



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:09 am GMT

PDB ID : 1JZ3
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-
GALACTOSYL ENZYME INTERMEDIATE
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 1.75 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

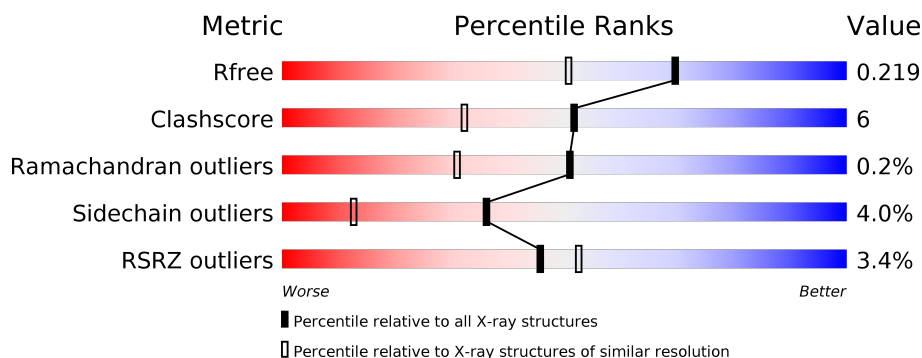
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	100719	1762 (1.76-1.76)
Clashscore	112137	1889 (1.76-1.76)
Ramachandran outliers	110173	1868 (1.76-1.76)
Sidechain outliers	110143	1868 (1.76-1.76)
RSRZ outliers	101464	1770 (1.76-1.76)

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> <div></div> <div>74%</div> <div>21%</div> <div>••</div> </div> </div>
1	B	1023	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>••</div> </div> </div>
1	C	1023	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>22%</div> <div>••</div> </div> </div>
1	D	1023	<div> <div>4%</div> <div> <div></div> <div>75%</div> <div>20%</div> <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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	2DG	A	2001	-	-	-	X
5	BTB	A	2002	-	-	-	X
6	DMS	A	8404	-	-	-	X
6	DMS	A	8406	-	-	-	X
6	DMS	A	8407	-	-	-	X
6	DMS	A	8417	-	-	-	X
6	DMS	A	8420	-	-	-	X
6	DMS	A	8423	-	-	-	X
6	DMS	A	8501	-	-	-	X
6	DMS	B	8405	-	-	-	X
6	DMS	B	8406	-	-	-	X
6	DMS	B	8407	-	-	-	X
6	DMS	B	8408	-	-	-	X
6	DMS	B	8420	-	-	-	X
6	DMS	B	8423	-	-	-	X
6	DMS	B	8425	-	-	-	X
6	DMS	B	8502	-	-	-	X
6	DMS	B	8508	-	-	-	X
6	DMS	C	8407	-	-	-	X
6	DMS	C	8419	-	-	-	X
6	DMS	C	8420	-	-	-	X
6	DMS	C	8423	-	-	-	X
6	DMS	C	8425	-	-	X	X
6	DMS	C	8501	-	-	-	X
6	DMS	D	8404	-	-	-	X
6	DMS	D	8407	-	-	-	X
6	DMS	D	8410	-	-	-	X
6	DMS	D	8417	-	-	-	X
6	DMS	D	8423	-	-	-	X
6	DMS	D	8425	-	-	-	X
6	DMS	D	8703	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 37369 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	1	0
			8131	5144	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:

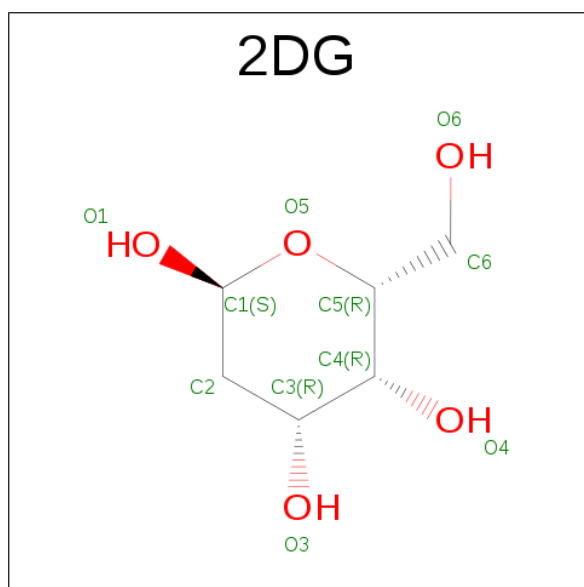
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	CLONING ARTIFACT	? P00722
A	2	SER	MET	CLONING ARTIFACT	? P00722
A	3	HIS	ILE	CLONING ARTIFACT	? P00722
A	4	MET	THR	CLONING ARTIFACT	? P00722
A	5	LEU	ASP	CLONING ARTIFACT	? P00722
A	6	GLU	SER	CLONING ARTIFACT	? P00722
A	7	ASP	LEU	CLONING ARTIFACT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

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

- Molecule 2 is SUGAR (2-DEOXY-BETA-D-GALACTOSE) (three-letter code: 2DG) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		
2	C	1	Total	C	O	0	0
			10	6	4		
2	D	1	Total	C	O	0	0
			10	6	4		

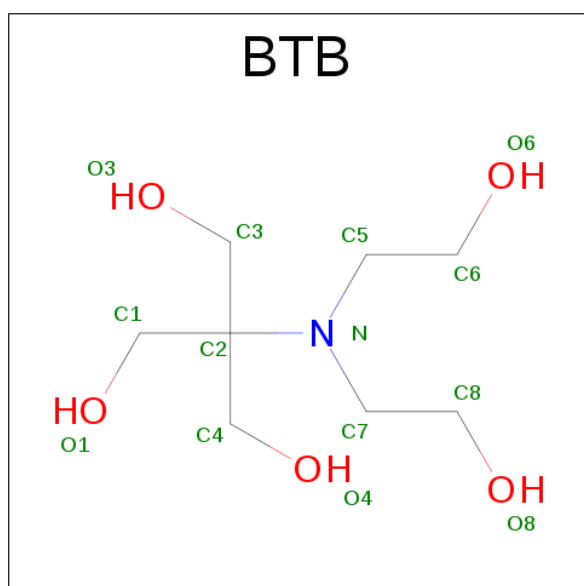
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	4	Total	Mg	0	0
			4	4		
3	D	4	Total	Mg	0	0
			4	4		
3	C	6	Total	Mg	0	0
			6	6		

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

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

- Molecule 5 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPAN E-1,3-DIOL (three-letter code: BTB) (formula: C₈H₁₉NO₅).



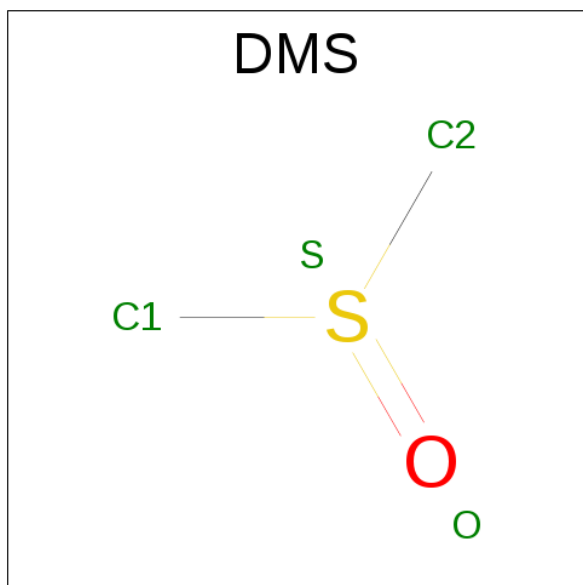
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 6 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1090	Total 1090	O 1090	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1091	Total 1091	O 1091	0	0
7	C	1034	Total 1034	O 1034	0	0
7	D	1079	Total 1079	O 1079	0	0

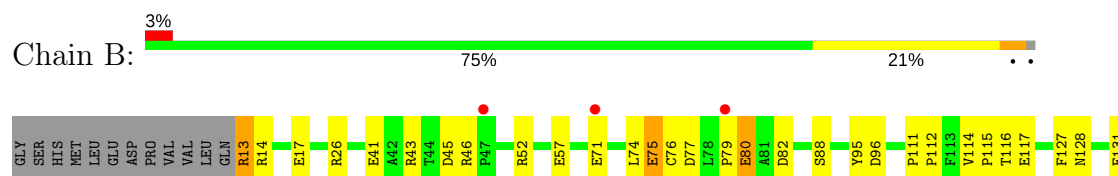
3 Residue-property plots

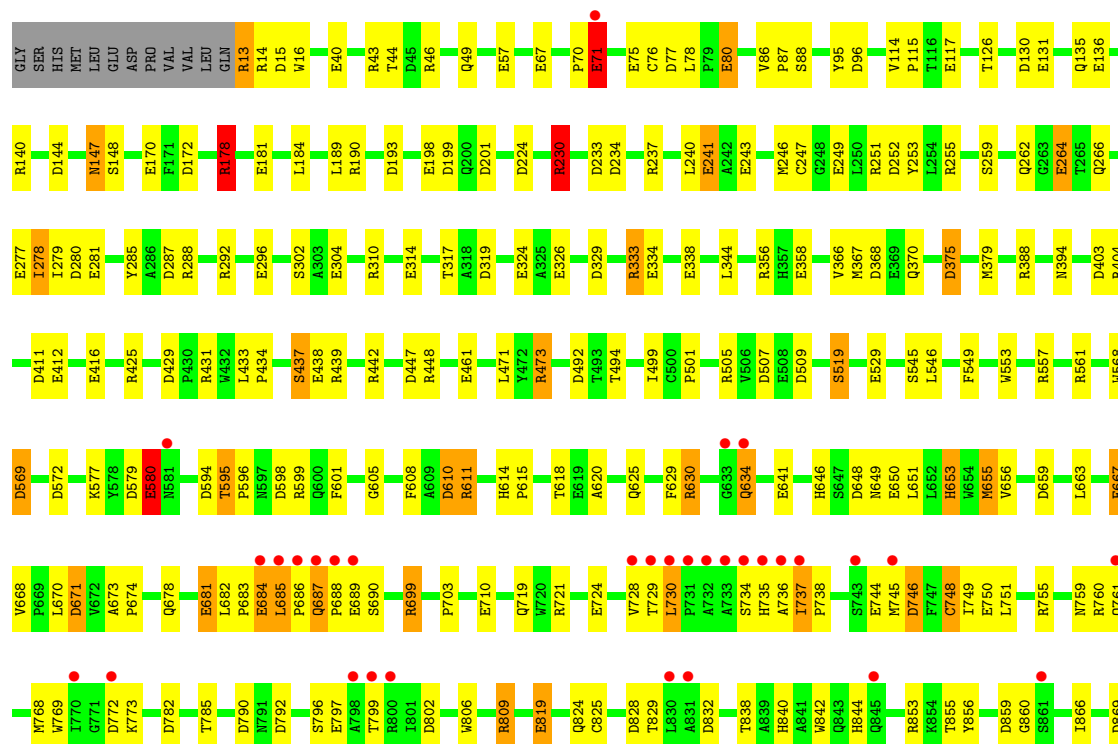
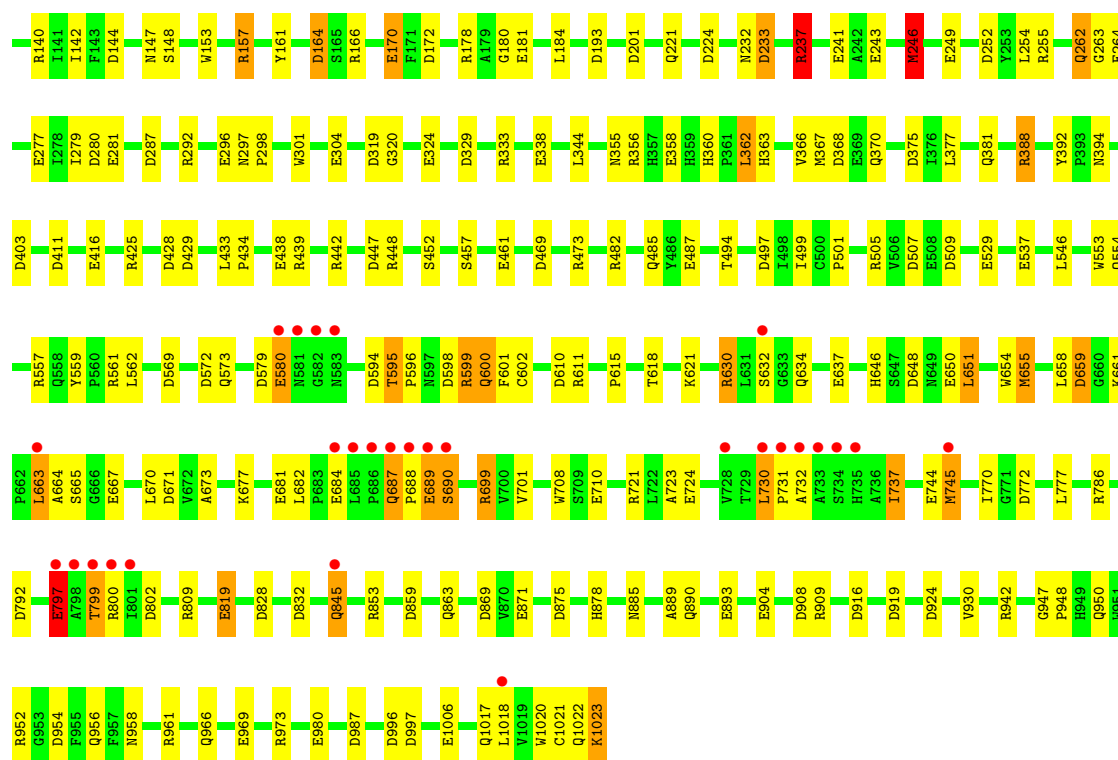
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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



