	842	TRP	CA-CB-CG	-5.73	102.82	113.70
1	C	889	ALA	N-CA-CB	-5.72	102.08	110.10
1	A	13	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	D	324	GLU	N-CA-CB	5.71	120.87	110.60
1	B	492	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	329	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	A	429	ASP	CB-CG-OD1	5.68	123.41	118.30
1	A	438	GLU	CG-CD-OE2	-5.67	106.95	118.30
1	A	546	LEU	N-CA-CB	5.67	121.74	110.40
1	B	875	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	D	210	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	287	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	A	954	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	C	828	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	416	GLU	CG-CD-OE1	5.62	129.54	118.30
1	A	771	GLY	N-CA-C	-5.62	99.06	113.10
1	B	997	ASP	N-CA-CB	5.62	120.71	110.60
1	D	251	ARG	CG-CD-NE	-5.61	100.02	111.80
1	A	440	VAL	CA-CB-CG2	-5.61	102.48	110.90
1	D	183	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	721	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	890	GLN	N-CA-CB	-5.60	100.52	110.60
1	D	869	ASP	CB-CG-OD2	-5.59	113.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	968	MET	CG-SD-CE	5.59	109.15	100.20
1	A	832	ASP	CB-CG-OD1	5.58	123.32	118.30
1	A	634	GLN	CB-CA-C	5.58	121.55	110.40
1	A	329	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	A	670	LEU	CB-CG-CD1	-5.56	101.55	111.00
1	B	832	ASP	N-CA-CB	-5.56	100.59	110.60
1	B	546	LEU	N-CA-CB	5.56	121.52	110.40
1	A	773	LYS	CB-CA-C	-5.55	99.30	110.40
1	C	746	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	B	746	ASP	CB-CA-C	-5.54	99.32	110.40
1	B	411	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	C	252	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	A	946	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	997	ASP	N-CA-CB	5.53	120.56	110.60
1	C	403	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	D	786	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	D	673	ALA	N-CA-CB	-5.52	102.37	110.10
1	A	469	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	699	ARG	CD-NE-CZ	5.51	131.31	123.60
1	C	578	TYR	CB-CG-CD1	-5.51	117.70	121.00
1	B	144	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	748	CYS	CA-CB-SG	-5.50	104.09	114.00
1	C	277	GLU	CA-CB-CG	-5.50	101.30	113.40
1	D	253	TYR	CB-CG-CD1	-5.50	117.70	121.00
1	C	546	LEU	N-CA-CB	5.50	121.39	110.40
1	D	987	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	252	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	909	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	568	TRP	CA-CB-CG	-5.48	103.28	113.70
1	D	917	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	A	996	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	591	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	C	147	ASN	N-CA-CB	-5.47	100.75	110.60
1	D	329	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	569	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	C	287	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	118	ASN	N-CA-CB	-5.44	100.80	110.60
1	C	210	ARG	N-CA-CB	5.44	120.39	110.60
1	C	699	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	C	875	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	A	164	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	255	ARG	NE-CZ-NH2	-5.43	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1018	LEU	CB-CG-CD2	-5.43	101.77	111.00
1	C	14	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	B	924	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	403	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	B	482	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	B	681	GLU	CB-CG-CD	-5.41	99.60	114.20
1	C	519	SER	N-CA-CB	-5.40	102.39	110.50
1	A	699	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	A	817	GLN	CB-CG-CD	-5.39	97.58	111.60
1	B	185	ALA	N-CA-CB	5.39	117.65	110.10
1	B	329	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	87	PRO	CA-N-CD	5.38	119.23	111.70
1	D	144	ASP	CB-CG-OD2	-5.38	113.46	118.30
1	C	344	LEU	CB-CG-CD2	5.38	120.14	111.00
1	C	768	MET	N-CA-CB	5.37	120.27	110.60
1	A	1018	LEU	CB-CA-C	-5.37	100.00	110.20
1	B	509	ASP	CB-CG-OD1	5.37	123.13	118.30
1	B	287	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	D	844	HIS	CA-CB-CG	-5.36	104.49	113.60
1	D	130	ASP	CB-CG-OD1	5.35	123.12	118.30
1	C	1017	GLN	CA-CB-CG	5.35	125.17	113.40
1	A	579	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	652	LEU	CB-CG-CD1	-5.34	101.92	111.00
1	C	403	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	234	ASP	CB-CG-OD2	-5.33	113.50	118.30
1	C	431	ARG	CA-CB-CG	-5.33	101.68	113.40
1	D	538	TYR	CB-CG-CD2	5.33	124.20	121.00
1	C	632	SER	N-CA-CB	5.33	118.49	110.50
1	C	594	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	952	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	D	43	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	C	630	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	D	653	HIS	N-CA-CB	5.32	120.17	110.60
1	D	958	ASN	N-CA-CB	5.31	120.16	110.60
1	C	790	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	519	SER	N-CA-CB	-5.30	102.55	110.50
1	C	371	THR	CA-CB-CG2	-5.30	104.98	112.40
1	B	447	ASP	CB-CG-OD1	5.30	123.07	118.30
1	C	802	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	D	472	TYR	CB-CG-CD1	5.29	124.17	121.00
1	A	772	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	D	319	ASP	CB-CG-OD2	-5.28	113.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	893	GLU	CB-CG-CD	5.27	128.44	114.20
1	C	193	ASP	CB-CG-OD1	5.27	123.05	118.30
1	C	267	VAL	CA-CB-CG2	-5.27	103.00	110.90
1	C	648	ASP	CB-CG-OD1	5.27	123.04	118.30
1	D	855	THR	N-CA-CB	5.27	120.31	110.30
1	D	164	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	838	THR	CA-CB-CG2	-5.26	105.04	112.40
1	D	233	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	144	ASP	CB-CG-OD2	-5.25	113.58	118.30
1	B	166	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	786	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	D	77	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	854	LYS	CB-CA-C	-5.24	99.91	110.40
1	B	399	TYR	CB-CG-CD1	-5.24	117.86	121.00
1	B	190	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	C	469	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	280	ASP	CB-CG-OD1	5.23	123.01	118.30