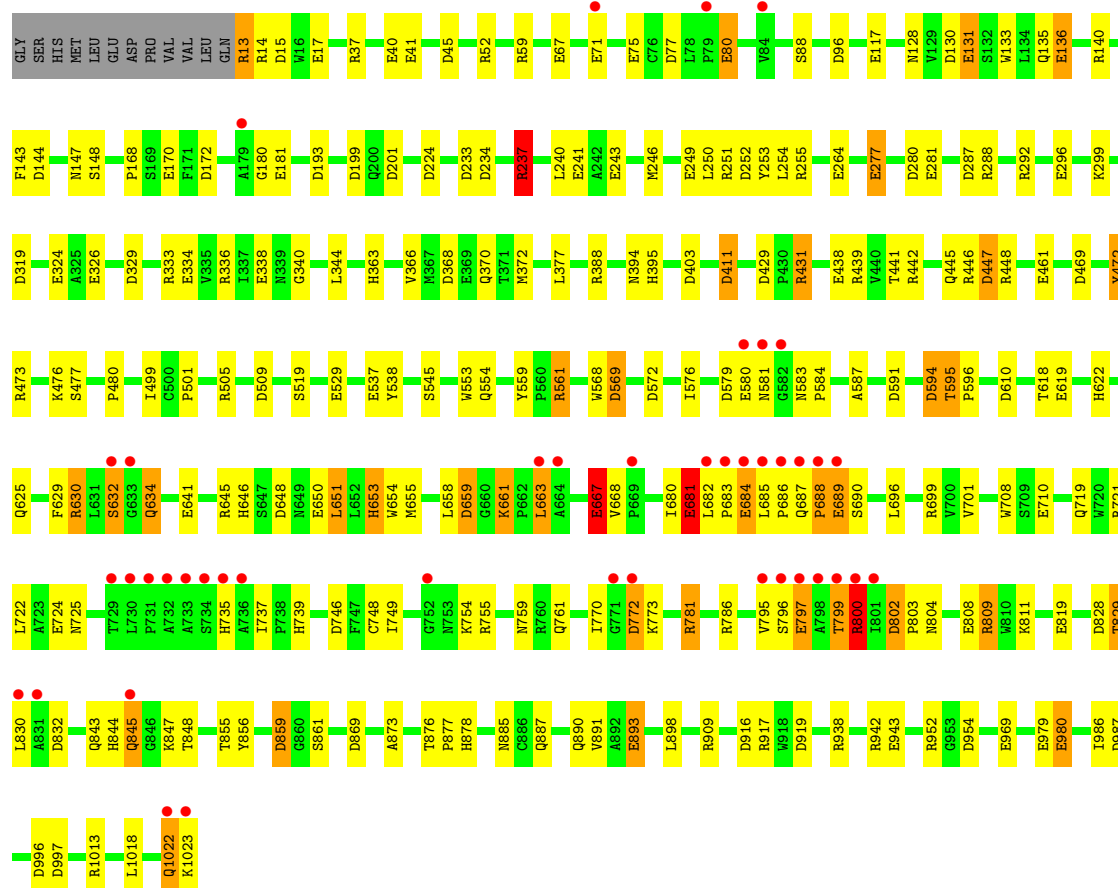
• Molecule 1: Beta-Galactosidase







• Molecule 1: Beta-Galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.56Å 168.19Å 200.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.00 – 1.75 15.97 – 1.75	Depositor EDS
% Data completeness (in resolution range)	93.8 (16.00-1.75) 93.4 (15.97-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 1.75Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.158 , 0.222 0.163 , 0.219	Depositor DCC
R_{free} test set	6833 reflections (1.47%)	DCC
Wilson B-factor (Å ²)	14.8	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 97.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	37369	wwPDB-VP
Average B, all atoms (Å ²)	23.0	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 36.43 % 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 5.0078e-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, 0.333 respectively for untwinned datasets, and 0.375, 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, 2DG, BTB

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.05	42/8367 (0.5%)	1.56	150/11415 (1.3%)
1	B	1.06	43/8379 (0.5%)	1.60	152/11431 (1.3%)
1	C	1.04	47/8367 (0.6%)	1.56	156/11415 (1.4%)
1	D	1.07	43/8367 (0.5%)	1.56	144/11415 (1.3%)
All	All	1.06	175/33480 (0.5%)	1.57	602/45676 (1.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	10.77	1.37	1.25
1	D	537	GLU	CD-OE2	8.83	1.35	1.25
1	B	461	GLU	CD-OE2	8.74	1.35	1.25
1	C	80	GLU	CD-OE2	8.60	1.35	1.25
1	D	75	GLU	CD-OE2	8.46	1.34	1.25
1	C	529	GLU	CD-OE2	8.33	1.34	1.25
1	B	650	GLU	CD-OE2	8.04	1.34	1.25
1	D	650	GLU	CD-OE2	7.95	1.34	1.25
1	A	487	GLU	CD-OE2	7.89	1.34	1.25
1	D	170	GLU	CD-OE2	7.78	1.34	1.25
1	A	537	GLU	CD-OE2	7.74	1.34	1.25
1	C	304	GLU	CD-OE2	7.70	1.34	1.25
1	D	461	GLU	CD-OE2	7.61	1.34	1.25
1	C	170	GLU	CD-OE2	7.61	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	243	GLU	CD-OE2	7.50	1.33	1.25
1	A	943	GLU	CD-OE2	7.48	1.33	1.25
1	B	71	GLU	CD-OE2	7.48	1.33	1.25
1	D	819	GLU	CD-OE2	7.38	1.33	1.25
1	D	980	GLU	CD-OE2	7.33	1.33	1.25
1	A	249	GLU	CD-OE2	7.33	1.33	1.25
1	B	689	GLU	CD-OE2	7.33	1.33	1.25
1	B	324	GLU	CD-OE2	7.30	1.33	1.25
1	A	681	GLU	CD-OE2	7.26	1.33	1.25
1	C	893	GLU	CD-OE2	7.21	1.33	1.25
1	D	40	GLU	CD-OE2	7.20	1.33	1.25
1	B	358	GLU	CD-OE2	7.09	1.33	1.25
1	A	296	GLU	CD-OE2	7.00	1.33	1.25
1	B	819	GLU	CD-OE2	6.97	1.33	1.25
1	A	969	GLU	CD-OE2	6.95	1.33	1.25
1	D	80	GLU	CD-OE2	6.93	1.33	1.25
1	C	461	GLU	CD-OE2	6.92	1.33	1.25
1	A	1006	GLU	CD-OE2	6.91	1.33	1.25
1	D	580	GLU	CD-OE2	6.90	1.33	1.25
1	C	416	GLU	CD-OE2	6.87	1.33	1.25
1	D	136	GLU	CD-OE2	6.83	1.33	1.25
1	A	689	GLU	CD-OE2	6.82	1.33	1.25
1	A	277	GLU	CD-OE2	6.81	1.33	1.25
1	A	580	GLU	CD-OE2	6.75	1.33	1.25
1	A	80	GLU	CD-OE2	6.74	1.33	1.25
1	C	744	GLU	CD-OE2	6.72	1.33	1.25
1	C	710	GLU	CD-OE2	6.68	1.32	1.25
1	D	681	GLU	CD-OE2	6.68	1.32	1.25
1	C	71	GLU	CD-OE2	6.67	1.32	1.25
1	D	667	GLU	CD-OE2	6.61	1.32	1.25
1	B	684	GLU	CD-OE2	6.60	1.32	1.25
1	A	71	GLU	CD-OE2	6.57	1.32	1.25
1	C	334	GLU	CD-OE2	6.56	1.32	1.25
1	C	934	GLU	CD-OE2	6.56	1.32	1.25
1	D	689	GLU	CD-OE2	6.55	1.32	1.25
1	A	170	GLU	CD-OE2	6.54	1.32	1.25
1	A	243	GLU	CD-OE2	6.53	1.32	1.25
1	C	684	GLU	CD-OE2	6.52	1.32	1.25
1	B	667	GLU	CD-OE2	6.50	1.32	1.25
1	B	1006	GLU	CD-OE2	6.50	1.32	1.25
1	A	819	GLU	CD-OE2	6.49	1.32	1.25
1	A	684	GLU	CD-OE2	6.48	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	GLU	CD-OE2	6.47	1.32	1.25
1	A	724	GLU	CD-OE2	6.45	1.32	1.25
1	C	580	GLU	CD-OE2	6.45	1.32	1.25
1	B	724	GLU	CD-OE2	6.44	1.32	1.25
1	B	529	GLU	CD-OE2	6.43	1.32	1.25
1	B	243	GLU	CD-OE2	6.42	1.32	1.25
1	D	979	GLU	CD-OE2	6.42	1.32	1.25
1	A	461	GLU	CD-OE2	6.41	1.32	1.25
1	B	710	GLU	CD-OE2	6.41	1.32	1.25
1	B	304	GLU	CD-OE2	6.36	1.32	1.25
1	A	980	GLU	CD-OE2	6.35	1.32	1.25
1	C	667	GLU	CD-OE2	6.35	1.32	1.25
1	D	893	GLU	CD-OE2	6.30	1.32	1.25
1	C	980	GLU	CD-OE2	6.30	1.32	1.25
1	C	819	GLU	CD-OE2	6.30	1.32	1.25
1	B	487	GLU	CD-OE2	6.29	1.32	1.25
1	B	580	GLU	CD-OE2	6.29	1.32	1.25
1	C	277	GLU	CD-OE2	6.28	1.32	1.25
1	A	710	GLU	CD-OE2	6.28	1.32	1.25
1	B	181	GLU	CD-OE2	6.28	1.32	1.25
1	C	281	GLU	CD-OE2	6.28	1.32	1.25
1	A	529	GLU	CD-OE2	6.25	1.32	1.25
1	B	744	GLU	CD-OE2	6.25	1.32	1.25
1	D	277	GLU	CD-OE2	6.24	1.32	1.25
1	C	198	GLU	CD-OE2	6.24	1.32	1.25
1	B	264	GLU	CD-OE2	6.22	1.32	1.25
1	D	684	GLU	CD-OE2	6.21	1.32	1.25
1	B	17	GLU	CD-OE2	6.20	1.32	1.25
1	B	980	GLU	CD-OE2	6.20	1.32	1.25
1	C	241	GLU	CD-OE2	6.18	1.32	1.25
1	A	979	GLU	CD-OE2	6.18	1.32	1.25
1	D	264	GLU	CD-OE2	6.18	1.32	1.25
1	C	136	GLU	CD-OE2	6.16	1.32	1.25
1	C	689	GLU	CD-OE2	6.14	1.32	1.25
1	C	326	GLU	CD-OE2	6.14	1.32	1.25
1	D	529	GLU	CD-OE2	6.10	1.32	1.25
1	B	797	GLU	CD-OE2	6.08	1.32	1.25
1	D	797	GLU	CD-OE2	6.07	1.32	1.25
1	C	296	GLU	CD-OE2	6.07	1.32	1.25
1	B	170	GLU	CD-OE2	6.05	1.32	1.25
1	D	17	GLU	CD-OE2	6.05	1.32	1.25
1	A	264	GLU	CD-OE2	6.05	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	277	GLU	CD-OE2	6.03	1.32	1.25
1	B	904	GLU	CD-OE2	6.03	1.32	1.25
1	C	75	GLU	CD-OE2	6.02	1.32	1.25
1	D	117	GLU	CD-OE2	6.02	1.32	1.25
1	A	131	GLU	CD-OE2	6.00	1.32	1.25
1	C	650	GLU	CD-OE2	6.00	1.32	1.25
1	A	797	GLU	CD-OE2	5.99	1.32	1.25
1	D	724	GLU	CD-OE2	5.99	1.32	1.25
1	B	969	GLU	CD-OE2	5.97	1.32	1.25
1	D	438	GLU	CD-OE2	5.94	1.32	1.25
1	D	943	GLU	CD-OE2	5.93	1.32	1.25
1	B	117	GLU	CD-OE2	5.89	1.32	1.25
1	B	241	GLU	CD-OE2	5.88	1.32	1.25
1	B	57	GLU	CD-OE2	5.86	1.32	1.25
1	B	537	GLU	CD-OE2	5.86	1.32	1.25
1	C	338	GLU	CD-OE2	5.86	1.32	1.25
1	C	681	GLU	CD-OE2	5.82	1.32	1.25
1	B	893	GLU	CD-OE2	5.79	1.32	1.25
1	A	641	GLU	CD-OE1	-5.78	1.19	1.25
1	A	338	GLU	CD-OE2	5.74	1.31	1.25
1	C	324	GLU	CD-OE2	5.71	1.31	1.25
1	C	724	GLU	CD-OE2	5.71	1.31	1.25
1	B	416	GLU	CD-OE2	5.69	1.31	1.25
1	C	750	GLU	CD-OE2	5.67	1.31	1.25
1	D	131	GLU	CD-OE2	5.66	1.31	1.25
1	D	334	GLU	CD-OE2	5.64	1.31	1.25
1	A	637	GLU	CD-OE2	5.64	1.31	1.25
1	B	80	GLU	CD-OE2	5.63	1.31	1.25
1	D	249	GLU	CD-OE2	5.63	1.31	1.25
1	D	241	GLU	CD-OE2	5.60	1.31	1.25
1	D	281	GLU	CD-OE2	5.60	1.31	1.25
1	B	131	GLU	CD-OE2	5.59	1.31	1.25
1	A	304	GLU	CD-OE2	5.58	1.31	1.25
1	C	57	GLU	CD-OE2	5.56	1.31	1.25
1	B	249	GLU	CD-OE2	5.55	1.31	1.25
1	B	296	GLU	CD-OE2	5.55	1.31	1.25
1	C	249	GLU	CD-OE2	5.55	1.31	1.25
1	B	871	GLU	CD-OE2	5.52	1.31	1.25
1	D	181	GLU	CD-OE2	5.51	1.31	1.25
1	D	710	GLU	CD-OE2	5.51	1.31	1.25
1	D	41	GLU	CD-OE1	-5.51	1.19	1.25
1	A	893	GLU	CD-OE2	5.50	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	117	GLU	CD-OE2	5.49	1.31	1.25
1	A	75	GLU	CD-OE2	5.48	1.31	1.25
1	D	324	GLU	CD-OE1	-5.45	1.19	1.25
1	C	314	GLU	CD-OE1	-5.45	1.19	1.25
1	C	412	GLU	CD-OE2	5.43	1.31	1.25
1	D	969	GLU	CD-OE2	5.42	1.31	1.25
1	C	641	GLU	CD-OE1	-5.40	1.19	1.25
1	C	358	GLU	CD-OE2	5.35	1.31	1.25
1	A	650	GLU	CD-OE2	5.35	1.31	1.25
1	D	338	GLU	CD-OE2	5.35	1.31	1.25
1	A	57	GLU	CD-OE2	5.30	1.31	1.25
1	B	75	GLU	CD-OE2	5.28	1.31	1.25
1	B	41	GLU	CD-OE2	5.28	1.31	1.25
1	A	667	GLU	CD-OE2	5.27	1.31	1.25
1	A	438	GLU	CD-OE2	5.25	1.31	1.25
1	C	243	GLU	CD-OE1	-5.24	1.19	1.25
1	A	198	GLU	CD-OE2	5.24	1.31	1.25
1	B	281	GLU	CD-OE2	5.24	1.31	1.25
1	B	681	GLU	CD-OE2	5.24	1.31	1.25
1	C	117	GLU	CD-OE2	5.24	1.31	1.25
1	D	296	GLU	CD-OE2	5.24	1.31	1.25
1	A	314	GLU	CD-OE1	-5.23	1.19	1.25
1	C	797	GLU	CD-OE2	5.20	1.31	1.25
1	D	641	GLU	CD-OE2	5.18	1.31	1.25
1	C	181	GLU	CD-OE2	5.17	1.31	1.25
1	A	41	GLU	CD-OE2	5.14	1.31	1.25
1	C	40	GLU	CD-OE2	5.14	1.31	1.25
1	A	41	GLU	CD-OE1	-5.10	1.20	1.25
1	C	969	GLU	CD-OE2	5.09	1.31	1.25
1	B	338	GLU	CD-OE2	5.07	1.31	1.25
1	D	67	GLU	CD-OE2	5.07	1.31	1.25
1	D	326	GLU	CD-OE2	5.03	1.31	1.25
1	C	67	GLU	CD-OE2	5.01	1.31	1.25
1	C	131	GLU	CD-OE2	5.01	1.31	1.25
1	C	264	GLU	CD-OE2	5.00	1.31	1.25

All (602) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	809	ARG	NE-CZ-NH1	21.36	130.98	120.30
1	B	699	ARG	NE-CZ-NH1	18.89	129.75	120.30
1	C	809	ARG	NE-CZ-NH1	17.33	128.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	699	ARG	NE-CZ-NH2	-16.56	112.02	120.30
1	B	809	ARG	NE-CZ-NH2	-15.81	112.39	120.30
1	B	442	ARG	NE-CZ-NH1	15.46	128.03	120.30
1	B	442	ARG	NE-CZ-NH2	-13.59	113.51	120.30
1	C	442	ARG	NE-CZ-NH2	-13.45	113.57	120.30
1	A	997	ASP	CB-CG-OD2	-13.45	106.19	118.30
1	A	442	ARG	NE-CZ-NH2	-12.50	114.05	120.30
1	C	431	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	D	781	ARG	NE-CZ-NH1	12.35	126.48	120.30
1	D	431	ARG	NE-CZ-NH2	-12.25	114.17	120.30
1	D	699	ARG	NE-CZ-NH1	11.91	126.25	120.30
1	C	721	ARG	NE-CZ-NH1	11.84	126.22	120.30
1	C	809	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	A	442	ARG	NE-CZ-NH1	11.28	125.94	120.30
1	D	439	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	B	252	ASP	CB-CG-OD2	-10.84	108.55	118.30
1	C	909	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	610	ASP	CB-CG-OD1	10.26	127.53	118.30
1	A	224	ASP	CB-CG-OD1	10.22	127.50	118.30
1	A	144	ASP	CB-CG-OD1	10.08	127.37	118.30
1	D	336	ARG	NE-CZ-NH1	10.07	125.34	120.30
1	A	172	ASP	CB-CG-OD2	-10.01	109.29	118.30
1	A	594	ASP	CB-CG-OD1	9.97	127.27	118.30
1	D	429	ASP	CB-CG-OD2	-9.94	109.35	118.30
1	D	942	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	659	ASP	CB-CG-OD2	-9.73	109.54	118.30
1	D	429	ASP	CB-CG-OD1	9.69	127.02	118.30
1	C	425	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	B	287	ASP	CB-CG-OD1	9.58	126.92	118.30
1	D	446	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	D	746	ASP	CB-CG-OD2	-9.54	109.72	118.30
1	A	336	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	D	594	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	B	648	ASP	CB-CG-OD2	-9.51	109.74	118.30
1	A	755	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	C	473	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	224	ASP	CB-CG-OD1	9.42	126.78	118.30
1	A	166	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	C	199	ASP	CB-CG-OD1	9.34	126.71	118.30
1	B	368	ASP	CB-CG-OD2	-9.34	109.90	118.30
1	D	388	ARG	NE-CZ-NH2	-9.34	115.63	120.30
1	B	557	ARG	NE-CZ-NH2	-9.27	115.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	425	ARG	NE-CZ-NH1	9.27	124.94	120.30
1	B	13	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	D	952	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	B	388	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	C	13	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	C	224	ASP	CB-CG-OD1	9.18	126.56	118.30
1	D	172	ASP	CB-CG-OD2	-9.18	110.04	118.30
1	A	130	ASP	CB-CG-OD2	-9.12	110.09	118.30
1	D	287	ASP	CB-CG-OD1	9.04	126.44	118.30
1	B	368	ASP	CB-CG-OD1	9.04	126.43	118.30
1	B	572	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	C	961	ARG	NE-CZ-NH1	8.98	124.79	120.30
1	A	997	ASP	CB-CG-OD1	8.96	126.36	118.30
1	B	828	ASP	CB-CG-OD2	-8.96	110.24	118.30
1	B	425	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	A	233	ASP	CB-CG-OD2	-8.88	110.31	118.30
1	D	469	ASP	CB-CG-OD1	8.86	126.28	118.30
1	A	172	ASP	CB-CG-OD1	8.82	126.24	118.30
1	D	869	ASP	CB-CG-OD1	8.81	126.22	118.30
1	B	505	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	D	786	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	A	431	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	987	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	875	ASP	CB-CG-OD1	8.71	126.14	118.30
1	C	43	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	B	448	ARG	NE-CZ-NH2	-8.71	115.95	120.30
1	C	802	ASP	CB-CG-OD1	8.69	126.12	118.30
1	C	952	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	D	721	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	C	233	ASP	CB-CG-OD1	8.69	126.12	118.30
1	A	908	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	859	ASP	CB-CG-OD1	8.65	126.09	118.30
1	B	809	ARG	CD-NE-CZ	8.65	135.70	123.60
1	B	909	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	B	942	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	B	367	MET	CG-SD-CE	8.60	113.95	100.20
1	B	594	ASP	CB-CG-OD1	8.55	125.99	118.30
1	C	310	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	659	ASP	CB-CG-OD1	8.53	125.98	118.30
1	C	579	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	857	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	572	ASP	CB-CG-OD1	8.50	125.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	ASP	CB-CG-OD1	8.47	125.93	118.30
1	C	579	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	D	746	ASP	CB-CG-OD1	8.47	125.92	118.30
1	A	233	ASP	CB-CG-OD1	8.43	125.88	118.30
1	A	755	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	B	859	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	D	859	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	D	144	ASP	CB-CG-OD1	8.39	125.85	118.30
1	B	557	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	234	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	A	634	GLN	N-CA-CB	8.36	125.65	110.60
1	B	356	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	C	442	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	A	509	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	954	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	B	671	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	A	699	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	C	648	ASP	CB-CG-OD2	-8.24	110.89	118.30
1	A	447	ASP	CB-CG-OD1	8.20	125.68	118.30
1	C	659	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	D	828	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	D	368	ASP	CB-CG-OD2	-8.18	110.94	118.30
1	D	37	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	B	469	ASP	CB-CG-OD1	8.14	125.63	118.30
1	C	802	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	B	356	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	859	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	233	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	D	15	ASP	CB-CG-OD2	-8.09	111.02	118.30
1	D	809	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	A	869	ASP	CB-CG-OD1	8.07	125.56	118.30
1	C	908	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	446	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	C	909	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	D	130	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	A	987	ASP	CB-CG-OD1	8.02	125.52	118.30
1	C	230	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	428	ASP	CB-CG-OD1	8.00	125.50	118.30
1	C	594	ASP	CB-CG-OD1	7.99	125.49	118.30
1	D	246	MET	CG-SD-CE	-7.98	87.43	100.20
1	A	234	ASP	CB-CG-OD1	7.96	125.46	118.30
1	A	439	ARG	NE-CZ-NH2	-7.93	116.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	ARG	NE-CZ-NH1	7.93	124.26	120.30
1	D	659	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	A	509	ASP	CB-CG-OD2	-7.92	111.17	118.30
1	D	802	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	D	287	ASP	CB-CG-OD2	-7.90	111.19	118.30
1	D	201	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	190	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	411	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	B	363	HIS	CA-CB-CG	-7.87	100.22	113.60
1	B	671	ASP	CB-CG-OD1	7.87	125.38	118.30
1	D	802	ASP	CB-CG-OD1	7.87	125.38	118.30
1	B	287	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	D	52	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	A	648	ASP	CB-CG-OD1	7.83	125.35	118.30
1	D	772	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	C	310	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	C	659	ASP	CB-CG-OD1	7.81	125.33	118.30
1	D	45	ASP	CB-CG-OD1	7.80	125.32	118.30
1	A	469	ASP	CB-CG-OD1	7.77	125.30	118.30
1	B	648	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	996	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	D	987	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	C	431	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	D	938	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	987	ASP	CB-CG-OD2	-7.69	111.38	118.30
1	C	509	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	403	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	746	ASP	CB-CG-OD2	-7.64	111.42	118.30
1	A	224	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	C	611	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	D	869	ASP	CB-CG-OD2	-7.61	111.45	118.30
1	B	828	ASP	CB-CG-OD1	7.61	125.15	118.30
1	A	411	ASP	CB-CG-OD1	7.56	125.10	118.30
1	A	403	ASP	CB-CG-OD1	7.55	125.10	118.30
1	C	996	ASP	CB-CG-OD1	7.54	125.09	118.30
1	A	859	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	C	557	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	D	917	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	C	439	ARG	NE-CZ-NH1	7.49	124.04	120.30
1	B	559	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	C	610	ASP	CB-CG-OD1	7.46	125.02	118.30
1	D	233	ASP	CB-CG-OD1	7.45	125.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	572	ASP	CB-CG-OD2	-7.44	111.60	118.30
1	A	388	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	B	45	ASP	CB-CG-OD1	7.43	124.99	118.30
1	C	875	ASP	CB-CG-OD1	7.38	124.94	118.30
1	B	594	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	A	210	ARG	NE-CZ-NH2	-7.35	116.63	120.30
1	B	699	ARG	CD-NE-CZ	7.33	133.87	123.60
1	C	961	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	C	997	ASP	CB-CG-OD1	7.33	124.89	118.30
1	A	201	ASP	CB-CG-OD2	-7.33	111.71	118.30
1	C	144	ASP	CB-CG-OD1	7.33	124.89	118.30
1	C	388	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	B	553	TRP	CA-CB-CG	-7.32	99.79	113.70
1	B	561	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	C	439	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	469	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	D	632	SER	N-CA-CB	7.25	121.38	110.50
1	D	469	ASP	CB-CG-OD2	-7.24	111.78	118.30
1	B	958	ASN	N-CA-CB	7.24	123.62	110.60
1	B	572	ASP	CB-CG-OD1	7.23	124.80	118.30
1	B	319	ASP	CB-CG-OD1	7.20	124.78	118.30
1	C	772	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	C	828	ASP	CB-CG-OD2	-7.18	111.84	118.30
1	C	924	ASP	CB-CG-OD1	7.18	124.76	118.30
1	C	509	ASP	CB-CG-OD2	-7.17	111.85	118.30
1	D	786	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	C	610	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	B	429	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	C	13	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	C	594	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	D	59	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	B	792	ASP	CB-CG-OD1	7.11	124.70	118.30
1	B	255	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	D	403	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	C	375	ASP	CB-CG-OD1	7.09	124.68	118.30
1	C	572	ASP	CB-CG-OD2	-7.07	111.93	118.30
1	D	172	ASP	CB-CG-OD1	7.07	124.66	118.30
1	A	632	SER	N-CA-CB	7.07	121.10	110.50
1	D	237	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	C	505	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	246	MET	CG-SD-CE	-7.04	88.94	100.20
1	C	561	ARG	NE-CZ-NH2	-7.02	116.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	594	ASP	CB-CG-OD1	7.02	124.62	118.30
1	D	648	ASP	CB-CG-OD2	-7.02	111.98	118.30
1	D	431	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	A	594	ASP	CB-CG-OD2	-6.96	112.03	118.30
1	C	507	ASP	CB-CG-OD1	6.96	124.56	118.30
1	C	473	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	610	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	D	579	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	802	ASP	CB-CG-OD1	6.93	124.53	118.30
1	C	368	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	D	447	ASP	CB-CG-OD1	6.92	124.53	118.30
1	C	76	CYS	N-CA-CB	-6.89	98.19	110.60
1	B	77	ASP	CB-CG-OD2	-6.88	112.10	118.30
1	B	233	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	B	853	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	448	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	802	ASP	CB-CG-OD1	6.83	124.45	118.30
1	A	247	CYS	CA-CB-SG	-6.82	101.72	114.00
1	B	786	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	329	ASP	CB-CG-OD2	-6.81	112.17	118.30
1	B	319	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	916	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	857	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	B	869	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	C	388	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	853	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	D	193	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	13	ARG	NE-CZ-NH2	-6.73	116.93	120.30
1	C	77	ASP	CB-CG-OD1	6.73	124.36	118.30
1	D	288	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	D	559	TYR	CB-CG-CD2	-6.71	116.97	121.00
1	C	43	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	B	569	ASP	CB-CG-OD1	6.69	124.32	118.30
1	C	190	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	C	719	GLN	CB-CA-C	-6.68	97.03	110.40
1	C	429	ASP	CB-CG-OD1	6.68	124.31	118.30
1	D	233	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	D	832	ASP	CB-CG-OD2	-6.64	112.32	118.30
1	C	553	TRP	CA-CB-CG	-6.64	101.09	113.70
1	A	996	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	166	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	B	832	ASP	CB-CG-OD1	6.62	124.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	D	800	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	996	ASP	CB-CG-OD1	6.56	124.20	118.30
1	B	611	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	853	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	C	199	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	C	869	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	439	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	428	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	15	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	A	439	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	746	ASP	CB-CA-C	-6.52	97.36	110.40
1	B	721	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	C	630	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	A	809	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	497	ASP	CB-CG-OD1	6.51	124.16	118.30
1	B	96	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	C	411	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	403	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	D	252	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	772	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	C	404	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	336	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	659	ASP	CB-CG-OD1	6.47	124.12	118.30
1	C	869	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	595	THR	CA-CB-CG2	-6.46	103.35	112.40
1	A	469	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	D	800	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	671	ASP	CB-CG-OD2	-6.45	112.50	118.30
1	C	924	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	C	859	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	909	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	792	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	D	996	ASP	CB-CG-OD2	-6.42	112.53	118.30
1	D	442	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	D	919	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	B	1018	LEU	CB-CA-C	-6.41	98.03	110.20
1	B	473	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	579	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	B	908	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	772	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	280	ASP	CB-CG-OD1	6.40	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ASP	CB-CG-OD1	6.38	124.04	118.30