1	D	507	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	193	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	D	787	ALA	N-CA-CB	-5.22	102.79	110.10
1	A	591	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	507	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	854	LYS	CB-CA-C	-5.21	99.98	110.40
1	B	252	ASP	CB-CG-OD1	5.21	122.99	118.30
1	C	279	ILE	CA-CB-CG2	5.20	121.31	110.90
1	C	375	ASP	CB-CG-OD1	5.20	122.98	118.30
1	B	894	ARG	CB-CA-C	-5.20	100.00	110.40
1	D	157	ARG	CG-CD-NE	5.19	122.70	111.80
1	D	875	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	685	LEU	N-CA-CB	5.18	120.76	110.40
1	D	840	HIS	CB-CA-C	-5.18	100.04	110.40
1	A	781	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	C	367	MET	CB-CA-C	-5.17	100.06	110.40
1	A	157	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	B	663	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	C	772	ASP	CB-CG-OD1	5.16	122.95	118.30
1	C	411	ASP	CB-CG-OD1	5.16	122.95	118.30
1	A	280	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	962	TYR	CB-CG-CD1	-5.16	117.91	121.00
1	B	569	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	997	ASP	N-CA-CB	5.16	119.88	110.60
1	C	553	TRP	CA-CB-CG	-5.14	103.94	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	792	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	45	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	C	832	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	746	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	369	GLU	CB-CG-CD	-5.13	100.35	114.20
1	B	52	ARG	CB-CA-C	-5.13	100.14	110.40
1	D	80	GLU	CG-CD-OE2	-5.13	108.04	118.30
1	D	519	SER	N-CA-CB	-5.13	102.81	110.50
1	B	280	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	973	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	14	ARG	NE-CZ-NH2	5.12	122.86	120.30
1	D	77	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	A	225	PHE	N-CA-CB	5.11	119.81	110.60
1	A	746	ASP	CB-CA-C	-5.11	100.17	110.40
1	D	279	ILE	CA-CB-CG2	5.11	121.12	110.90
1	B	164	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	D	572	ASP	CB-CA-C	-5.10	100.19	110.40
1	D	707	ALA	CB-CA-C	-5.10	102.45	110.10
1	C	239	VAL	CG1-CB-CG2	-5.10	102.75	110.90
1	B	292	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	A	292	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	799	THR	N-CA-CB	-5.08	100.64	110.30
1	C	161	TYR	N-CA-CB	-5.08	101.45	110.60
1	C	853	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	199	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	442	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	673	ALA	N-CA-CB	-5.08	103.00	110.10
1	A	446	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	184	LEU	CB-CA-C	-5.07	100.57	110.20
1	B	1022	GLN	N-CA-CB	5.06	119.71	110.60
1	D	686	PRO	N-CA-CB	5.06	109.37	103.30
1	B	280	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	193	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	100	TYR	CA-CB-CG	-5.05	103.80	113.40
1	D	916	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	416	GLU	CG-CD-OE2	-5.05	108.20	118.30
1	D	184	LEU	CB-CA-C	-5.04	100.62	110.20
1	A	871	GLU	CB-CG-CD	-5.04	100.59	114.20
1	A	800	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	131	GLU	CG-CD-OE1	5.04	128.37	118.30
1	A	319	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	A	477	SER	CB-CA-C	-5.03	100.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	B	855	THR	N-CA-CB	5.03	119.85	110.30
1	B	1021	CYS	CA-CB-SG	-5.03	104.95	114.00
1	A	285	TYR	CG-CD1-CE1	5.02	125.32	121.30
1	B	438	GLU	CG-CD-OE2	-5.02	108.25	118.30
1	D	952	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	987	ASP	CB-CG-OD1	5.02	122.82	118.30
1	B	572	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	832	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	400	THR	CA-CB-CG2	-5.01	105.39	112.40
1	C	800	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

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	8125	0	7716	97	0
1	B	8125	0	7716	81	0
1	C	8125	0	7716	89	0
1	D	8125	0	7716	78	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	112	0	168	10	0
4	B	108	0	162	5	0
4	C	112	0	168	4	0
4	D	116	0	174	7	0
5	A	1134	0	0	20	0
5	B	1104	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1072	0	0	12	0
5	D	1114	0	0	13	0
All	All	37408	0	31536	358	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (358) 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)
4:D:8407:DMS:S	4:D:8407:DMS:C1	2.02	1.47
4:A:8413:DMS:S	4:A:8413:DMS:C2	2.01	1.46
4:B:8415:DMS:C1	4:B:8415:DMS:S	2.03	1.45
4:B:8407:DMS:S	4:B:8407:DMS:C1	2.06	1.44
4:B:8508:DMS:C2	4:B:8508:DMS:S	2.10	1.40
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.38	1.19
1:C:634:GLN:H	1:C:634:GLN:NE2	1.41	1.17
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.48	1.12
1:B:655:MET:HE2	1:B:665:SER:HB3	1.32	1.06
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.24	1.01
1:B:600:GLN:H	1:B:600:GLN:HE21	1.15	0.94
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.32	0.93
1:A:809:ARG:HH11	1:A:809:ARG:HG2	1.37	0.88
1:C:634:GLN:H	1:C:634:GLN:HE21	1.22	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.03	0.87
1:C:634:GLN:N	1:C:634:GLN:NE2	2.24	0.86
1:A:773:LYS:N	1:A:773:LYS:HE2	1.91	0.86
1:A:687:GLN:HG3	5:A:9507:HOH:O	1.78	0.83
1:B:634:GLN:HE22	1:B:685:LEU:HG	1.45	0.82
1:D:658:LEU:O	1:D:661:LYS:HG3	1.79	0.82
1:A:600:GLN:H	1:A:600:GLN:HE21	1.30	0.80
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.63	0.80
4:A:8420:DMS:H11	5:D:9556:HOH:O	1.82	0.78
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.49	0.78
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.64	0.78
1:B:634:GLN:NE2	1:B:685:LEU:HG	2.00	0.77
1:B:684:GLU:O	1:B:686:PRO:HD3	1.83	0.77
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.68	0.76
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.17	0.74
1:C:748:CYS:C	1:C:749:ILE:HD12	2.08	0.74
1:B:890:GLN:HG3	1:B:891:VAL:N	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:9722:HOH:O	1:B:530:THR:HG22	1.86	0.74
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.69	0.74
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.74