1	C	367	MET	CB-CA-C	-6.38	97.64	110.40
1	C	193	ASP	CB-CG-OD1	6.37	124.04	118.30
1	A	859	ASP	CB-CG-OD1	6.37	124.03	118.30
1	C	859	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	C	140	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	D	224	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	B	832	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	C	997	ASP	CB-CG-OD2	-6.33	112.60	118.30
1	C	856	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	B	659	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	B	375	ASP	CB-CG-OD1	6.32	123.98	118.30
1	D	439	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	954	ASP	CB-CG-OD1	6.29	123.96	118.30
1	D	329	ASP	CB-CG-OD1	6.29	123.96	118.30
1	A	572	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	630	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	429	ASP	CB-CG-OD1	6.28	123.95	118.30
1	A	1021	CYS	CA-CB-SG	-6.28	102.70	114.00
1	C	790	ASP	CB-CG-OD1	6.25	123.93	118.30
1	B	632	SER	N-CA-CB	6.25	119.88	110.50
1	C	403	ASP	CB-CG-OD2	-6.25	112.67	118.30
1	A	924	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	B	997	ASP	N-CA-CB	6.24	121.82	110.60
1	A	559	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	C	987	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	482	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	C	492	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	B	996	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	76	CYS	CA-CB-SG	-6.20	102.84	114.00
1	A	579	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	D	561	ARG	NE-CZ-NH1	6.20	123.40	120.30
1	C	178	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	D	255	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	D	446	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	B	954	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	C	184	LEU	CB-CA-C	-6.17	98.48	110.20
1	A	832	ASP	CB-CG-OD1	6.16	123.85	118.30
1	A	252	ASP	CB-CG-OD2	-6.16	112.75	118.30
1	B	13	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	46	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	D	15	ASP	CB-CG-OD1	6.15	123.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	770	ILE	CA-CB-CG1	-6.15	99.32	111.00
1	B	579	ASP	CB-CG-OD1	6.14	123.83	118.30
1	D	448	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	C	881	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	C	130	ASP	CB-CG-OD1	6.12	123.81	118.30
1	D	509	ASP	CB-CG-OD1	6.12	123.80	118.30
1	B	869	ASP	CB-CG-OD1	6.11	123.80	118.30
1	D	411	ASP	CB-CG-OD1	6.09	123.78	118.30
1	D	130	ASP	CB-CG-OD1	6.06	123.76	118.30
1	D	699	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	1018	LEU	CB-CA-C	-6.06	98.68	110.20
1	A	438	GLU	CG-CD-OE2	-6.06	106.18	118.30
1	A	82	ASP	CB-CG-OD1	6.06	123.75	118.30
1	C	333	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	C	746	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	D	193	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	43	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	B	45	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	C	429	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	D	997	ASP	N-CA-CB	5.99	121.38	110.60
1	A	672	VAL	CG1-CB-CG2	5.98	120.47	110.90
1	A	178	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	172	ASP	CB-CG-OD1	5.97	123.67	118.30
1	A	648	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	A	768	MET	CA-CB-CG	5.96	123.42	113.30
1	B	507	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	509	ASP	CB-CG-OD1	5.95	123.65	118.30
1	A	828	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	199	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	96	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	280	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	D	856	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	A	211	ASP	CB-CG-OD1	5.93	123.64	118.30
1	C	234	ASP	CB-CG-OD1	5.93	123.64	118.30
1	D	199	ASP	CB-CG-OD1	5.93	123.64	118.30
1	A	96	ASP	N-CA-CB	5.92	121.26	110.60
1	C	958	ASN	N-CA-CB	5.92	121.25	110.60
1	B	77	ASP	CB-CG-OD1	5.91	123.62	118.30
1	C	630	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	A	917	ARG	NE-CZ-NH1	-5.91	117.34	120.30
1	D	855	THR	N-CA-CB	5.91	121.53	110.30
1	C	147	ASN	N-CA-CB	-5.89	100.00	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	719	GLN	CB-CA-C	-5.89	98.62	110.40
1	D	45	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	D	288	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	782	ASP	CB-CG-OD2	-5.88	113.00	118.30
1	C	77	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	B	723	ALA	CB-CA-C	-5.87	101.30	110.10
1	A	497	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	C	598	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	D	234	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	144	ASP	CB-CG-OD2	-5.84	113.05	118.30
1	A	890	GLN	N-CA-CB	-5.84	100.09	110.60
1	B	280	ASP	CB-CG-OD2	-5.84	113.04	118.30
1	A	251	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	A	579	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	832	ASP	N-CA-CB	-5.83	100.10	110.60
1	B	246	MET	CG-SD-CE	-5.83	90.86	100.20
1	B	193	ASP	CB-CG-OD1	5.83	123.55	118.30
1	C	832	ASP	CB-CG-OD1	5.83	123.55	118.30
1	D	980	GLU	C-N-CA	-5.83	110.06	122.30
1	C	748	CYS	CA-CB-SG	-5.82	103.52	114.00
1	A	46	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	648	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	438	GLU	CG-CD-OE2	-5.81	106.68	118.30
1	D	52	ARG	CB-CA-C	-5.81	98.78	110.40
1	B	505	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	653	HIS	N-CA-CB	5.79	121.02	110.60
1	D	96	ASP	N-CA-CB	5.78	121.00	110.60
1	B	237	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	172	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	A	553	TRP	CA-CB-CG	-5.75	102.77	113.70
1	C	906	TYR	CB-CG-CD2	-5.75	117.55	121.00
1	A	429	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	477	SER	N-CA-CB	5.75	119.12	110.50
1	D	13	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	D	553	TRP	CA-CB-CG	-5.75	102.78	113.70
1	C	782	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	746	ASP	CB-CG-OD1	5.74	123.47	118.30
1	C	792	ASP	CB-CG-OD1	5.74	123.47	118.30
1	B	292	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	D	140	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	253	TYR	CB-CG-CD1	-5.73	117.56	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	772	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	909	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	C	572	ASP	CB-CG-OD1	5.71	123.44	118.30
1	C	996	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	428	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	140	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	867	THR	CA-CB-CG2	-5.69	104.43	112.40
1	B	279	ILE	CA-CB-CG2	5.69	122.28	110.90
1	D	630	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	C	259	SER	CB-CA-C	5.68	120.90	110.10
1	C	721	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	C	890	GLN	N-CA-CB	-5.67	100.39	110.60
1	B	201	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	C	140	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	D	772	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	193	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	875	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	B	329	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	832	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	43	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	D	559	TYR	CB-CG-CD1	5.63	124.38	121.00
1	D	144	ASP	CB-CG-OD2	-5.62	113.24	118.30
1	A	147	ASN	N-CA-CB	-5.61	100.50	110.60
1	A	15	ASP	CB-CG-OD1	5.61	123.35	118.30
1	B	201	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	587	ALA	CB-CA-C	-5.61	101.69	110.10
1	B	329	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	252	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	82	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	494	THR	CA-CB-CG2	-5.59	104.57	112.40
1	B	52	ARG	CB-CA-C	-5.59	99.22	110.40
1	C	252	ASP	CB-CG-OD2	-5.58	113.27	118.30
1	D	234	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	800	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	B	908	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	741	THR	CA-CB-CG2	-5.57	104.61	112.40
1	B	924	ASP	CB-CG-OD1	5.56	123.30	118.30
1	C	302	SER	N-CA-CB	5.55	118.83	110.50
1	A	924	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	908	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	B	916	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	329	ASP	CB-CG-OD1	5.53	123.28	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	GLN	N-CA-CB	-5.53	100.64	110.60
1	A	61	ALA	N-CA-CB	5.51	117.82	110.10
1	C	671	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	B	116	THR	CA-CB-CG2	-5.51	104.69	112.40
1	A	546	LEU	N-CA-CB	5.50	121.41	110.40
1	A	952	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	771	GLY	C-N-CA	-5.49	107.96	121.70
1	B	772	ASP	CB-CG-OD1	5.48	123.23	118.30
1	D	781	ARG	CD-NE-CZ	5.48	131.28	123.60
1	A	782	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	431	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	310	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	599	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	A	14	ARG	N-CA-CB	-5.47	100.76	110.60
1	A	356	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	C	411	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	280	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	442	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	A	329	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	D	610	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	95	TYR	CB-CG-CD2	-5.43	117.74	121.00
1	C	96	ASP	N-CA-CB	5.42	120.36	110.60
1	C	447	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	A	909	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	234	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	569	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	329	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	D	579	ASP	CB-CG-OD1	5.41	123.17	118.30
1	C	201	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	B	610	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	770	ILE	N-CA-C	-5.40	96.42	111.00
1	A	201	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	699	ARG	CB-CA-C	-5.38	99.63	110.40
1	A	13	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	D	505	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	247	CYS	CA-CB-SG	-5.36	104.35	114.00
1	D	388	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	C	403	ASP	CB-CG-OD1	5.36	123.12	118.30
1	B	919	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	C	15	ASP	CB-CG-OD1	5.34	123.11	118.30
1	A	225	PHE	N-CA-CB	5.34	120.21	110.60
1	B	659	ASP	CB-CG-OD1	5.34	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	919	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	287	ASP	CB-CG-OD1	5.33	123.09	118.30
1	B	392	TYR	CG-CD2-CE2	5.33	125.56	121.30
1	D	538	TYR	CB-CG-CD2	5.33	124.20	121.00
1	C	126	THR	CA-CB-CG2	-5.32	104.95	112.40
1	D	324	GLU	N-CA-CB	5.32	120.18	110.60
1	B	954	ASP	CB-CG-OD1	5.32	123.09	118.30
1	D	252	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	369	GLU	CG-CD-OE2	-5.31	107.68	118.30
1	B	224	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	224	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	C	230	ARG	CD-NE-CZ	5.30	131.02	123.60
1	A	1018	LEU	CB-CA-C	-5.29	100.15	110.20
1	B	438	GLU	CG-CD-OE2	-5.29	107.73	118.30
1	B	144	ASP	CB-CG-OD1	5.28	123.06	118.30
1	A	185	ALA	N-CA-CB	5.28	117.49	110.10
1	B	157	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	D	472	TYR	CB-CG-CD1	5.28	124.17	121.00
1	D	591	ASP	CB-CG-OD1	5.27	123.04	118.30
1	B	509	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	B	598	ASP	CB-CG-OD2	-5.26	113.57	118.30
1	D	80	GLU	OE1-CD-OE2	5.26	129.61	123.30
1	D	591	ASP	CB-CG-OD2	-5.25	113.57	118.30
1	A	45	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	634	GLN	CB-CA-C	5.24	120.88	110.40
1	C	130	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	942	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	C	368	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	144	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	997	ASP	N-CA-CB	5.23	120.01	110.60
1	B	598	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	255	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	A	251	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	645	ARG	NE-CZ-NH1	-5.21	117.69	120.30
1	D	916	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	714	ILE	CA-CB-CG1	-5.21	101.10	111.00
1	B	164	ASP	CB-CG-OD1	5.20	122.98	118.30
1	C	287	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	497	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	1019	VAL	CA-CB-CG2	-5.18	103.12	110.90
1	C	906	TYR	CB-CG-CD1	5.18	124.11	121.00
1	A	672	VAL	CA-CB-CG1	5.18	118.67	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	782	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	280	ASP	CB-CG-OD1	5.17	122.96	118.30
1	C	601	PHE	CB-CG-CD2	-5.17	117.18	120.80
1	A	519	SER	N-CA-CB	-5.17	102.74	110.50
1	A	869	ASP	CB-CG-OD2	-5.17	113.65	118.30
1	C	855	THR	N-CA-CB	5.15	120.09	110.30
1	A	319	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	D	280	ASP	CB-CG-OD1	5.15	122.93	118.30
1	C	319	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	1020	TRP	CB-CA-C	-5.14	100.11	110.40
1	D	319	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	C	519	SER	N-CA-CB	-5.14	102.79	110.50
1	C	569	ASP	CB-CG-OD1	5.14	122.92	118.30
1	D	645	ARG	NE-CZ-NH2	5.13	122.87	120.30
1	B	403	ASP	CB-CG-OD2	-5.13	113.68	118.30
1	A	721	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	B	161	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	C	344	LEU	CA-CB-CG	-5.13	103.51	115.30
1	A	991	MET	CG-SD-CE	5.12	108.40	100.20
1	D	829	THR	N-CA-CB	5.12	120.03	110.30
1	B	95	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	C	448	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	288	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	958	ASN	N-CA-CB	5.12	119.81	110.60
1	C	842	TRP	CA-CB-CG	-5.12	103.98	113.70
1	D	954	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	C	840	HIS	CB-CA-C	-5.11	100.18	110.40
1	A	447	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	A	368	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	D	77	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	292	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	D	719	GLN	CB-CA-C	-5.09	100.21	110.40
1	C	545	SER	N-CA-CB	-5.09	102.86	110.50
1	D	14	ARG	N-CA-CB	-5.09	101.44	110.60
1	A	96	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	497	ASP	CB-CG-OD2	-5.08	113.72	118.30
1	D	832	ASP	CB-CG-OD1	5.08	122.87	118.30
1	C	681	GLU	C-N-CA	-5.08	109.00	121.70
1	C	838	THR	CA-CB-CG2	-5.07	105.30	112.40
1	D	809	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	B	924	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	D	477	SER	N-CA-CB	5.07	118.10	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	ARG	CD-NE-CZ	5.06	130.68	123.60
1	B	987	ASP	CB-CG-OD1	5.05	122.85	118.30
1	D	411	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	26	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	140	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	172	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	C	388	ARG	CG-CD-NE	5.01	122.33	111.80
1	C	629	PHE	CB-CA-C	-5.01	100.38	110.40
1	D	319	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	221	GLN	N-CA-CB	-5.01	101.59	110.60
1	A	285	TYR	CB-CG-CD2	-5.00	118.00	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	634	GLN	CA