1:A:797:GLU:O	1:A:801:ILE:HD13	1.87	0.73
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.00	0.73
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.01	0.72
1:C:178:ARG:HD2	5:C:9619:HOH:O	1.90	0.71
1:A:787:ALA:HA	1:A:968:MET:HG3	1.73	0.71
1:D:277:GLU:H	1:D:277:GLU:CD	1.95	0.70
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.11	0.70
1:B:262:GLN:HE21	1:B:263:GLY:N	1.89	0.70
1:B:878:HIS:HD2	5:B:8694:HOH:O	1.74	0.69
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.27	0.69
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.57	0.69
1:A:237:ARG:HG2	1:A:296:GLU:OE1	1.93	0.68
1:A:648:ASP:OD2	5:A:9590:HOH:O	2.11	0.68
1:D:893:GLU:HG2	1:D:894:ARG:HG2	1.76	0.68
1:D:748:CYS:C	1:D:749:ILE:HD12	2.13	0.68
1:A:720:TRP:HA	4:A:8427:DMS:H21	1.76	0.68
1:D:634:GLN:NE2	1:D:682:LEU:O	2.25	0.68
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.75	0.68
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.21	0.67
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.27	0.67
1:D:749:ILE:N	1:D:749:ILE:HD12	2.07	0.67
1:D:237:ARG:NH1	5:D:9291:HOH:O	2.27	0.67
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.26	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.07	0.66
1:A:277:GLU:H	1:A:277:GLU:CD	1.99	0.66
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.08	0.66
1:D:719:GLN:O	4:D:8427:DMS:H22	1.96	0.66
1:D:618:THR:HG21	5:D:9064:HOH:O	1.95	0.65
1:B:730:LEU:H	1:B:730:LEU:CD1	2.02	0.65
1:D:651:LEU:HD12	1:D:652:LEU:N	2.12	0.65
1:D:887:GLN:NE2	1:D:980:GLU:O	2.30	0.65
1:A:878:HIS:HD2	5:A:8676:HOH:O	1.80	0.65
1:D:292:ARG:HH12	4:D:8412:DMS:C1	2.10	0.64
1:C:878:HIS:HD2	5:C:8705:HOH:O	1.80	0.64
1:B:730:LEU:HD12	1:B:730:LEU:H	1.63	0.63
1:D:878:HIS:HD2	5:D:8819:HOH:O	1.81	0.63
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.06	0.62
1:A:635:THR:OG1	1:A:681:GLU:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.80	0.62
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.14	0.62
1:A:431:ARG:HG3	5:A:9618:HOH:O	1.99	0.61
1:C:749:ILE:HD12	1:C:749:ILE:N	2.14	0.61
1:C:835:LEU:HD11	1:C:855:THR:HB	1.80	0.61
1:D:128:ASN:HB3	1:D:180:GLY:O	2.00	0.61
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.83	0.61
1:A:116:THR:HG22	5:A:9689:HOH:O	2.01	0.61
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.99	0.61
1:D:135:GLN:O	1:D:136:GLU:HG2	2.00	0.60
4:A:8502:DMS:H22	5:A:9384:HOH:O	2.00	0.60
1:D:595:THR:HA	1:D:596:PRO:C	2.19	0.60
1:A:832:ASP:OD1	1:A:832:ASP:N	2.34	0.60
1:A:178:ARG:HD2	5:A:9537:HOH:O	2.02	0.60
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.84	0.59
1:A:595:THR:HA	1:A:596:PRO:C	2.23	0.59
1:C:278:ILE:HD13	1:C:278:ILE:N	2.17	0.59
1:B:1017:GLN:HB2	5:B:9639:HOH:O	2.02	0.59
1:D:847:LYS:HG3	1:D:848:THR:N	2.13	0.59
1:B:262:GLN:HE21	1:B:262:GLN:C	2.05	0.59
1:D:135:GLN:C	1:D:136:GLU:HG2	2.22	0.59
1:B:797:GLU:O	1:B:801:ILE:HD13	2.02	0.59
4:D:8427:DMS:H11	5:D:9189:HOH:O	2.02	0.59
1:B:745:MET:HE1	5:B:9702:HOH:O	2.03	0.59
1:A:685:LEU:O	1:A:687:GLN:NE2	2.36	0.59
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.84	0.58
1:D:292:ARG:HH12	4:D:8412:DMS:H12	1.67	0.58
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.67	0.58
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.18	0.58
1:D:893:GLU:O	1:D:893:GLU:HG3	2.03	0.58
1:A:646:HIS:ND1	5:A:9499:HOH:O	2.29	0.58
1:D:254:LEU:HD12	5:D:9691:HOH:O	2.02	0.58
1:D:651:LEU:C	1:D:651:LEU:HD12	2.23	0.58
1:C:595:THR:HA	1:C:596:PRO:C	2.23	0.58
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.18	0.58
1:C:356:ARG:HD2	1:C:379:MET:CE	2.32	0.58
1:C:651:LEU:C	1:C:651:LEU:HD12	2.23	0.58
1:A:887:GLN:NE2	1:A:980:GLU:O	2.36	0.58
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.72	0.57
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.34	0.57
1:D:893:GLU:HG2	1:D:894:ARG:CD	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.85	0.57
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.26	0.57
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.33	0.57
1:A:861:SER:OG	1:A:863:GLN:HG3	2.05	0.57
1:B:381:GLN:O	1:B:621:LYS:HE3	2.05	0.56
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.20	0.56
1:D:646:HIS:ND1	5:D:9625:HOH:O	2.33	0.56
1:A:651:LEU:HD12	1:A:651:LEU:C	2.25	0.56
1:C:266:GLN:HE21	4:C:8602:DMS:C1	2.19	0.56
1:C:690:SER:HB2	5:C:9407:HOH:O	2.06	0.56
1:C:49:GLN:HG2	5:C:9592:HOH:O	2.05	0.56
1:A:88:SER:HA	1:A:366:VAL:HG21	1.88	0.56
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.88	0.56
1:A:809:ARG:NH1	1:A:809:ARG:HG2	2.13	0.56
4:A:8427:DMS:H23	5:A:9005:HOH:O	2.05	0.55
1:C:655:MET:HE2	1:C:665:SER:HB3	1.88	0.55
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.34	0.55
1:C:844:HIS:HD2	5:C:9519:HOH:O	1.90	0.55
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.89	0.55
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.22	0.55
4:C:8407:DMS:H11	5:C:9628:HOH:O	2.05	0.55
1:C:651:LEU:O	1:C:651:LEU:HD12	2.06	0.55
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.20	0.54
1:A:237:ARG:NH1	5:A:9146:HOH:O	2.40	0.54
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.40	0.54
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.07	0.54
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.89	0.54
1:A:663:LEU:HD11	1:A:688:PRO:HG3	1.89	0.54
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.43	0.54
1:B:595:THR:HA	1:B:596:PRO:C	2.28	0.54
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.44	0.53
1:D:893:GLU:HG2	1:D:894:ARG:CG	2.39	0.53
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.08	0.53
1:C:569:ASP:HB2	5:C:9458:HOH:O	2.07	0.53
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.91	0.53
1:C:429:ASP:OD1	1:C:431:ARG:HG3	2.09	0.53
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.09	0.53
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.76	0.53
1:B:600:GLN:N	1:B:600:GLN:HE21	1.96	0.53
1:A:719:GLN:O	4:A:8427:DMS:H22	2.09	0.52
1:D:618:THR:HG23	5:D:9080:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:H	1:A:773:LYS:HE2	1.73	0.52
1:A:655:MET:HE2	1:A:656:VAL:N	2.25	0.52
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.91	0.52
1:C:667:GLU:C	1:C:668:VAL:HG23	2.31	0.51
1:C:890:GLN:HG3	1:C:891:VAL:N	2.25	0.51
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.22	0.51