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8125	0	7716	105	0
1	B	8131	0	7721	88	0
1	C	8125	0	7716	105	0
1	D	8125	0	7716	105	0
2	A	10	0	9	0	0
2	B	10	0	9	0	0
2	C	10	0	9	0	0
2	D	10	0	10	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	6	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	14	0	19	0	0
5	B	14	0	19	0	0
5	C	14	0	19	1	0
5	D	14	0	19	1	0
6	A	108	0	162	9	0
6	B	108	0	162	7	0
6	C	112	0	168	10	0
6	D	112	0	168	9	0
7	A	1090	0	0	17	1
7	B	1091	0	0	9	1
7	C	1034	0	0	14	0
7	D	1079	0	0	19	0
All	All	37369	0	31642	415	1

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

All (415) 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)
6:B:8508:DMS:C1	6:B:8508:DMS:S	2.06	1.42
6:B:8407:DMS:S	6:B:8407:DMS:C2	2.10	1.39
1:C:634:GLN:H	1:C:634:GLN:NE2	1.37	1.21
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.41	1.16
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.41	1.16
1:B:655:MET:HE2	1:B:665:SER:HB3	1.31	1.08
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.25	1.02
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.25	0.97
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.49	0.94
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.84	0.92
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.34	0.90
1:A:804:ASN:HA	1:A:809:ARG:NH1	1.87	0.89
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.04	0.88
1:B:600:GLN:H	1:B:600:GLN:HE21	1.18	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.04	0.87
1:C:634:GLN:NE2	1:C:634:GLN:N	2.22	0.87
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.57	0.86
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.40	0.82
1:D:237:ARG:HG2	1:D:237:ARG:HH11	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:658:LEU:O	1:D:661:LYS:HG3	1.81	0.81
1:A:787:ALA:HA	1:A:968:MET:HG3	1.63	0.81
1:C:703:PRO:HG2	6:C:8425:DMS:H13	1.63	0.80
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.62	0.80
1:D:663:LEU:CD1	1:D:686:PRO:HG2	2.11	0.80
1:A:237:ARG:HB3	1:A:237:ARG:NH1	1.97	0.80
1:A:797:GLU:O	1:A:801:ILE:HD13	1.83	0.77
1:B:651:LEU:O	1:B:651:LEU:HD23	1.83	0.77
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.65	0.77
1:D:663:LEU:HD13	1:D:686:PRO:HG2	1.66	0.77
1:A:1022:GLN:HG2	1:A:1023:LYS:N	1.99	0.77
1:A:237:ARG:HH11	1:A:237:ARG:CB	1.98	0.77
6:A:8503:DMS:H23	7:A:8976:HOH:O	1.85	0.77
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.66	0.76
1:C:634:GLN:H	1:C:634:GLN:HE21	1.27	0.76
1:D:629:PHE:O	1:D:630:ARG:HD3	1.86	0.75
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.68	0.75
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.67	0.74
1:D:887:GLN:NE2	1:D:980:GLU:O	2.20	0.74
1:B:737:ILE:HD11	7:B:9591:HOH:O	1.88	0.74
1:A:600:GLN:H	1:A:600:GLN:HE21	1.35	0.73
1:C:230:ARG:HD2	7:C:8959:HOH:O	1.89	0.71
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.72	0.70
1:C:824:GLN:HG2	1:C:825:CYS:N	2.05	0.70
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.27	0.70
1:C:703:PRO:HG2	6:C:8425:DMS:C1	2.20	0.70
1:D:748:CYS:C	1:D:749:ILE:HD12	2.13	0.69
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.72	0.69
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.08	0.69
6:A:8420:DMS:H21	7:D:9523:HOH:O	1.92	0.69
1:A:800:ARG:HB3	7:A:9395:HOH:O	1.92	0.68
1:A:832:ASP:OD1	1:A:832:ASP:N	2.27	0.68
1:D:749:ILE:N	1:D:749:ILE:HD12	2.08	0.68
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.75	0.68
1:B:262:GLN:HE21	1:B:263:GLY:N	1.92	0.68
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.24	0.68
1:B:878:HIS:HD2	7:B:8695:HOH:O	1.76	0.68
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.08	0.68
1:D:133:TRP:HE1	6:D:8703:DMS:H23	1.59	0.67
1:C:749:ILE:HD12	1:C:749:ILE:N	2.10	0.67
6:B:8410:DMS:H13	7:B:9151:HOH:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:878:HIS:HD2	7:C:8695:HOH:O	1.76	0.67
1:B:845:GLN:OE1	1:B:845:GLN:HA	1.95	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.07	0.66
1:A:878:HIS:HD2	7:A:8674:HOH:O	1.78	0.66
1:D:128:ASN:HB3	1:D:180:GLY:O	1.95	0.66
1:B:494:THR:HB	1:C:473:ARG:NH2	2.11	0.66
1:C:356:ARG:HD2	1:C:379:MET:CE	2.23	0.66
1:C:690:SER:HB2	7:C:9380:HOH:O	1.95	0.66
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.26	0.66
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.11	0.66
1:D:237:ARG:NH1	7:D:9273:HOH:O	2.28	0.66
6:D:8703:DMS:H23	7:D:9706:HOH:O	1.96	0.66
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.60	0.65
1:A:754:LYS:NZ	7:A:9527:HOH:O	2.30	0.65
1:D:685:LEU:HB3	1:D:686:PRO:HD2	1.77	0.65
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.31	0.65
1:A:887:GLN:NE2	1:A:980:GLU:O	2.29	0.65
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.77	0.65
1:D:653:HIS:CE1	1:D:701:VAL:HG21	2.32	0.64
1:C:748:CYS:C	1:C:749:ILE:HD12	2.17	0.64
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.08	0.64
1:A:277:GLU:H	1:A:277:GLU:CD	1.99	0.64
6:D:8421:DMS:H11	7:D:9361:HOH:O	1.97	0.64
1:C:651:LEU:C	1:C:651:LEU:HD12	2.17	0.64
1:A:655:MET:HE2	1:A:656:VAL:N	2.12	0.64
1:C:651:LEU:O	1:C:651:LEU:HD12	1.98	0.64
1:D:254:LEU:HD12	7:D:9641:HOH:O	1.97	0.63
1:D:292:ARG:HH12	6:D:8412:DMS:C2	2.11	0.63
1:A:431:ARG:HG3	7:A:9378:HOH:O	1.97	0.63
1:A:648:ASP:OD2	7:A:9548:HOH:O	2.15	0.63
1:B:262:GLN:HE21	1:B:262:GLN:C	2.01	0.62
1:C:278:ILE:HD13	1:C:278:ILE:N	2.13	0.62
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.80	0.62
1:B:797:GLU:CG	1:B:799:THR:HG23	2.28	0.62
1:B:637:GLU:OE2	1:B:677:LYS:HE3	2.00	0.62
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.80	0.62
1:D:725:ASN:HB2	7:D:9581:HOH:O	1.99	0.61
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.33	0.61
1:A:976:LEU:HB2	6:A:8423:DMS:H11	1.82	0.61
1:D:1022:GLN:O	1:D:1022:GLN:HG3	1.98	0.61
1:A:658:LEU:O	1:A:661:LYS:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:SER:HA	1:C:366:VAL:HG21	1.82	0.61
1:D:878:HIS:HD2	7:D:8814:HOH:O	1.83	0.61
1:D:135:GLN:C	1:D:136:GLU:HG2	2.22	0.60
1:C:730:LEU:HD23	1:C:730:LEU:N	2.16	0.60
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.83	0.60
1:C:237:ARG:CB	1:C:237:ARG:HH11	2.13	0.60
1:A:241:GLU:OE2	1:A:292:ARG:NE	2.28	0.60
1:A:809:ARG:CG	1:A:809:ARG:HH11	2.15	0.60
1:D:292:ARG:HH12	6:D:8412:DMS:H21	1.66	0.60
1:D:663:LEU:HD13	1:D:686:PRO:CG	2.32	0.59
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.85	0.59
1:D:618:THR:HG21	7:D:9054:HOH:O	2.02	0.59
1:D:809:ARG:NH1	1:D:809:ARG:HG2	2.09	0.59
1:C:890:GLN:HG3	1:C:891:VAL:N	2.18	0.59
1:C:703:PRO:HD2	6:C:8425:DMS:H11	1.84	0.59
1:B:599:ARG:NH1	1:B:601[A]:PHE:CD1	2.71	0.59
1:A:687:GLN:HG3	7:A:9467:HOH:O	2.02	0.59
1:C:595:THR:HA	1:C:596:PRO:C	2.23	0.58
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.03	0.58
6:C:8427:DMS:H21	7:C:9057:HOH:O	2.02	0.58
1:A:699:ARG:NH2	7:A:9471:HOH:O	2.35	0.57
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.39	0.57
1:D:809:ARG:CG	1:D:809:ARG:HH11	2.14	0.57
1:C:240:LEU:HD23	1:C:240:LEU:C	2.25	0.57
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.73	0.57
1:A:237:ARG:NH1	7:A:9138:HOH:O	2.29	0.57
1:C:687:GLN:HE21	1:C:687:GLN:HA	1.69	0.57
1:C:730:LEU:HD23	1:C:730:LEU:H	1.67	0.57
1:D:595:THR:HA	1:D:596:PRO:C	2.25	0.56
5:C:2002:BTB:O8	5:C:2002:BTB:H62	2.05	0.56
1:C:730:LEU:CD2	1:C:730:LEU:H	2.18	0.56
1:D:799:THR:OG1	1:D:800:ARG:N	2.38	0.56
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.88	0.56
1:A:651:LEU:HD12	1:A:651:LEU:C	2.26	0.56
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.39	0.56
1:C:866:ILE:O	1:C:1017:GLN:NE2	2.36	0.56
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.88	0.56
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.06	0.56
1:A:803:PRO:O	1:A:809:ARG:NH1	2.38	0.55
1:A:473:ARG:HH12	1:A:476:LYS:HB2	1.71	0.55
1:B:157:ARG:HD3	7:B:9476:HOH:O	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:GLU:OE1	1:B:75:GLU:HA	2.06	0.55
1:A:595:THR:HA	1:A:596:PRO:C	2.27	0.55
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.88	0.55
1:C:649:ASN:HA	6:C:8425:DMS:C1	2.37	0.55
1:B:950:GLN:OE1	1:B:952:ARG:HD3	2.07	0.55
1:A:735:HIS:O	1:A:736:ALA:HB2	2.07	0.54
1:B:615:PRO:O	1:B:618:THR:HG22	2.08	0.54
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.43	0.54
1:A:178:ARG:HD2	7:A:9497:HOH:O	2.07	0.54
1:D:133:TRP:HE1	6:D:8703:DMS:C2	2.20	0.54
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.42	0.54
1:B:79:PRO:HD2	1:B:80:GLU:OE2	2.07	0.54
1:D:878:HIS:HE1	7:D:9399:HOH:O	1.91	0.54
1:B:320:GLY:O	6:B:8406:DMS:O	2.26	0.54
1:B:595:THR:HA	1:B:596:PRO:C	2.28	0.54
1:D:135:GLN:O	1:D:136:GLU:HG2	2.07	0.54
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.73	0.54
1:A:88:SER:HA	1:A:366:VAL:HG21	1.90	0.54
1:D:847:LYS:HG3	1:D:848:THR:N	2.17	0.54
1:A:718:GLN:CD	6:A:8503:DMS:H13	2.28	0.53
1:B:178:ARG:HG3	1:B:178:ARG:O	2.08	0.53
1:C:649:ASN:HA	6:C:8425:DMS:H12	1.90	0.53
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.76	0.53
1:C:745:MET:HE3	1:C:745:MET:HA	1.91	0.53
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.92	0.53
1:C:241:GLU:OE1	1:C:292:ARG:NE	2.41	0.53
1:D:685:LEU:HB3	1:D:686:PRO:CD	2.39	0.52
1:A:1017:GLN:HG3	1:A:1018:LEU:N	2.16	0.52
6:A:8423:DMS:H13	7:A:9155:HOH:O	2.09	0.52
1:C:266:GLN:O	6:C:8602:DMS:H22	2.09	0.52
1:B:651:LEU:C	1:B:651:LEU:HD23	2.29	0.52
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.44	0.52
1:A:1022:GLN:C	1:A:1023:LYS:HG3	2.30	0.52
1:C:178:ARG:HD2	7:C:9553:HOH:O	2.09	0.52
1:D:554:GLN:NE2	7:D:9666:HOH:O	2.24	0.52
1:B:634:GLN:HG2	1:B:682:LEU:O	2.10	0.52
1:B:596:PRO:HB3	7:B:9423:HOH:O	2.09	0.52
6:C:8407:DMS:H21	7:C:9561:HOH:O	2.08	0.52
1:B:599:ARG:HH11	1:B:599:ARG:CG	2.16	0.51
1:C:46:ARG:HG2	7:C:9538:HOH:O	2.10	0.51
1:A:768:MET:HE3	1:A:1020:TRP:CZ2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:615:PRO:O	1:A:618:THR:HG22	2.11	0.51
1:B:797:GLU:HG2	1:B:799:THR:CG2	2.38	0.51
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.92	0.51
1:D:749:ILE:N	1:D:749:ILE:CD1	2.73	0.51
6:B:8407:DMS:C1	6:B:8407:DMS:C2	2.88	0.51
1:A:264:GLU:HG3	7:A:9518:HOH:O	2.11	0.51
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.46	0.51
1:B:599:ARG:HH12	1:B:601[A]:PHE:HE1	1.50	0.50
1:D:754:LYS:HE2	1:D:1022:GLN:HG2	1.92	0.50
1:D:584:PRO:HD2	7:D:9453:HOH:O	2.11	0.50
1:C:630:ARG:HH11	1:C:630:ARG:CB	2.25	0.50
1:D:651:LEU:HD12	1:D:651:LEU:O	2.11	0.50
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.09	0.50
1:C:736:ALA:O	1:C:860:GLY:HA3	2.12	0.50
1:D:363:HIS:HD2	7:D:9324:HOH:O	1.93	0.50
1:C:13:ARG:O	1:C:14:ARG:C	2.50	0.49
1:C:16:TRP:CG	1:C:189:LEU:HD13	2.47	0.49
1:C:759:ASN:OD1	1:C:761:GLN:N	2.44	0.49
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.42	0.49
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.30	0.49
1:D:131:GLU:OE2	1:D:131:GLU:O	2.30	0.49
1:D:651:LEU:HD12	1:D:651:LEU:C	2.33	0.49
1:D:859:ASP:OD1	1:D:861:SER:HB2	2.12	0.49
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.95	0.49
1:B:689:GLU:O	1:B:690:SER:OG	2.29	0.49
1:D:797:GLU:HB3	1:D:799:THR:HG23	1.95	0.49
1:D:844:HIS:O	1:D:845:GLN:HB2	2.13	0.49
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.28	0.49
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.47	0.49
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.73	0.49
1:C:634:GLN:H	1:C:634:GLN:CD	2.08	0.49
1:A:680:ILE:HG12	7:A:9249:HOH:O	2.13	0.48
1:C:728:VAL:O	1:C:730:LEU:HD23	2.13	0.48
1:C:824:GLN:CG	1:C:825:CYS:N	2.75	0.48
1:D:809:ARG:CG	1:D:809:ARG:NH1	2.75	0.48
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.95	0.48
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.14	0.48
1:D:795:VAL:HG12	6:D:8506:DMS:C1	2.43	0.48
1:B:88:SER:HA	1:B:366:VAL:HG21	1.95	0.48
1:D:441:THR:O	1:D:445:GLN:HG3	2.13	0.48
1:D:843:GLN:HB3	1:D:847:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.13	0.48
1:D:634:GLN:NE2	1:D:682:LEU:O	2.46	0.48
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.32	0.48
1:B:381:GLN:O	1:B:621:LYS:HE3	2.14	0.48
1:C:671:ASP:N	1:C:678:GLN:OE1	2.28	0.48
1:A:809:ARG:HH11	1:A:809:ARG:HG3	1.79	0.48
1:A:890:GLN:HG3	1:A:891:VAL:N	2.28	0.48
1:C:44:THR:OG1	1:C:46:ARG:HD3	2.14	0.47
1:D:739:HIS:HB2	7:D:9753:HOH:O	2.15	0.47
1:D:795:VAL:HG12	6:D:8506:DMS:H13	1.96	0.47
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.49	0.47
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.79	0.47
1:B:573:GLN:HB2	1:B:602:CYS:O	2.13	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.49	0.47
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.77	0.47
1:D:890:GLN:HG3	1:D:891:VAL:N	2.30	0.47
1:A:372:MET:HE1	1:A:395:HIS:HB3	1.97	0.47
1:A:668:VAL:HG12	1:A:669:PRO:O	2.14	0.47
1:C:651:LEU:CD1	1:C:653:HIS:ND1	2.77	0.47
1:B:1017:GLN:HB2	7:B:9592:HOH:O	2.14	0.47
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.47
1:D:340:GLY:O	1:D:561:ARG:HG2	2.15	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.58	0.47
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.43	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.95	0.47
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.73	0.47
1:C:749:ILE:N	1:C:749:ILE:CD1	2.77	0.47
1:C:86:VAL:HG13	1:C:87:PRO:HA	1.97	0.47
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.49	0.47
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.30	0.46
6:A:8409:DMS:O	7:A:9110:HOH:O	2.20	0.46
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.97	0.46
1:B:127:PHE:N	1:B:127:PHE:CD2	2.83	0.46
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.98	0.46
1:B:730:LEU:H	1:B:730:LEU:HG	1.27	0.46
1:A:809:ARG:CG	1:A:809:ARG:NH1	2.78	0.46
1:B:595:THR:O	1:B:595:THR:HG23	2.15	0.46
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.97	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.16	0.46
1:D:653:HIS:ND1	1:D:701:VAL:CG2	2.77	0.46
1:D:696:LEU:HB2	1:D:722:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.75	0.46
1:B:494:THR:HB	1:C:473:ARG:HH21	1.81	0.46
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.66	0.46
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.98	0.46
1:C:751:LEU:HD21	1:C:860:GLY:O	2.16	0.46
1:D:250:LEU:O	1:D:251:ARG:HG2	2.17	0.45
1:C:745:MET:HE3	1:C:745:MET:CA	2.45	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.45
1:A:663:LEU:HD11	1:A:688:PRO:HG3	1.96	0.45
1:B:777:LEU:HG	1:B:889:ALA:HA	1.99	0.45
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.45
1:A:178:ARG:HG3	7:A:9497:HOH:O	2.16	0.45
1:B:147:ASN:HA	1:B:148:SER:HA	1.59	0.45
1:D:688:PRO:C	1:D:690:SER:H	2.20	0.45
1:A:128:ASN:HB2	7:A:9543:HOH:O	2.17	0.45
1:A:251:ARG:HH11	6:A:8416:DMS:H11	1.82	0.45
1:C:646:HIS:HB3	7:C:9488:HOH:O	2.17	0.45
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.52	0.45
1:B:377:LEU:O	1:B:381:GLN:HG3	2.16	0.45
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.52	0.45
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.43	0.45
1:B:599:ARG:NH1	1:B:601[A]:PHE:CE1	2.74	0.45
1:C:253:TYR:CD1	1:C:317:THR:HG22	2.52	0.45
1:D:545:SER:O	1:D:909:ARG:HD3	2.17	0.45
1:A:361:PRO:HB2	1:A:576:ILE:HG12	1.99	0.44
1:C:114:VAL:HB	1:C:115:PRO:CD	2.47	0.44
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.72	0.44
1:A:742:THR:HG22	1:A:743:SER:N	2.31	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.60	0.44
1:C:433:LEU:O	1:C:437:SER:HB3	2.17	0.44
1:D:808:GLU:OE2	1:D:811:LYS:NZ	2.49	0.44
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.80	0.44
1:C:577:LYS:HE3	1:C:577:LYS:HB3	1.88	0.44
1:C:667:GLU:C	1:C:668:VAL:HG23	2.38	0.44
1:D:668:VAL:HG11	1:D:680:ILE:HG12	1.99	0.44
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.52	0.44
1:D:133:TRP:NE1	6:D:8703:DMS:H23	2.30	0.44
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.99	0.44
1:A:84:VAL:HA	6:A:8414:DMS:O	2.17	0.44
6:C:8410:DMS:H13	7:C:8966:HOH:O	2.17	0.44
1:C:844:HIS:HD2	7:C:9471:HOH:O	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:687:GLN:HE21	1:B:687:GLN:N	2.15	0.44
1:D:651:LEU:CD1	1:D:653:HIS:CE1	3.00	0.44
1:D:663:LEU:HD11	1:D:686:PRO:HG2	1.96	0.44
1:B:599:ARG:NH1	1:B:601[A]:PHE:HD1	2.16	0.43
7:B:9403:HOH:O	6:C:8420:DMS:H21	2.17	0.43
1:B:630:ARG:HH21	1:B:637:GLU:CD	2.21	0.43
1:C:569:ASP:O	1:C:605:GLY:HA2	2.19	0.43
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.54	0.43
1:D:802:ASP:O	1:D:808:GLU:HG3	2.18	0.43
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.54	0.43
1:D:659:ASP:HB3	1:D:898:LEU:HD21	2.01	0.43
1:A:127:PHE:CD2	1:A:127:PHE:N	2.86	0.43
1:A:843:GLN:HA	1:A:847:LYS:O	2.18	0.43
1:B:114:VAL:HB	1:B:115:PRO:HD2	2.01	0.43
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.18	0.43
1:B:128:ASN:HA	1:B:180:GLY:O	2.19	0.43
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.86	0.43
1:D:829:THR:O	1:D:830:LEU:HD23	2.19	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.18	0.43
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.54	0.43
1:D:651:LEU:C	1:D:651:LEU:CD1	2.87	0.43
1:A:433:LEU:N	1:A:434:PRO:CD	2.82	0.43
1:A:600:GLN:N	1:A:600:GLN:HE21	2.09	0.42
1:B:745:MET:SD	1:B:745:MET:N	2.75	0.42
1:D:843:GLN:HA	1:D:847:LYS:O	2.19	0.42
1:D:873:ALA:O	1:D:876:THR:HG22	2.19	0.42
1:C:230:ARG:HB3	7:C:9557:HOH:O	2.18	0.42
1:C:49:GLN:HG2	7:C:9326:HOH:O	2.18	0.42
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.42
1:A:658:LEU:O	1:A:659:ASP:C	2.55	0.42
1:B:13:ARG:O	1:B:14:ARG:C	2.57	0.42
1:B:233:ASP:HA	6:B:8417:DMS:C1	2.49	0.42
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.42
1:B:663:LEU:HD22	1:B:663:LEU:HA	1.60	0.42
1:D:646:HIS:ND1	7:D:9585:HOH:O	2.37	0.42
1:A:873:ALA:O	1:A:876:THR:HG22	2.20	0.42
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.45	0.42
1:A:701:VAL:O	1:A:703:PRO:HD3	2.20	0.42
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.84	0.42
1:C:785:THR:O	1:C:881:ARG:HD2	2.19	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:HH11	6:A:8416:DMS:C1	2.33	0.42
1:B:246:MET:HE1	1:B:254:LEU:HD13	2.02	0.42
1:D:372:MET:HE1	1:D:395:HIS:HB3	2.01	0.42
1:D:681:GLU:HG2	7:D:9468:HOH:O	2.19	0.42
1:B:297:ASN:N	1:B:298:PRO:CD	2.83	0.42
5:D:2002:BTB:H51	5:D:2002:BTB:H31	1.73	0.42
1:D:619:GLU:HG2	1:D:909:ARG:HG3	2.02	0.42
1:A:781:ARG:NH1	7:A:9346:HOH:O	2.53	0.42
1:B:433:LEU:N	1:B:434:PRO:CD	2.83	0.42
1:C:580:GLU:HG3	1:C:580:GLU:H	1.26	0.42
1:D:622:HIS:O	1:D:625:GLN:HG3	2.20	0.42
1:A:685:LEU:HD22	1:A:686:PRO:HD2	2.01	0.41
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.84	0.41
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.57	0.41
1:C:285:TYR:HB3	1:C:288:ARG:HG3	2.01	0.41
1:D:377:LEU:HD22	1:D:708:TRP:HA	2.02	0.41
1:A:742:THR:CG2	1:A:743:SER:N	2.84	0.41
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.02	0.41
1:D:682:LEU:HA	1:D:682:LEU:HD23	1.77	0.41
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.35	0.41
1:A:990:HIS:HD2	1:A:991:MET:O	2.03	0.41
1:B:966:GLN:HG3	7:B:9663:HOH:O	2.20	0.41
1:A:685:LEU:CD2	1:A:686:PRO:HD3	2.51	0.41
1:A:753:ASN:OD1	1:A:753:ASN:N	2.53	0.41
1:C:670:LEU:HA	1:C:670:LEU:HD23	1.89	0.41
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.55	0.41
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.20	0.41
1:A:745:MET:HE2	1:A:745:MET:HB3	1.75	0.41
1:C:279:ILE:HA	1:C:279:ILE:HD13	1.87	0.41
1:C:625:GLN:NE2	7:C:8824:HOH:O	2.50	0.41
1:D:654:TRP:CZ2	1:D:683:PRO:HG2	2.56	0.41
1:D:781:ARG:NH1	7:D:9479:HOH:O	2.36	0.41
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.41
1:A:753:ASN:OD1	1:A:754:LYS:HG3	2.20	0.41
1:B:890:GLN:HB3	7:B:9443:HOH:O	2.21	0.41
1:C:655:MET:SD	1:C:656:VAL:N	2.93	0.41
1:D:240:LEU:HD23	1:D:240:LEU:C	2.41	0.41
1:D:618:THR:HG23	7:D:9070:HOH:O	2.20	0.41
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.50	0.41
1:A:427:THR:HG21	1:A:462:SER:HB3	2.02	0.41
1:B:961:ARG:HG3	6:B:8508:DMS:H23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LEU:CD2	1:C:730:LEU:N	2.78	0.41
1:C:883:GLY:HA3	1:C:987:ASP:HA	2.03	0.41
1:D:143:PHE:O	1:D:168:PRO:HA	2.20	0.41
1:D:472:TYR:O	1:D:476:LYS:HG2	2.20	0.41
1:A:685:LEU:CD2	1:A:686:PRO:CD	2.99	0.41
1:A:804:ASN:HA	1:A:809:ARG:CZ	2.50	0.41
1:A:473:ARG:HA	1:A:473:ARG:HD2	1.85	0.41
1:B:1023:LYS:HE3	1:B:1023:LYS:HB3	1.66	0.41
1:B:658:LEU:O	1:B:659:ASP:C	2.58	0.41
1:C:71:GLU:N	7:C:9383:HOH:O	2.53	0.40
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.21	0.40
1:A:337:ILE:HA	1:A:341:LEU:O	2.21	0.40
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.21	0.40
1:B:301:TRP:CH2	1:B:452:SER:HA	2.56	0.40
1:B:562:LEU:HA	1:B:562:LEU:HD23	1.83	0.40
1:B:655:MET:HE2	1:B:664:ALA:O	2.22	0.40
1:B:930:VAL:HA	1:B:973:ARG:HD3	2.03	0.40
1:C:471:LEU:HA	1:C:471:LEU:HD23	1.95	0.40
1:B:111:PRO:HA	1:B:112:PRO:HA	1.86	0.40
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.02	0.40
1:B:457:SER:HA	1:B:485:GLN:O	2.22	0.40
1:A:557:ARG:HD2	1:A:557:ARG:HH11	1.72	0.40
1:A:685:LEU:CB	1:A:686:PRO:CD	2.99	0.40
1:A:861:SER:OG	1:A:863:GLN:HG3	2.22	0.40
1:D:431:ARG:HD2	7:D:9514:HOH:O	2.21	0.40
1:D:583:ASN:HB3	7:D:9453:HOH:O	2.20	0.40
1:D:759:ASN:OD1	1:D:761:GLN:N	2.47	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:9544:HOH:O	7:B:9658:HOH:O[2_454]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1009/1023 (99%)	974 (96%)	34 (3%)	1 (0%)	55 35
1	B	1010/1023 (99%)	969 (96%)	36 (4%)	5 (0%)	32 13
1	C	1009/1023 (99%)	975 (97%)	34 (3%)	0	100 100
1	D	1009/1023 (99%)	970 (96%)	38 (4%)	1 (0%)	55 35
All	All	4037/4092 (99%)	3888 (96%)	142 (4%)	7 (0%)	51 31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	731	PRO
1	B	732	ALA
1	D	688	PRO
1	B	690	SER
1	A	164	ASP
1	B	164	ASP
1	B	688	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	864/875 (99%)	834 (96%)	30 (4%)	41 16
1	B	865/875 (99%)	835 (96%)	30 (4%)	41 16
1	C	864/875 (99%)	824 (95%)	40 (5%)	31 10
1	D	864/875 (99%)	825 (96%)	39 (4%)	32 10
All	All	3457/3500 (99%)	3318 (96%)	139 (4%)	36 13