1:B:689:GLU:O	1:B:690:SER:OG	2.26	0.51
1:D:681:GLU:HG2	5:D:9499:HOH:O	2.11	0.51
1:B:600:GLN:H	1:B:600:GLN:NE2	1.97	0.51
1:B:745:MET:SD	1:B:745:MET:N	2.79	0.51
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.93	0.51
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.76	0.51
1:B:615:PRO:O	1:B:618:THR:HG22	2.11	0.51
1:B:730:LEU:HD12	1:B:730:LEU:N	2.25	0.50
1:A:521:LYS:HE2	5:A:9035:HOH:O	2.10	0.50
1:A:735:HIS:O	1:A:736:ALA:HB2	2.11	0.50
1:B:262:GLN:NE2	1:B:263:GLY:N	2.57	0.50
1:B:157:ARG:HD3	5:B:9508:HOH:O	2.11	0.50
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.93	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.93	0.50
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.41	0.50
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.93	0.50
1:C:240:LEU:HD23	1:C:240:LEU:C	2.32	0.50
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.76	0.49
1:B:178:ARG:HG3	1:B:178:ARG:O	2.10	0.49
1:B:494:THR:HB	1:C:473:ARG:NH2	2.27	0.49
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.77	0.49
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.47	0.49
1:C:13:ARG:O	1:C:14:ARG:C	2.51	0.49
1:D:667:GLU:C	1:D:668:VAL:HG23	2.33	0.49
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.96	0.49
1:D:277:GLU:N	1:D:277:GLU:OE1	2.41	0.49
1:A:737:ILE:O	1:A:737:ILE:HD13	2.13	0.49
1:B:863:GLN:CG	1:B:1021:CYS:HB3	2.39	0.49
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.43	0.49
1:D:581:ASN:HD22	1:D:583:ASN:HD22	1.60	0.49
1:A:754:LYS:NZ	5:A:9569:HOH:O	2.46	0.48
4:A:8425:DMS:H11	5:A:9441:HOH:O	2.13	0.48
1:D:749:ILE:N	1:D:749:ILE:CD1	2.73	0.48
1:A:724:GLU:O	1:B:847:LYS:NZ	2.38	0.48
1:C:829:THR:HG22	1:C:830:LEU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.63	0.48
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.97	0.48
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.96	0.48
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.49	0.48
1:D:682:LEU:HA	1:D:682:LEU:HD23	1.70	0.48
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.44	0.48
1:B:804:ASN:HD22	1:B:809:ARG:HH21	1.61	0.48
1:D:88:SER:HA	1:D:366:VAL:HG21	1.96	0.47
1:B:655:MET:SD	1:B:656:VAL:N	2.87	0.47
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.96	0.47
1:D:622:HIS:O	1:D:625:GLN:HG3	2.14	0.47
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.96	0.47
1:C:753:ASN:OD1	1:C:754:LYS:NZ	2.26	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.63	0.47
1:A:890:GLN:HG3	1:A:891:VAL:N	2.28	0.47
4:B:8407:DMS:C1	4:B:8407:DMS:C2	2.84	0.47
1:B:651:LEU:C	1:B:651:LEU:HD23	2.32	0.47
1:C:431:ARG:HG3	5:C:8631:HOH:O	2.13	0.47
1:C:730:LEU:HG	1:C:730:LEU:H	1.29	0.47
1:D:843:GLN:HA	1:D:847:LYS:O	2.15	0.47
1:D:861:SER:OG	1:D:863:GLN:HG3	2.14	0.47
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.97	0.47
1:D:240:LEU:HD23	1:D:240:LEU:C	2.35	0.47
1:C:750:GLU:HG2	5:C:9510:HOH:O	2.15	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.55	0.47
1:C:655:MET:SD	1:C:656:VAL:N	2.88	0.47
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.50	0.47
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.96	0.47
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.27	0.46
1:A:844:HIS:HD2	5:A:9496:HOH:O	1.98	0.46
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.96	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.16	0.46
1:C:819:GLU:H	1:C:819:GLU:HG2	1.24	0.46
1:D:340:GLY:O	1:D:561:ARG:HG2	2.15	0.46
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.73	0.46
4:A:8409:DMS:O	5:A:9118:HOH:O	2.20	0.46
1:B:232:ASN:ND2	1:B:237:ARG:CG	2.78	0.46
1:A:533:LEU:C	1:A:533:LEU:HD23	2.36	0.46
1:D:991:MET:HE2	1:D:1003:VAL:HG21	1.98	0.46
1:A:71:GLU:O	1:A:71:GLU:HG3	2.16	0.46
1:C:114:VAL:HB	1:C:115:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:720:TRP:HA	4:D:8427:DMS:C2	2.46	0.45
1:D:363:HIS:HD2	5:D:9341:HOH:O	1.99	0.45
1:A:279:ILE:HD13	1:A:279:ILE:HG21	1.60	0.45
1:C:749:ILE:N	1:C:749:ILE:CD1	2.80	0.45
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.32	0.45
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.51	0.45
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.78	0.45
1:C:781:ARG:NH1	5:C:9397:HOH:O	2.49	0.45
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.50	0.45
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.63	0.45
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.98	0.45
5:B:9426:HOH:O	4:C:8420:DMS:H11	2.16	0.45
1:B:320:GLY:O	4:B:8406:DMS:O	2.35	0.45
1:C:745:MET:HG2	5:C:9513:HOH:O	2.15	0.45
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.99	0.45
1:D:773:LYS:HG3	1:D:773:LYS:O	2.08	0.45
1:C:658:LEU:O	1:C:659:ASP:C	2.53	0.45
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.52	0.45
1:D:660:GLY:O	1:D:662:PRO:HD3	2.17	0.44
1:B:655:MET:HE2	1:B:664:ALA:O	2.18	0.44
1:A:737:ILE:HD13	1:A:737:ILE:C	2.37	0.44
1:D:736:ALA:C	1:D:737:ILE:HG22	2.37	0.44
1:B:240:LEU:HD23	1:B:240:LEU:C	2.38	0.44
1:B:581:ASN:ND2	5:B:9529:HOH:O	2.51	0.44
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.00	0.44
1:D:634:GLN:HB2	1:D:682:LEU:HB2	2.00	0.44
1:C:266:GLN:HE21	4:C:8602:DMS:H12	1.82	0.44
1:D:768:MET:HB2	1:D:768:MET:HE2	1.86	0.44
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.52	0.44
1:B:889:ALA:HB3	5:B:9650:HOH:O	2.18	0.44
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.47	0.44
1:A:649:ASN:HA	4:A:8425:DMS:H21	2.00	0.44
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.99	0.44
1:A:680:ILE:HG12	5:A:9265:HOH:O	2.16	0.43
1:A:773:LYS:CA	1:A:773:LYS:HE2	2.30	0.43
1:A:781:ARG:NH1	5:A:9369:HOH:O	2.50	0.43
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.54	0.43
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.81	0.43
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.99	0.43
1:A:660:GLY:O	1:A:662:PRO:HD3	2.18	0.43
1:C:673:ALA:HB1	1:C:674:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:GLU:HA	1:C:181:GLU:OE1	2.19	0.43
1:C:797:GLU:O	1:C:801:ILE:HD13	2.18	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.63	0.43
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.48	0.43
1:D:545:SER:O	1:D:909:ARG:HD3	2.19	0.43
1:A:600:GLN:N	1:A:600:GLN:HE21	2.08	0.43
1:C:356:ARG:HD2	1:C:379:MET:HE3	1.99	0.43
1:B:634:GLN:HG3	1:B:682:LEU:O	2.18	0.43