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	237	ARG
1	A	333	ARG
1	A	370	GLN
1	A	394	ASN
1	A	519	SER
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	655	MET
1	A	661	LYS
1	A	663	LEU
1	A	667	GLU
1	A	684	GLU
1	A	729	THR
1	A	730	LEU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	796	SER
1	A	797	GLU
1	A	799	THR
1	A	800	ARG
1	A	801	ILE
1	A	809	ARG
1	A	817	GLN
1	A	885	ASN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	237	ARG
1	B	246	MET
1	B	262	GLN
1	B	333	ARG
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	394	ASN
1	B	546	LEU
1	B	554	GLN
1	B	580	GLU
1	B	599	ARG
1	B	600	GLN

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Mol	Chain	Res	Type
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	687	GLN
1	B	699	ARG
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	797	GLU
1	B	799	THR
1	B	800	ARG
1	B	819	GLU
1	B	845	GLN
1	B	885	ASN
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	230	ARG
1	C	251	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	370	GLN
1	C	394	ASN
1	C	437	SER
1	C	519	SER
1	C	546	LEU
1	C	580	GLU
1	C	595	THR
1	C	634	GLN
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN

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Mol	Chain	Res	Type
1	C	699	ARG
1	C	729	THR
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	773	LYS
1	C	796	SER
1	C	799	THR
1	C	819	GLU
1	C	829	THR
1	C	893	GLU
1	C	986	ILE
1	C	1017	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	80	GLU
1	D	237	ARG
1	D	277	GLU
1	D	299	LYS
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	480	PRO
1	D	519	SER
1	D	581	ASN
1	D	594	ASP
1	D	595	THR
1	D	632	SER
1	D	634	GLN
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	667	GLU
1	D	681	GLU
1	D	684	GLU
1	D	687	GLN
1	D	689	GLU
1	D	735	HIS
1	D	737	ILE

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Mol	Chain	Res	Type
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	796	SER
1	D	799	THR
1	D	800	ARG
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1013	ARG
1	D	1022	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	600	GLN
1	A	624	GLN
1	A	675	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	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	687	GLN
1	B	863	GLN
1	B	878	HIS
1	B	977	HIS
1	C	163	GLN
1	C	266	GLN
1	C	614	HIS
1	C	624	GLN
1	C	634	GLN
1	C	646	HIS
1	C	687	GLN
1	C	817	GLN

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Mol	Chain	Res	Type
1	C	878	HIS
1	D	135	GLN
1	D	363	HIS
1	D	624	GLN
1	D	628	GLN
1	D	704	ASN
1	D	804	ASN
1	D	878	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 151 ligands modelled in this entry, 33 are monoatomic - leaving 118 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2DG	A	2001	1,4	10,10,11	0.79	0	10,13,15	1.69	1 (10%)
5	BTB	A	2002	-	13,13,13	1.54	3 (23%)	9,16,16	1.21	1 (11%)
6	DMS	A	8401	-	3,3,3	0.73	0	3,3,3	0.47	0
6	DMS	A	8402	-	3,3,3	0.99	0	3,3,3	0.49	0
6	DMS	A	8403	-	3,3,3	2.02	2 (66%)	3,3,3	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	A	8404	-	3,3,3	1.10	0	3,3,3	0.18	0
6	DMS	A	8405	-	3,3,3	0.50	0	3,3,3	0.47	0
6	DMS	A	8406	-	3,3,3	0.61	0	3,3,3	0.86	0
6	DMS	A	8407	-	3,3,3	1.55	0	3,3,3	0.66	0
6	DMS	A	8408	-	3,3,3	0.66	0	3,3,3	0.44	0
6	DMS	A	8409	-	3,3,3	2.35	1 (33%)	3,3,3	0.19	0
6	DMS	A	8410	-	3,3,3	0.73	0	3,3,3	0.84	0
6	DMS	A	8411	-	3,3,3	0.91	0	3,3,3	0.39	0
6	DMS	A	8412	-	3,3,3	0.39	0	3,3,3	0.25	0
6	DMS	A	8413	-	3,3,3	1.56	0	3,3,3	0.08	0
6	DMS	A	8414	-	3,3,3	1.11	0	3,3,3	0.23	0
6	DMS	A	8416	-	3,3,3	0.48	0	3,3,3	0.36	0
6	DMS	A	8417	-	3,3,3	1.26	0	3,3,3	0.13	0
6	DMS	A	8419	-	3,3,3	0.57	0	3,3,3	0.32	0
6	DMS	A	8420	-	3,3,3	0.79	0	3,3,3	1.06	0
6	DMS	A	8421	-	3,3,3	0.79	0	3,3,3	0.50	0
6	DMS	A	8423	-	3,3,3	1.28	1 (33%)	3,3,3	0.26	0
6	DMS	A	8425	4	3,3,3	1.38	1 (33%)	3,3,3	0.56	0
6	DMS	A	8501	-	3,3,3	1.16	0	3,3,3	0.12	0
6	DMS	A	8502	-	3,3,3	1.94	1 (33%)	3,3,3	1.07	0
6	DMS	A	8503	-	3,3,3	0.46	0	3,3,3	0.30	0
6	DMS	A	8504	-	3,3,3	0.60	0	3,3,3	0.26	0
6	DMS	A	8506	-	3,3,3	1.02	0	3,3,3	0.42	0
6	DMS	A	8602	-	3,3,3	0.67	0	3,3,3	0.29	0
2	2DG	B	2001	1,4	10,10,11	0.91	0	10,13,15	1.01	0
5	BTB	B	2002	-	13,13,13	1.38	2 (15%)	9,16,16	1.00	0
6	DMS	B	8401	-	3,3,3	0.35	0	3,3,3	0.36	0
6	DMS	B	8402	-	3,3,3	0.97	0	3,3,3	0.70	0
6	DMS	B	8403	-	3,3,3	1.03	0	3,3,3	0.24	0
6	DMS	B	8404	-	3,3,3	0.77	0	3,3,3	0.22	0
6	DMS	B	8405	-	3,3,3	1.35	1 (33%)	3,3,3	0.52	0
6	DMS	B	8406	-	3,3,3	1.18	0	3,3,3	0.44	0
6	DMS	B	8407	-	3,3,3	2.91	2 (66%)	3,3,3	0.30	0
6	DMS	B	8408	-	3,3,3	0.45	0	3,3,3	0.06	0
6	DMS	B	8409	-	3,3,3	1.45	1 (33%)	3,3,3	0.76	0
6	DMS	B	8410	-	3,3,3	0.59	0	3,3,3	0.47	0
6	DMS	B	8411	-	3,3,3	1.22	0	3,3,3	0.56	0
6	DMS	B	8412	-	3,3,3	0.90	0	3,3,3	0.27	0
6	DMS	B	8413	-	3,3,3	1.84	1 (33%)	3,3,3	0.43	0
6	DMS	B	8414	-	3,3,3	0.94	0	3,3,3	0.33	0
6	DMS	B	8415	-	3,3,3	1.98	1 (33%)	3,3,3	1.18	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	B	8416	-	3,3,3	1.45	1 (33%)	3,3,3	0.51	0
6	DMS	B	8417	-	3,3,3	0.46	0	3,3,3	0.48	0
6	DMS	B	8420	-	3,3,3	1.65	1 (33%)	3,3,3	0.79	0
6	DMS	B	8421	-	3,3,3	0.27	0	3,3,3	0.45	0
6	DMS	B	8423	-	3,3,3	0.55	0	3,3,3	0.58	0
6	DMS	B	8425	4	3,3,3	2.27	2 (66%)	3,3,3	0.32	0
6	DMS	B	8427	-	3,3,3	0.74	0	3,3,3	0.16	0
6	DMS	B	8502	-	3,3,3	0.76	0	3,3,3	1.27	1 (33%)
6	DMS	B	8504	-	3,3,3	0.66	0	3,3,3	0.67	0
6	DMS	B	8506	-	3,3,3	1.00	0	3,3,3	0.49	0
6	DMS	B	8508	-	3,3,3	2.61	1 (33%)	3,3,3	0.60	0
6	DMS	B	8601	-	3,3,3	1.52	1 (33%)	3,3,3	0.46	0
2	2DG	C	2001	1,4	10,10,11	1.05	1 (10%)	10,13,15	2.49	3 (30%)
5	BTB	C	2002	-	13,13,13	1.77	4 (30%)	9,16,16	1.07	0
6	DMS	C	8401	-	3,3,3	0.69	0	3,3,3	0.14	0
6	DMS	C	8402	-	3,3,3	1.38	1 (33%)	3,3,3	0.13	0
6	DMS	C	8403	-	3,3,3	0.86	0	3,3,3	0.65	0
6	DMS	C	8404	-	3,3,3	0.49	0	3,3,3	1.05	0
6	DMS	C	8405	-	3,3,3	1.05	0	3,3,3	0.59	0
6	DMS	C	8407	-	3,3,3	1.37	0	3,3,3	0.04	0
6	DMS	C	8408	-	3,3,3	0.62	0	3,3,3	0.71	0
6	DMS	C	8409	-	3,3,3	1.33	1 (33%)	3,3,3	1.24	1 (33%)
6	DMS	C	8410	-	3,3,3	1.06	0	3,3,3	0.19	0
6	DMS	C	8411	-	3,3,3	0.96	0	3,3,3	0.33	0
6	DMS	C	8412	-	3,3,3	0.88	0	3,3,3	0.57	0
6	DMS	C	8413	-	3,3,3	2.27	1 (33%)	3,3,3	0.13	0
6	DMS	C	8414	-	3,3,3	0.51	0	3,3,3	0.78	0
6	DMS	C	8415	-	3,3,3	1.09	0	3,3,3	0.36	0
6	DMS	C	8416	-	3,3,3	0.59	0	3,3,3	0.37	0
6	DMS	C	8417	-	3,3,3	0.75	0	3,3,3	0.29	0
6	DMS	C	8419	-	3,3,3	0.70	0	3,3,3	0.24	0
6	DMS	C	8420	-	3,3,3	1.28	1 (33%)	3,3,3	0.33	0
6	DMS	C	8421	-	3,3,3	0.58	0	3,3,3	0.56	0
6	DMS	C	8423	-	3,3,3	0.67	0	3,3,3	0.10	0
6	DMS	C	8425	4	3,3,3	1.41	1 (33%)	3,3,3	0.22	0
6	DMS	C	8427	-	3,3,3	0.42	0	3,3,3	0.21	0
6	DMS	C	8501	-	3,3,3	0.89	0	3,3,3	0.84	0
6	DMS	C	8503	-	3,3,3	0.87	0	3,3,3	0.54	0
6	DMS	C	8504	-	3,3,3	0.54	0	3,3,3	0.20	0
6	DMS	C	8506	-	3,3,3	1.18	0	3,3,3	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	C	8601	-	3,3,3	1.40	1 (33%)	3,3,3	0.77	0
6	DMS	C	8602	-	3,3,3	0.91	0	3,3,3	0.15	0
2	2DG	D	2001	1,4	10,10,11	0.72	0	10,13,15	2.17	2 (20%)
5	BTB	D	2002	-	13,13,13	1.34	1 (7%)	9,16,16	1.08	0
6	DMS	D	8401	-	3,3,3	1.02	0	3,3,3	0.15	0
6	DMS	D	8402	-	3,3,3	1.07	0	3,3,3	0.21	0
6	DMS	D	8403	-	3,3,3	0.58	0	3,3,3	0.20	0
6	DMS	D	8404	-	3,3,3	1.40	1 (33%)	3,3,3	0.28	0
6	DMS	D	8405	-	3,3,3	0.70	0	3,3,3	0.82	0
6	DMS	D	8406	-	3,3,3	0.97	0	3,3,3	0.66	0
6	DMS	D	8407	-	3,3,3	0.80	0	3,3,3	0.63	0
6	DMS	D	8408	-	3,3,3	1.19	0	3,3,3	0.31	0
6	DMS	D	8409	-	3,3,3	1.38	1 (33%)	3,3,3	0.58	0
6	DMS	D	8410	-	3,3,3	0.93	0	3,3,3	0.22	0
6	DMS	D	8411	-	3,3,3	0.48	0	3,3,3	0.21	0
6	DMS	D	8412	-	3,3,3	0.59	0	3,3,3	0.75	0
6	DMS	D	8413	-	3,3,3	0.95	0	3,3,3	0.25	0
6	DMS	D	8414	-	3,3,3	0.24	0	3,3,3	0.33	0
6	DMS	D	8415	-	3,3,3	2.84	1 (33%)	3,3,3	0.32	0
6	DMS	D	8416	-	3,3,3	0.57	0	3,3,3	0.47	0
6	DMS	D	8417	-	3,3,3	1.65	1 (33%)	3,3,3	0.59	0
6	DMS	D	8419	-	3,3,3	0.93	0	3,3,3	0.09	0
6	DMS	D	8421	-	3,3,3	0.29	0	3,3,3	0.14	0
6	DMS	D	8423	-	3,3,3	1.30	0	3,3,3	0.33	0
6	DMS	D	8425	4	3,3,3	0.26	0	3,3,3	0.36	0
6	DMS	D	8501	-	3,3,3	0.54	0	3,3,3	0.41	0
6	DMS	D	8503	-	3,3,3	0.63	0	3,3,3	0.95	0
6	DMS	D	8506	-	3,3,3	1.01	0	3,3,3	0.16	0
6	DMS	D	8508	-	3,3,3	1.69	1 (33%)	3,3,3	0.52	0
6	DMS	D	8701	-	3,3,3	2.22	2 (66%)	3,3,3	0.45	0
6	DMS	D	8703	-	3,3,3	1.59	1 (33%)	3,3,3	0.28	0
6	DMS	D	8705	-	3,3,3	1.89	1 (33%)	3,3,3	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2DG	A	2001	1,4	-	0/2/16/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BTB	A	2002	-	-	0/21/21/21	0/0/0/0
6	DMS	A	8401	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8402	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8403	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8404	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8405	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8406	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8407	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8408	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8409	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8410	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8411	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8412	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8413	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8414	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8416	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8417	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8419	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8420	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8421	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8423	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8425	4	-	0/0/0/0	0/0/0/0
6	DMS	A	8501	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8502	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8503	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8504	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8506	-	-	0/0/0/0	0/0/0/0
6	DMS	A	8602	-	-	0/0/0/0	0/0/0/0
2	2DG	B	2001	1,4	-	0/2/16/18	0/1/1/1
5	BTB	B	2002	-	-	0/21/21/21	0/0/0/0
6	DMS	B	8401	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8402	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8403	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8404	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8405	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8406	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8407	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8408	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8409	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8410	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8411	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8412	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DMS	B	8413	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8414	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8415	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8416	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8417	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8420	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8421	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8423	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8425	4	-	0/0/0/0	0/0/0/0
6	DMS	B	8427	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8502	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8504	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8506	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8508	-	-	0/0/0/0	0/0/0/0
6	DMS	B	8601	-	-	0/0/0/0	0/0/0/0
2	2DG	C	2001	1,4	-	0/2/16/18	0/1/1/1
5	BTB	C	2002	-	-	0/21/21/21	0/0/0/0
6	DMS	C	8401	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8402	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8403	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8404	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8405	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8407	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8408	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8409	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8410	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8411	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8412	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8413	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8414	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8415	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8416	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8417	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8419	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8420	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8421	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8423	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8425	4	-	0/0/0/0	0/0/0/0
6	DMS	C	8427	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8501	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8503	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8504	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	DMS	C	8506	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8601	-	-	0/0/0/0	0/0/0/0
6	DMS	C	8602	-	-	0/0/0/0	0/0/0/0
2	2DG	D	2001	1,4	-	0/2/16/18	0/1/1/1
5	BTB	D	2002	-	-	0/21/21/21	0/0/0/0
6	DMS	D	8401	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8402	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8403	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8404	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8405	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8406	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8407	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8408	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8409	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8410	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8411	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8412	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8413	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8414	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8415	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8416	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8417	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8419	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8421	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8423	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8425	4	-	0/0/0/0	0/0/0/0
6	DMS	D	8501	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8503	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8506	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8508	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8701	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8703	-	-	0/0/0/0	0/0/0/0
6	DMS	D	8705	-	-	0/0/0/0	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2002	BTB	C1-C2	-4.19	1.48	1.53
5	A	2002	BTB	C1-C2	-3.02	1.49	1.53
5	D	2002	BTB	C1-C2	-2.83	1.49	1.53
5	B	2002	BTB	C1-C2	-2.68	1.50	1.53
6	A	8425	DMS	O-S	2.00	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2002	BTB	O3-C3	2.03	1.48	1.42
6	D	8417	DMS	O-S	2.05	1.64	1.50
6	B	8407	DMS	O-S	2.07	1.64	1.50
6	B	8413	DMS	O-S	2.09	1.64	1.50
6	D	8703	DMS	O-S	2.09	1.64	1.50
6	B	8415	DMS	C2-S	2.11	1.91	1.75
6	A	8423	DMS	C1-S	2.12	1.91	1.75
6	C	8420	DMS	O-S	2.12	1.64	1.50
6	D	8409	DMS	O-S	2.12	1.64	1.50
6	B	8601	DMS	C2-S	2.13	1.91	1.75
6	D	8404	DMS	C2-S	2.15	1.92	1.75
6	B	8425	DMS	C2-S	2.16	1.92	1.75
6	B	8405	DMS	O-S	2.17	1.64	1.50
6	A	8403	DMS	C2-S	2.17	1.92	1.75
6	C	8425	DMS	O-S	2.23	1.65	1.50
5	C	2002	BTB	C7-N	2.23	1.51	1.48
6	D	8701	DMS	C1-S	2.24	1.92	1.75
6	C	8409	DMS	O-S	2.25	1.65	1.50
6	C	8601	DMS	C2-S	2.29	1.93	1.75
6	C	8402	DMS	C2-S	2.39	1.93	1.75
6	B	8409	DMS	O-S	2.39	1.66	1.50
5	A	2002	BTB	C3-C2	2.41	1.56	1.53
2	C	2001	2DG	C3-C4	2.43	1.55	1.52
6	B	8416	DMS	O-S	2.44	1.66	1.50
5	A	2002	BTB	C5-N	2.53	1.51	1.48
5	B	2002	BTB	C3-C2	2.53	1.56	1.53
6	D	8508	DMS	O-S	2.67	1.68	1.50
6	A	8502	DMS	C1-S	2.70	1.96	1.75
6	B	8420	DMS	C2-S	2.70	1.96	1.75
6	D	8701	DMS	O-S	2.70	1.68	1.50
6	A	8403	DMS	O-S	2.74	1.68	1.50
6	D	8705	DMS	O-S	2.85	1.69	1.50
5	C	2002	BTB	C3-C2	3.08	1.57	1.53
6	B	8425	DMS	O-S	3.28	1.72	1.50
6	C	8413	DMS	O-S	3.41	1.73	1.50
6	A	8409	DMS	O-S	3.76	1.75	1.50
6	B	8508	DMS	C1-S	4.00	2.06	1.75
6	D	8415	DMS	O-S	4.52	1.80	1.50
6	B	8407	DMS	C2-S	4.58	2.10	1.75