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.00	0.43
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.01	0.43
1:B:533:LEU:HD23	1:B:533:LEU:C	2.40	0.42
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.54	0.42
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.55	0.42
1:B:809:ARG:NH1	1:B:809:ARG:HG2	2.34	0.42
1:D:725:ASN:HB2	5:D:9621:HOH:O	2.18	0.42
1:D:431:ARG:HD2	5:D:8744:HOH:O	2.19	0.42
1:B:673:ALA:HB1	1:B:674:PRO:HD2	2.01	0.42
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.01	0.42
1:B:181:GLU:HG3	5:B:9652:HOH:O	2.18	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.54	0.42
1:B:127:PHE:CD2	1:B:127:PHE:N	2.88	0.42
1:B:127:PHE:HE2	1:B:184:LEU:HG	1.84	0.42
1:B:513:PRO:O	1:B:514:ALA:HB3	2.19	0.42
1:C:580:GLU:HG3	1:C:580:GLU:H	1.44	0.42
1:B:297:ASN:N	1:B:298:PRO:CD	2.83	0.42
1:C:663:LEU:HA	1:C:663:LEU:HD22	1.80	0.42
1:A:634:GLN:OE1	1:A:634:GLN:CA	2.67	0.42
1:D:738:PRO:HG3	1:D:751:LEU:HD13	2.02	0.42
1:A:262:GLN:NE2	1:A:299:LYS:HD3	2.34	0.42
1:C:615:PRO:O	1:C:618:THR:HG22	2.18	0.42
4:A:8405:DMS:O	5:A:9310:HOH:O	2.22	0.42
1:A:668:VAL:HG13	1:A:669:PRO:HD2	2.00	0.42
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.52	0.42
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.36	0.42
1:B:663:LEU:HA	1:B:663:LEU:HD22	1.48	0.42
1:A:427:THR:HG21	1:A:462:SER:HB3	2.01	0.42
1:D:736:ALA:HB1	1:D:737:ILE:H	1.69	0.42
1:A:959:ILE:HD13	1:A:959:ILE:HG21	1.91	0.42
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.86	0.42
1:A:830:LEU:HD12	1:A:833:ALA:HB3	2.02	0.42
1:D:131:GLU:OE2	1:D:131:GLU:O	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:LEU:CD1	1:A:686:PRO:CG	2.99	0.41
1:D:893:GLU:CG	1:D:894:ARG:HD2	2.50	0.41
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.45	0.41
1:B:634:GLN:HE22	1:B:685:LEU:CG	2.26	0.41
4:D:8703:DMS:H13	5:D:9766:HOH:O	2.19	0.41
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.60	0.41
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.56	0.41
1:A:843:GLN:HA	1:A:847:LYS:O	2.20	0.41
1:A:835:LEU:HD11	1:A:855:THR:HB	2.01	0.41
1:C:674:PRO:O	1:C:675:GLN:HB2	2.21	0.41
1:B:658:LEU:O	1:B:659:ASP:C	2.57	0.41
1:C:861:SER:OG	1:C:863:GLN:HG3	2.21	0.41
1:A:651:LEU:HD23	1:A:703:PRO:HG3	2.03	0.41
1:D:737:ILE:HA	1:D:738:PRO:HD3	1.95	0.41
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.56	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.21	0.41
1:C:613:PRO:HB3	1:C:617:LEU:HD23	2.03	0.41
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.21	0.41
1:C:785:THR:O	1:C:881:ARG:HD2	2.20	0.41
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.91	0.41
1:B:937:LEU:HA	1:B:957:PHE:O	2.21	0.41
1:B:340:GLY:O	1:B:561:ARG:HG2	2.21	0.40
1:B:299:LYS:HE2	5:B:9327:HOH:O	2.19	0.40
1:C:655:MET:SD	1:C:656:VAL:O	2.80	0.40
1:B:542:MET:HA	1:B:604:ASN:HA	2.02	0.40
1:A:753:ASN:OD1	1:A:754:LYS:HG3	2.21	0.40
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.56	0.40
1:B:801:ILE:HA	1:B:801:ILE:HD13	1.74	0.40
1:A:473:ARG:HD2	1:A:473:ARG:HA	1.95	0.40
1:A:855:THR:HG23	5:A:9379:HOH:O	2.20	0.40
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.56	0.40
1:C:995:GLY:O	1:C:996:ASP:C	2.59	0.40
1:C:367:MET:HA	1:C:367:MET:HE3	2.03	0.40
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.40
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.85	0.40
1:C:49:GLN:CG	5:C:9592:HOH:O	2.66	0.40
1:B:88:SER:HA	1:B:366:VAL:HG21	2.02	0.40
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.75	0.40
1:C:157:ARG:HD3	1:C:157:ARG:HH11	1.73	0.40
1:C:930:VAL:O	1:C:932:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

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	1009/1023 (99%)	974 (96%)	34 (3%)	1 (0%)	56	35
1	B	1009/1023 (99%)	971 (96%)	34 (3%)	4 (0%)	39	20
1	C	1009/1023 (99%)	973 (96%)	35 (4%)	1 (0%)	56	35
1	D	1009/1023 (99%)	977 (97%)	31 (3%)	1 (0%)	56	35
All	All	4036/4092 (99%)	3895 (96%)	134 (3%)	7 (0%)	52	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA
1	B	690	SER
1	B	731	PRO
1	C	734	SER
1	A	164	ASP
1	B	164	ASP
1	D	164	ASP

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	864/875 (99%)	835 (97%)	29 (3%)	44	21
1	B	864/875 (99%)	834 (96%)	30 (4%)	43	20
1	C	864/875 (99%)	833 (96%)	31 (4%)	42	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	864/875 (99%)	830 (96%)	34 (4%)	39	16
All	All	3456/3500 (99%)	3332 (96%)	124 (4%)	42	19

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	131	GLU
1	A	237	ARG
1	A	250	LEU
1	A	333	ARG
1	A	394	ASN
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
1	A	634	GLN
1	A	655	MET
1	A	663	LEU
1	A	671	ASP
1	A	684	GLU
1	A	689	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	801	ILE
1	A	817	GLN
1	A	819	GLU
1	A	885	ASN
1	A	910	LEU
1	A	956	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1017	GLN
1	A	1023	LYS
1	B	76	CYS
1	B	80	GLU
1	B	262	GLN
1	B	264	GLU
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU

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Mol	Chain	Res	Type
1	B	370	GLN
1	B	394	ASN
1	B	554	GLN
1	B	580	GLU
1	B	600	GLN
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	687	GLN
1	B	690	SER
1	B	699	ARG
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	799	THR
1	B	819	GLU
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	890	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	230	ARG
1	C	262	GLN
1	C	278	ILE
1	C	333	ARG
1	C	392	TYR
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	595	THR
1	C	634	GLN
1	C	655	MET
1	C	663	LEU
1	C	681	GLU

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Mol	Chain	Res	Type
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	750	GLU
1	C	773	LYS
1	C	800	ARG
1	C	819	GLU
1	C	1023	LYS
1	D	71	GLU
1	D	80	GLU
1	D	112	PRO
1	D	237	ARG
1	D	277	GLU
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	594	ASP
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	667	GLU
1	D	684	GLU
1	D	687	GLN
1	D	689	GLU
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	845	GLN

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Mol	Chain	Res	Type
1	D	885	ASN
1	D	893	GLU
1	D	1022	GLN
1	D	1023	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	135	GLN
1	A	262	GLN
1	A	583	ASN
1	A	600	GLN
1	A	624	GLN
1	A	675	GLN
1	A	757	GLN
1	A	761	GLN
1	A	817	GLN
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	804	ASN
1	B	817	GLN
1	B	878	HIS
1	C	163	GLN
1	C	266	GLN
1	C	634	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	363	HIS
1	D	583	ASN
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	804	ASN

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Mol	Chain	Res	Type
1	D	878	HIS
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 148 ligands modelled in this entry, 36 are monoatomic - leaving 112 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	$\# Z > 2$
4	DMS	A	8401	-	3,3,3	0.65	0	3,3,3	0.52	0
4	DMS	A	8402	-	3,3,3	1.07	0	3,3,3	0.36	0
4	DMS	A	8403	-	3,3,3	1.56	1 (33%)	3,3,3	0.42	0
4	DMS	A	8404	-	3,3,3	1.30	0	3,3,3	0.04	0
4	DMS	A	8405	-	3,3,3	0.77	0	3,3,3	0.64	0
4	DMS	A	8406	-	3,3,3	1.28	0	3,3,3	0.73	0
4	DMS	A	8407	-	3,3,3	2.37	2 (66%)	3,3,3	0.54	0
4	DMS	A	8408	-	3,3,3	0.43	0	3,3,3	0.60	0
4	DMS	A	8409	-	3,3,3	2.22	1 (33%)	3,3,3	0.65	0
4	DMS	A	8410	-	3,3,3	1.47	1 (33%)	3,3,3	1.00	0
4	DMS	A	8411	-	3,3,3	1.11	0	3,3,3	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	A	8412	-	3,3,3	0.82	0	3,3,3	0.28	0
4	DMS	A	8413	-	3,3,3	2.82	3 (100%)	3,3,3	0.62	0
4	DMS	A	8414	-	3,3,3	1.21	0	3,3,3	0.29	0
4	DMS	A	8415	-	3,3,3	2.05	2 (66%)	3,3,3	0.57	0
4	DMS	A	8416	-	3,3,3	0.88	0	3,3,3	0.56	0
4	DMS	A	8417	-	3,3,3	1.06	0	3,3,3	0.17	0
4	DMS	A	8419	-	3,3,3	0.77	0	3,3,3	0.32	0
4	DMS	A	8420	-	3,3,3	0.70	0	3,3,3	1.07	0
4	DMS	A	8421	-	3,3,3	1.01	0	3,3,3	1.09	0
4	DMS	A	8423	-	3,3,3	1.54	0	3,3,3	0.52	0
4	DMS	A	8425	3	3,3,3	1.79	1 (33%)	3,3,3	0.43	0
4	DMS	A	8427	-	3,3,3	0.64	0	3,3,3	0.68	0
4	DMS	A	8501	-	3,3,3	1.55	1 (33%)	3,3,3	0.32	0
4	DMS	A	8502	-	3,3,3	2.32	2 (66%)	3,3,3	1.49	1 (33%)
4	DMS	A	8503	-	3,3,3	1.22	0	3,3,3	0.31	0
4	DMS	A	8504	-	3,3,3	0.24	0	3,3,3	0.53	0
4	DMS	A	8602	-	3,3,3	0.90	0	3,3,3	0.43	0
4	DMS	B	8401	-	3,3,3	0.43	0	3,3,3	0.33	0
4	DMS	B	8402	-	3,3,3	1.39	0	3,3,3	0.20	0
4	DMS	B	8403	-	3,3,3	1.19	0	3,3,3	0.77	0
4	DMS	B	8404	-	3,3,3	0.43	0	3,3,3	0.37	0
4	DMS	B	8405	-	3,3,3	1.33	0	3,3,3	0.58	0
4	DMS	B	8406	-	3,3,3	1.37	0	3,3,3	0.35	0
4	DMS	B	8407	-	3,3,3	2.91	3 (100%)	3,3,3	0.33	0
4	DMS	B	8408	-	3,3,3	0.20	0	3,3,3	0.69	0
4	DMS	B	8409	-	3,3,3	1.84	1 (33%)	3,3,3	0.64	0
4	DMS	B	8410	-	3,3,3	1.25	0	3,3,3	0.49	0
4	DMS	B	8411	-	3,3,3	0.81	0	3,3,3	0.61	0
4	DMS	B	8412	-	3,3,3	0.65	0	3,3,3	0.42	0
4	DMS	B	8413	-	3,3,3	2.68	2 (66%)	3,3,3	0.72	0
4	DMS	B	8414	-	3,3,3	1.08	0	3,3,3	0.87	0
4	DMS	B	8415	-	3,3,3	2.56	2 (66%)	3,3,3	1.54	1 (33%)
4	DMS	B	8416	-	3,3,3	1.32	1 (33%)	3,3,3	0.68	0
4	DMS	B	8417	-	3,3,3	0.67	0	3,3,3	0.56	0
4	DMS	B	8420	-	3,3,3	1.33	1 (33%)	3,3,3	0.37	0
4	DMS	B	8421	-	3,3,3	0.29	0	3,3,3	0.53	0
4	DMS	B	8423	-	3,3,3	0.47	0	3,3,3	0.66	0
4	DMS	B	8425	3	3,3,3	3.12	2 (66%)	3,3,3	0.45	0
4	DMS	B	8427	-	3,3,3	1.12	0	3,3,3	0.10	0
4	DMS	B	8502	-	3,3,3	0.87	0	3,3,3	1.50	1 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8504	-	3,3,3	0.73	0	3,3,3	0.31	0
4	DMS	B	8506	-	3,3,3	1.67	1 (33%)	3,3,3	0.44	0
4	DMS	B	8508	-	3,3,3	2.87	1 (33%)	3,3,3	0.86	0
4	DMS	B	8601	-	3,3,3	2.02	1 (33%)	3,3,3	0.66	0
4	DMS	C	8401	-	3,3,3	0.81	0	3,3,3	0.27	0
4	DMS	C	8402	-	3,3,3	1.60	1 (33%)	3,3,3	0.24	0
4	DMS	C	8403	-	3,3,3	0.82	0	3,3,3	0.33	0
4	DMS	C	8404	-	3,3,3	0.78	0	3,3,3	1.35	1 (33%)
4	DMS	C	8405	-	3,3,3	1.48	0	3,3,3	0.52	0
4	DMS	C	8407	-	3,3,3	1.69	1 (33%)	3,3,3	0.40	0
4	DMS	C	8408	-	3,3,3	0.42	0	3,3,3	0.77	0
4	DMS	C	8409	-	3,3,3	2.05	1 (33%)	3,3,3	1.01	0
4	DMS	C	8410	-	3,3,3	1.16	0	3,3,3	0.04	0
4	DMS	C	8411	-	3,3,3	1.04	0	3,3,3	0.19	0
4	DMS	C	8412	-	3,3,3	1.19	0	3,3,3	0.53	0
4	DMS	C	8413	-	3,3,3	1.62	1 (33%)	3,3,3	0.09	0
4	DMS	C	8414	-	3,3,3	1.85	1 (33%)	3,3,3	0.91	0
4	DMS	C	8415	-	3,3,3	1.83	1 (33%)	3,3,3	0.82	0
4	DMS	C	8416	-	3,3,3	1.12	0	3,3,3	0.63	0
4	DMS	C	8417	-	3,3,3	0.73	0	3,3,3	0.72	0
4	DMS	C	8419	-	3,3,3	0.57	0	3,3,3	0.35	0
4	DMS	C	8420	-	3,3,3	1.31	1 (33%)	3,3,3	0.60	0
4	DMS	C	8421	-	3,3,3	0.62	0	3,3,3	1.63	1 (33%)
4	DMS	C	8423	-	3,3,3	0.90	0	3,3,3	0.19	0
4	DMS	C	8425	3	3,3,3	1.86	1 (33%)	3,3,3	0.39	0
4	DMS	C	8427	-	3,3,3	0.92	0	3,3,3	0.28	0
4	DMS	C	8501	-	3,3,3	0.96	0	3,3,3	0.96	0
4	DMS	C	8503	-	3,3,3	0.90	0	3,3,3	0.32	0
4	DMS	C	8504	-	3,3,3	0.52	0	3,3,3	0.37	0
4	DMS	C	8506	-	3,3,3	1.47	1 (33%)	3,3,3	0.83	0
4	DMS	C	8601	-	3,3,3	1.30	1 (33%)	3,3,3	1.02	0
4	DMS	C	8602	-	3,3,3	1.55	1 (33%)	3,3,3	0.52	0
4	DMS	D	8401	-	3,3,3	1.13	0	3,3,3	0.34	0
4	DMS	D	8402	-	3,3,3	1.17	0	3,3,3	0.29	0
4	DMS	D	8403	-	3,3,3	1.50	1 (33%)	3,3,3	0.46	0
4	DMS	D	8404	-	3,3,3	1.42	1 (33%)	3,3,3	0.24	0
4	DMS	D	8405	-	3,3,3	0.88	0	3,3,3	0.83	0
4	DMS	D	8406	-	3,3,3	0.97	0	3,3,3	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	D	8407	-	3,3,3	2.54	2 (66%)	3,3,3	1.39	1 (33%)
4	DMS	D	8408	-	3,3,3	1.16	0	3,3,3	0.12	0
4	DMS	D	8409	-	3,3,3	2.06	1 (33%)	3,3,3	0.74	0
4	DMS	D	8410	-	3,3,3	1.18	0	3,3,3	0.49	0
4	DMS	D	8411	-	3,3,3	1.04	0	3,3,3	0.27	0
4	DMS	D	8412	-	3,3,3	0.45	0	3,3,3	0.47	0
4	DMS	D	8413	-	3,3,3	1.47	0	3,3,3	0.92	0
4	DMS	D	8414	-	3,3,3	0.47	0	3,3,3	0.36	0
4	DMS	D	8415	-	3,3,3	2.17	1 (33%)	3,3,3	0.47	0
4	DMS	D	8416	-	3,3,3	0.36	0	3,3,3	0.32	0
4	DMS	D	8417	-	3,3,3	1.20	0	3,3,3	0.37	0
4	DMS	D	8419	-	3,3,3	0.30	0	3,3,3	0.39	0
4	DMS	D	8421	-	3,3,3	0.60	0	3,3,3	0.34	0
4	DMS	D	8423	-	3,3,3	1.35	0	3,3,3	0.24	0
4	DMS	D	8425	3	3,3,3	0.62	0	3,3,3	0.73	0
4	DMS	D	8427	-	3,3,3	0.82	0	3,3,3	0.11	0
4	DMS	D	8501	-	3,3,3	0.44	0	3,3,3	0.20	0
4	DMS	D	8503	-	3,3,3	1.00	0	3,3,3	0.60	0
4	DMS	D	8506	-	3,3,3	1.77	1 (33%)	3,3,3	0.29	0
4	DMS	D	8508	-	3,3,3	1.66	1 (33%)	3,3,3	0.49	0
4	DMS	D	8701	-	3,3,3	2.26	3 (100%)	3,3,3	0.76	0
4	DMS	D	8703	-	3,3,3	1.72	1 (33%)	3,3,3	0.32	0
4	DMS	D	8705	-	3,3,3	1.94	1 (33%)	3,3,3	1.03	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
4	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8411	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	A	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8420	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	B	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8506	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	C	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8504	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8506	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
4	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8412	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8415	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8425	3	-	0/0/0/0	0/0/0/0
4	DMS	D	8427	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8506	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
4	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	8602	DMS	C1-S	-2.63	1.55	1.75
4	C	8414	DMS	C2-S	-2.48	1.56	1.75
4	B	8407	DMS	C2-S	-2.07	1.59	1.75
4	B	8425	DMS	C1-S	2.01	1.91	1.75
4	A	8415	DMS	C1-S	2.02	1.91	1.75
4	D	8403	DMS	O-S	2.03	1.64	1.50
4	C	8506	DMS	C1-S	2.03	1.91	1.75
4	B	8413	DMS	C1-S	2.04	1.91	1.75
4	A	8403	DMS	C1-S	2.04	1.91	1.75
4	D	8701	DMS	C1-S	2.10	1.92	1.75
4	C	8601	DMS	C1-S	2.12	1.92	1.75
4	B	8416	DMS	O-S	2.13	1.64	1.50
4	D	8701	DMS	C2-S	2.14	1.92	1.75
4	B	8415	DMS	C2-S	2.16	1.92	1.75
4	B	8420	DMS	C1-S	2.17	1.92	1.75
4	C	8407	DMS	C1-S	2.19	1.92	1.75
4	D	8404	DMS	C1-S	2.20	1.92	1.75
4	C	8420	DMS	O-S	2.22	1.65	1.50
4	C	8415	DMS	C1-S	2.28	1.93	1.75
4	B	8407	DMS	O-S	2.33	1.66	1.50
4	A	8415	DMS	O-S	2.34	1.66	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	8705	DMS	O-S	2.40	1.66	1.50
4	A	8413	DMS	O-S	2.41	1.66	1.50
4	C	8413	DMS	O-S	2.43	1.66	1.50
4	A	8410	DMS	C2-S	2.48	1.94	1.75
4	D	8701	DMS	O-S	2.50	1.67	1.50
4	D	8703	DMS	O-S	2.51	1.67	1.50
4	D	8508	DMS	O-S	2.55	1.67	1.50
4	A	8501	DMS	O-S	2.56	1.67	1.50
4	A	8502	DMS	C1-S	2.57	1.95	1.75
4	B	8506	DMS	O-S	2.58	1.67	1.50
4	A	8413	DMS	C1-S	2.59	1.95	1.75
4	D	8407	DMS	O-S	2.64	1.68	1.50
4	A	8407	DMS	C1-S	2.66	1.96	1.75
4	C	8402	DMS	C1-S	2.71	1.96	1.75
4	A	8425	DMS	O-S	2.73	1.69	1.50
4	A	8502	DMS	C2-S	2.91	1.98	1.75
4	A	8407	DMS	O-S	2.96	1.70	1.50
4	D	8506	DMS	O-S	3.03	1.71	1.50
4	B	8409	DMS	O-S	3.09	1.71	1.50
4	D	8409	DMS	O-S	3.11	1.71	1.50
4	B	8601	DMS	C1-S	3.12	1.99	1.75
4	C	8425	DMS	O-S	3.12	1.71	1.50
4	D	8415	DMS	O-S	3.13	1.71	1.50
4	A	8413	DMS	C2-S	3.37	2.01	1.75
4	D	8407	DMS	C1-S	3.52	2.02	1.75
4	C	8409	DMS	O-S	3.53	1.74	1.50
4	B	8415	DMS	C1-S	3.56	2.03	1.75
4	A	8409	DMS	O-S	3.63	1.75	1.50
4	B	8413	DMS	O-S	3.67	1.75	1.50
4	B	8407	DMS	C1-S	3.97	2.06	1.75
4	B	8508	DMS	C2-S	4.46	2.10	1.75
4	B	8425	DMS	O-S	5.01	1.84	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8421	DMS	C2-S-C1	-2.81	83.96	98.46
4	C	8404	DMS	C2-S-C1	2.28	110.23	98.46
4	D	8407	DMS	C2-S-C1	2.40	110.84	98.46
4	B	8415	DMS	C2-S-C1	2.44	111.09	98.46
4	B	8502	DMS	C2-S-C1	2.56	111.71	98.46
4	A	8502	DMS	C2-S-C1	2.58	111.79	98.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8405	DMS	1	0
4	A	8409	DMS	1	0
4	A	8413	DMS	1	0
4	A	8420	DMS	1	0
4	A	8425	DMS	2	0
4	A	8427	DMS	3	0
4	A	8502	DMS	1	0
4	B	8406	DMS	1	0
4	B	8407	DMS	2	0
4	B	8415	DMS	1	0
4	B	8508	DMS	1	0
4	C	8407	DMS	1	0
4	C	8420	DMS	1	0
4	C	8602	DMS	2	0
4	D	8407	DMS	1	0
4	D	8412	DMS	2	0
4	D	8427	DMS	3	0
4	D	8703	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.14	28 (2%) 56 61	9, 15, 43, 100	0
1	B	1011/1023 (98%)	-0.15	25 (2%) 61 65	8, 15, 43, 95	0
1	C	1011/1023 (98%)	-0.12	28 (2%) 56 61	9, 16, 45, 96	0
1	D	1011/1023 (98%)	-0.14	34 (3%) 49 53	9, 16, 46, 95	0
All	All	4044/4092 (98%)	-0.14	115 (2%) 56 61	8, 16, 45, 100	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	11.5
1	A	686	PRO	11.4
1	D	735	HIS	10.1
1	C	732	ALA	9.3
1	D	732	ALA	8.7
1	D	734	SER	8.5
1	C	731	PRO	8.4
1	B	685	LEU	8.0
1	A	687	GLN	7.4
1	C	730	LEU	7.3
1	C	735	HIS	6.9
1	A	732	ALA	6.5
1	A	685	LEU	6.2
1	B	733	ALA	6.1
1	A	733	ALA	6.0
1	B	689	GLU	5.9
1	C	733	ALA	5.8
1	B	730	LEU	5.8
1	B	731	PRO	5.8
1	A	580	GLU	5.6
1	B	732	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	C	686	PRO	5.5
1	D	733	ALA	5.3
1	C	685	LEU	5.2
1	D	689	GLU	5.1
1	A	689	GLU	5.1
1	C	687	GLN	5.0
1	B	686	PRO	5.0
1	C	689	GLU	4.8
1	B	684	GLU	4.7
1	D	580	GLU	4.6
1	A	582	GLY	4.5
1	D	686	PRO	4.5
1	A	799	THR	4.5
1	D	730	LEU	4.4
1	A	731	PRO	4.3
1	D	581	ASN	4.3
1	D	684	GLU	4.2
1	B	799	THR	4.2
1	A	736	ALA	4.2
1	A	730	LEU	4.1
1	B	735	HIS	4.1
1	D	771	GLY	4.0
1	D	687	GLN	3.9
1	A	734	SER	3.9
1	A	684	GLU	3.6
1	D	685	LEU	3.6
1	D	800	ARG	3.6
1	B	687	GLN	3.5
1	D	799	THR	3.4
1	C	684	GLU	3.4
1	D	582	GLY	3.3
1	C	800	ARG	3.3
1	D	798	ALA	3.3
1	D	683	PRO	3.3
1	C	734	SER	3.3
1	D	845	GLN	3.3
1	A	1023	LYS	3.2
1	D	736	ALA	3.2
1	B	734	SER	3.2
1	D	772	ASP	3.2
1	A	581	ASN	3.1
1	C	798	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	861	SER	3.0
1	C	799	THR	3.0
1	A	800	ARG	3.0
1	A	688	PRO	3.0
1	C	582	GLY	2.9
1	C	729	THR	2.9
1	A	737	ILE	2.9
1	D	737	ILE	2.9
1	B	798	ALA	2.9
1	C	745	MET	2.9
1	D	731	PRO	2.9
1	B	580	GLU	2.9
1	D	663	LEU	2.9
1	D	79	PRO	2.8
1	D	688	PRO	2.8
1	A	801	ILE	2.8
1	B	745	MET	2.8
1	A	682	LEU	2.8
1	B	79	PRO	2.7
1	A	845	GLN	2.7
1	C	581	ASN	2.7
1	B	581	ASN	2.6
1	B	845	GLN	2.5
1	C	76	CYS	2.5
1	D	729	THR	2.5
1	C	634	GLN	2.5
1	C	688	PRO	2.4
1	C	761	GLN	2.4
1	A	71	GLU	2.4
1	B	688	PRO	2.4
1	D	634	GLN	2.4
1	D	682	LEU	2.3
1	A	729	THR	2.3
1	D	579	ASP	2.3
1	C	578	TYR	2.3
1	B	582	GLY	2.3
1	A	683	PRO	2.3
1	C	633	GLY	2.2
1	C	580	GLU	2.2
1	D	861	SER	2.2
1	D	681	GLU	2.2
1	C	71	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	663	LEU	2.1
1	B	253	TYR	2.1
1	D	728	VAL	2.1
1	D	679	LEU	2.1
1	A	846	GLY	2.1
1	A	634	GLN	2.0
1	B	583	ASN	2.0
1	C	583	ASN	2.0
1	B	728	VAL	2.0
1	B	683	PRO	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
4	DMS	B	8407	4/4	0.92	0.18	17.19	28,30,40,44	0
4	DMS	D	8703	4/4	0.89	0.17	13.82	32,49,51,100	0
4	DMS	B	8420	4/4	0.92	0.18	11.97	50,62,76,100	0
4	DMS	C	8420	4/4	0.94	0.14	11.44	42,45,67,100	0
4	DMS	B	8406	4/4	0.83	0.19	10.74	33,40,56,80	0
4	DMS	B	8508	4/4	0.94	0.11	8.15	21,30,45,49	0
4	DMS	A	8407	4/4	0.95	0.15	8.05	23,24,33,36	0
4	DMS	D	8404	4/4	0.94	0.11	7.23	22,23,40,100	0
4	DMS	D	8407	4/4	0.88	0.15	6.25	30,32,39,45	0
4	DMS	A	8406	4/4	0.91	0.19	6.12	15,43,66,76	0
4	DMS	C	8506	4/4	0.94	0.12	5.12	34,34,45,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	B	8506	4/4	0.97	0.10	4.22	42,43,45,47	0
4	DMS	D	8425	4/4	0.88	0.22	4.09	19,20,30,32	4
4	DMS	D	8423	4/4	0.93	0.16	3.90	35,52,61,69	0
4	DMS	C	8419	4/4	0.87	0.17	3.89	40,44,52,66	0
4	DMS	C	8410	4/4	0.97	0.15	3.83	24,33,35,36	0
4	DMS	A	8420	4/4	0.95	0.11	3.36	35,38,40,58	0
4	DMS	B	8425	4/4	0.94	0.15	3.35	24,31,35,42	0
4	DMS	A	8417	4/4	0.90	0.22	3.19	28,29,56,92	0
4	DMS	D	8417	4/4	0.89	0.17	3.18	27,30,32,100	0
4	DMS	C	8407	4/4	0.96	0.14	3.03	27,33,35,41	0
4	DMS	A	8423	4/4	0.91	0.15	2.79	34,53,63,100	0
4	DMS	C	8425	4/4	0.96	0.17	2.60	29,34,40,62	0
4	DMS	C	8423	4/4	0.91	0.12	2.57	32,41,45,57	0
4	DMS	B	8502	4/4	0.96	0.14	2.46	25,26,36,36	0
4	DMS	D	8408	4/4	0.98	0.10	2.36	18,28,29,34	0
3	NA	D	3103	1/1	0.97	0.11	2.36	33,33,33,33	0
4	DMS	B	8423	4/4	0.95	0.10	2.00	33,34,57,82	0
4	DMS	B	8408	4/4	0.97	0.11	1.72	28,30,37,48	0
3	NA	B	3104	1/1	0.97	0.12	1.63	29,29,29,29	0
4	DMS	D	8705	4/4	0.92	0.15	1.63	22,30,36,36	0
4	DMS	A	8412	4/4	0.96	0.15	1.62	30,33,36,100	0
4	DMS	B	8417	4/4	0.92	0.15	1.57	26,32,64,100	0
4	DMS	C	8602	4/4	0.91	0.13	1.55	33,53,55,72	0
4	DMS	A	8401	4/4	0.99	0.09	1.53	12,13,14,16	0
4	DMS	D	8403	4/4	0.98	0.08	1.51	16,22,27,34	0
4	DMS	C	8417	4/4	0.89	0.17	1.51	31,33,56,69	0
4	DMS	D	8506	4/4	0.86	0.14	1.41	35,45,47,55	0
4	DMS	D	8405	4/4	0.99	0.09	1.26	22,23,33,39	0
4	DMS	D	8406	4/4	0.97	0.09	1.15	23,24,25,32	0
4	DMS	D	8410	4/4	0.98	0.12	1.03	27,29,32,37	0
4	DMS	C	8501	4/4	0.96	0.09	1.03	24,28,37,39	0
4	DMS	D	8419	4/4	0.97	0.09	0.88	27,36,41,47	0
4	DMS	D	8501	4/4	0.94	0.08	0.86	27,29,33,46	0
4	DMS	C	8403	4/4	0.98	0.09	0.82	18,20,22,23	0
4	DMS	D	8508	4/4	0.95	0.09	0.79	30,34,36,45	0
4	DMS	A	8404	4/4	0.96	0.08	0.64	19,24,28,31	0
3	NA	C	3104	1/1	0.98	0.10	0.63	28,28,28,28	0
4	DMS	B	8401	4/4	0.99	0.08	0.55	14,17,18,19	0
4	DMS	A	8502	4/4	0.94	0.12	0.54	24,25,48,56	0
4	DMS	A	8504	4/4	0.97	0.08	0.51	22,36,38,65	0
4	DMS	D	8412	4/4	0.98	0.12	0.47	23,25,29,41	0
4	DMS	B	8403	4/4	0.99	0.09	0.45	15,19,24,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	C	8411	4/4	0.99	0.11	0.44	21,26,27,34	0
4	DMS	C	8412	4/4	0.98	0.11	0.39	29,33,33,100	0
4	DMS	D	8701	4/4	0.98	0.10	0.33	14,14,19,32	0
4	DMS	A	8425	4/4	0.97	0.10	0.30	32,36,39,39	0
4	DMS	D	8402	4/4	0.98	0.07	0.25	15,20,20,23	0
3	NA	A	3104	1/1	0.98	0.08	0.21	25,25,25,25	0
4	DMS	B	8405	4/4	0.97	0.08	0.21	25,27,28,29	0
4	DMS	C	8405	4/4	0.98	0.07	0.11	23,23,24,27	0
4	DMS	A	8419	4/4	0.96	0.09	0.09	37,41,49,51	0
4	DMS	C	8408	4/4	0.98	0.08	0.07	21,34,35,36	0
4	DMS	C	8404	4/4	0.98	0.07	0.03	18,18,24,27	0
4	DMS	B	8504	4/4	0.95	0.09	0.01	23,36,42,46	0
2	MG	C	3002	1/1	1.00	0.07	-0.04	13,13,13,13	0
4	DMS	C	8402	4/4	0.98	0.07	-0.10	14,19,24,26	0
4	DMS	B	8402	4/4	0.98	0.07	-0.10	13,16,19,21	0
4	DMS	A	8501	4/4	0.95	0.09	-0.11	17,22,33,34	0
4	DMS	B	8412	4/4	0.98	0.09	-0.12	25,30,31,32	0
4	DMS	D	8411	4/4	0.98	0.09	-0.17	22,23,27,62	0
4	DMS	A	8402	4/4	0.98	0.07	-0.19	14,16,20,26	0
4	DMS	C	8401	4/4	0.99	0.07	-0.23	15,15,19,19	0
3	NA	D	3104	1/1	0.94	0.08	-0.25	34,34,34,34	0
4	DMS	A	8405	4/4	0.99	0.07	-0.29	20,24,25,33	0
4	DMS	A	8411	4/4	0.98	0.07	-0.62	27,27,27,37	0
4	DMS	A	8408	4/4	0.97	0.07	-0.73	15,33,34,49	0
3	NA	A	3102	1/1	1.00	0.08	-0.80	12,12,12,12	0
2	MG	B	3002	1/1	0.99	0.06	-0.94	15,15,15,15	0
4	DMS	B	8404	4/4	0.97	0.06	-0.97	21,24,32,33	0
3	NA	C	3102	1/1	0.99	0.06	-0.98	14,14,14,14	0
3	NA	A	3101	1/1	0.99	0.06	-0.99	16,16,16,16	0
2	MG	D	3002	1/1	0.99	0.06	-1.01	15,15,15,15	0
3	NA	B	3103	1/1	0.99	0.07	-1.14	23,23,23,23	0
3	NA	D	3102	1/1	1.00	0.06	-1.14	12,12,12,12	0
4	DMS	B	8411	4/4	0.99	0.06	-1.26	23,26,29,80	0
4	DMS	A	8403	4/4	0.99	0.06	-1.34	20,21,21,25	0
2	MG	B	3001	1/1	1.00	0.06	-1.46	12,12,12,12	0
3	NA	C	3101	1/1	1.00	0.06	-1.51	13,13,13,13	0
4	DMS	D	8401	4/4	0.99	0.06	-1.67	12,13,16,17	0
3	NA	B	3101	1/1	0.99	0.06	-1.71	14,14,14,14	0
3	NA	A	3103	1/1	0.98	0.07	-2.07	26,26,26,26	0
2	MG	A	3001	1/1	1.00	0.06	-2.29	16,16,16,16	0
2	MG	A	3002	1/1	0.99	0.05	-2.30	15,15,15,15	0
3	NA	B	3102	1/1	1.00	0.05	-2.44	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	D	3001	1/1	0.99	0.05	-2.86	13,13,13,13	0
3	NA	D	3101	1/1	1.00	0.05	-3.06	16,16,16,16	0
3	NA	C	3103	1/1	0.98	0.06	-3.51	23,23,23,23	0
2	MG	C	3001	1/1	1.00	0.04	-3.54	13,13,13,13	0
4	DMS	C	8427	4/4	0.93	0.14	-	45,60,64,73	0
4	DMS	C	8504	4/4	0.95	0.12	-	31,35,50,66	0
4	DMS	B	8414	4/4	0.95	0.13	-	29,46,48,100	0
4	DMS	C	8414	4/4	0.98	0.09	-	21,30,46,50	0
4	DMS	D	8427	4/4	0.93	0.17	-	53,58,61,100	0
4	DMS	A	8414	4/4	0.96	0.14	-	29,30,52,100	0
4	DMS	D	8409	4/4	0.96	0.12	-	27,29,37,40	0
4	DMS	A	8413	4/4	0.94	0.13	-	31,40,40,44	0
4	DMS	C	8601	4/4	0.96	0.12	-	29,42,47,56	0
2	MG	D	3005	1/1	0.99	0.08	-	21,21,21,21	0
3	NA	A	3105	1/1	0.69	0.30	-	35,35,35,35	1
4	DMS	B	8416	4/4	0.94	0.16	-	30,40,50,52	0
4	DMS	A	8427	4/4	0.91	0.22	-	42,70,92,100	0
4	DMS	C	8503	4/4	0.93	0.14	-	28,49,51,55	0
4	DMS	A	8416	4/4	0.91	0.20	-	23,34,99,100	0
4	DMS	A	8410	4/4	0.97	0.12	-	22,33,34,34	0
4	DMS	B	8427	4/4	0.92	0.10	-	34,34,63,64	0
4	DMS	C	8416	4/4	0.94	0.20	-	40,48,58,61	0
3	NA	C	3105	1/1	0.90	0.13	-	28,28,28,28	1
2	MG	C	3004	1/1	0.95	0.19	-	36,36,36,36	0
4	DMS	A	8602	4/4	0.95	0.21	-	35,49,100,100	0
2	MG	A	3005	1/1	0.94	0.10	-	30,30,30,30	0
4	DMS	B	8410	4/4	0.95	0.14	-	25,34,35,42	0
4	DMS	D	8503	4/4	0.94	0.10	-	26,52,54,54	0
4	DMS	C	8415	4/4	0.93	0.10	-	22,33,34,42	0
4	DMS	D	8414	4/4	0.98	0.14	-	22,39,95,100	0
4	DMS	A	8421	4/4	0.92	0.18	-	49,54,57,60	0
2	MG	C	3006	1/1	0.98	0.16	-	27,27,27,27	0
4	DMS	C	8421	4/4	0.95	0.15	-	28,43,46,72	0
4	DMS	A	8409	4/4	0.97	0.17	-	24,32,43,100	0
2	MG	C	3003	1/1	0.92	0.11	-	22,22,22,22	1
4	DMS	B	8413	4/4	0.92	0.17	-	34,35,45,47	0
2	MG	D	3003	1/1	0.94	0.19	-	47,47,47,47	0
4	DMS	D	8413	4/4	0.97	0.14	-	26,34,34,44	0
3	NA	B	3105	1/1	0.91	0.11	-	31,31,31,31	1
2	MG	B	3003	1/1	0.91	0.12	-	34,34,34,34	0
4	DMS	C	8409	4/4	0.97	0.12	-	30,32,35,38	0
4	DMS	B	8415	4/4	0.89	0.12	-	26,29,34,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	DMS	B	8601	4/4	0.97	0.10	-	38,38,41,42	0
4	DMS	B	8409	4/4	0.96	0.10	-	26,28,37,38	0
4	DMS	D	8415	4/4	0.89	0.14	-	24,41,60,70	0
4	DMS	A	8415	4/4	0.93	0.14	-	21,32,59,100	0
4	DMS	D	8421	4/4	0.97	0.09	-	42,48,75,100	0
4	DMS	D	8416	4/4	0.93	0.17	-	27,41,49,100	0
4	DMS	C	8413	4/4	0.97	0.15	-	30,33,36,39	0
4	DMS	B	8421	4/4	0.94	0.13	-	28,50,52,58	0
4	DMS	A	8503	4/4	0.93	0.12	-	32,40,42,44	0
3	NA	D	3105	1/1	0.94	0.13	-	29,29,29,29	1
2	MG	A	3003	1/1	0.89	0.22	-	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.