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	2DG	C3-C4-C5	-6.72	103.19	109.91
2	D	2001	2DG	C3-C4-C5	-4.63	105.28	109.91
2	A	2001	2DG	C3-C4-C5	-4.26	105.65	109.91
5	A	2002	BTB	C7-N-C2	-2.17	107.28	113.70
2	C	2001	2DG	C6-C5-C4	-2.07	108.16	113.00
6	C	8409	DMS	C2-S-C1	2.04	109.02	98.44
6	B	8502	DMS	C2-S-C1	2.16	109.66	98.44
2	C	2001	2DG	C1-O5-C5	2.47	116.41	112.03
2	D	2001	2DG	C1-O5-C5	4.43	119.89	112.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	8409	DMS	1	0
6	A	8414	DMS	1	0
6	A	8416	DMS	2	0
6	A	8420	DMS	1	0
6	A	8423	DMS	2	0
6	A	8503	DMS	2	0
6	B	8406	DMS	1	0
6	B	8407	DMS	2	0
6	B	8410	DMS	1	0
6	B	8417	DMS	1	0
6	B	8508	DMS	2	0
5	C	2002	BTB	1	0
6	C	8407	DMS	1	0
6	C	8410	DMS	1	0
6	C	8420	DMS	1	0
6	C	8425	DMS	5	0
6	C	8427	DMS	1	0
6	C	8602	DMS	1	0
5	D	2002	BTB	1	0
6	D	8412	DMS	2	0
6	D	8421	DMS	1	0
6	D	8506	DMS	2	0
6	D	8703	DMS	4	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.00	32 (3%)	48	55	11, 18, 46, 98	0
1	B	1011/1023 (98%)	0.03	31 (3%)	49	57	10, 18, 47, 97	0
1	C	1011/1023 (98%)	0.06	33 (3%)	47	54	11, 19, 49, 100	0
1	D	1011/1023 (98%)	0.05	43 (4%)	36	43	10, 18, 50, 100	0
All	All	4044/4092 (98%)	0.03	139 (3%)	46	52	10, 18, 48, 100	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	11.3
1	D	735	HIS	10.9
1	D	798	ALA	10.3
1	C	732	ALA	10.3
1	A	686	PRO	9.9
1	C	731	PRO	9.4
1	D	732	ALA	9.3
1	B	799	THR	8.4
1	D	799	THR	8.2
1	B	730	LEU	8.1
1	B	731	PRO	7.8
1	C	730	LEU	7.7
1	A	799	THR	7.7
1	B	733	ALA	7.6
1	B	689	GLU	7.4
1	A	687	GLN	7.4
1	D	800	ARG	7.4
1	B	685	LEU	7.3
1	C	689	GLU	6.9
1	B	798	ALA	6.9
1	D	734	SER	6.8

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Mol	Chain	Res	Type	RSRZ
1	C	735	HIS	6.6
1	D	730	LEU	6.3
1	A	732	ALA	6.3
1	A	730	LEU	6.0
1	A	689	GLU	5.6
1	C	799	THR	5.5
1	B	732	ALA	5.5
1	D	689	GLU	5.5
1	C	686	PRO	5.4
1	C	733	ALA	5.4
1	D	731	PRO	5.4
1	B	686	PRO	5.4
1	C	800	ARG	5.3
1	C	798	ALA	5.3
1	A	731	PRO	5.2
1	A	685	LEU	5.2
1	D	686	PRO	5.0
1	C	687	GLN	4.7
1	D	733	ALA	4.6
1	C	729	THR	4.6
1	D	771	GLY	4.6
1	A	733	ALA	4.5
1	A	800	ARG	4.5
1	D	685	LEU	4.4
1	D	684	GLU	4.4
1	C	772	ASP	4.3
1	A	801	ILE	4.3
1	A	1023	LYS	4.2
1	A	580	GLU	4.1
1	A	736	ALA	4.1
1	D	581	ASN	4.1
1	A	845	GLN	4.0
1	A	729	THR	4.0
1	D	687	GLN	4.0
1	C	685	LEU	3.8
1	D	797	GLU	3.8
1	C	633	GLY	3.8
1	C	634	GLN	3.8
1	D	845	GLN	3.8
1	B	684	GLU	3.7
1	D	580	GLU	3.7
1	B	800	ARG	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	581	ASN	3.6
1	D	729	THR	3.5
1	D	688	PRO	3.5
1	A	582	GLY	3.5
1	D	663	LEU	3.4
1	A	798	ALA	3.4
1	D	683	PRO	3.4
1	C	745	MET	3.4
1	D	664	ALA	3.3
1	D	633	GLY	3.3
1	D	682	LEU	3.2
1	B	797	GLU	3.2
1	D	772	ASP	3.2
1	C	71	GLU	3.2
1	B	687	GLN	3.1
1	D	801	ILE	3.1
1	B	734	SER	3.1
1	D	79	PRO	3.1
1	C	770	ILE	3.1
1	B	1018	LEU	3.1
1	A	734	SER	3.0
1	B	801	ILE	3.0
1	B	745	MET	2.9
1	D	632	SER	2.9
1	A	668	VAL	2.9
1	C	684	GLU	2.9
1	C	734	SER	2.9
1	A	684	GLU	2.9
1	C	736	ALA	2.9
1	B	580	GLU	2.8
1	A	632	SER	2.8
1	B	79	PRO	2.8
1	A	846	GLY	2.8
1	C	737	ILE	2.8
1	A	682	LEU	2.8
1	B	632	SER	2.8
1	A	688	PRO	2.8
1	D	1023	LYS	2.7
1	D	71	GLU	2.6
1	C	831	ALA	2.6
1	D	582	GLY	2.5
1	A	683	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	728	VAL	2.5
1	D	736	ALA	2.4
1	C	1023	LYS	2.4
1	C	761	GLN	2.4
1	A	829	THR	2.4
1	D	830	LEU	2.3
1	A	71	GLU	2.3
1	A	581	ASN	2.3
1	B	663	LEU	2.3
1	C	688	PRO	2.3
1	C	861	SER	2.3
1	D	179	ALA	2.3
1	B	582	GLY	2.3
1	A	79	PRO	2.2
1	D	1022	GLN	2.2
1	C	743	SER	2.2
1	D	796	SER	2.2
1	B	845	GLN	2.2
1	C	830	LEU	2.2
1	B	688	PRO	2.2
1	D	669	PRO	2.2
1	C	845	GLN	2.2
1	C	728	VAL	2.2
1	B	71	GLU	2.1
1	D	752	GLY	2.1
1	D	84	VAL	2.1
1	A	179	ALA	2.1
1	B	735	HIS	2.1
1	B	583	ASN	2.1
1	B	47	PRO	2.0
1	D	831	ALA	2.0
1	C	581	ASN	2.0
1	D	795	VAL	2.0
1	B	690	SER	2.0

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

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

6.3 Carbohydrates [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
6	DMS	D	8404	4/4	0.92	0.14	10.04	24,24,49,100	0
6	DMS	B	8420	4/4	0.92	0.17	9.96	52,54,69,77	0
6	DMS	A	8407	4/4	0.92	0.19	9.26	29,40,41,45	0
6	DMS	B	8407	4/4	0.90	0.23	7.50	34,34,41,47	0
6	DMS	C	8420	4/4	0.95	0.14	6.33	44,46,79,100	0
5	BTB	A	2002	14/14	0.89	0.16	5.87	11,20,31,34	14
6	DMS	B	8508	4/4	0.90	0.18	5.40	30,40,45,49	0
6	DMS	A	8417	4/4	0.93	0.19	4.94	32,34,90,100	0
2	2DG	A	2001	10/11	0.98	0.10	4.04	9,13,20,23	0
6	DMS	A	8423	4/4	0.89	0.19	3.84	39,68,81,100	0
6	DMS	D	8417	4/4	0.87	0.15	3.81	27,29,72,94	0
6	DMS	B	8406	4/4	0.85	0.20	3.70	32,40,52,59	0
6	DMS	B	8423	4/4	0.93	0.14	3.67	34,35,59,100	0
6	DMS	B	8408	4/4	0.95	0.16	3.66	28,34,40,90	0
6	DMS	A	8501	4/4	0.92	0.16	3.50	20,32,36,41	0
6	DMS	D	8407	4/4	0.72	0.15	3.44	21,34,71,100	0
6	DMS	C	8425	4/4	0.96	0.16	3.39	34,43,58,100	0
6	DMS	A	8420	4/4	0.93	0.12	3.20	37,43,45,66	0
6	DMS	D	8423	4/4	0.89	0.19	3.12	39,55,62,70	0
6	DMS	A	8404	4/4	0.96	0.10	3.12	23,27,36,37	0
6	DMS	C	8423	4/4	0.91	0.15	3.02	39,39,54,61	0
6	DMS	A	8406	4/4	0.93	0.12	2.95	23,33,65,73	0
6	DMS	C	8501	4/4	0.93	0.14	2.84	20,30,36,46	0
6	DMS	B	8425	4/4	0.92	0.13	2.83	23,34,44,50	0
6	DMS	D	8410	4/4	0.97	0.14	2.73	33,35,39,44	0
6	DMS	B	8502	4/4	0.96	0.14	2.47	25,30,42,46	0
6	DMS	C	8407	4/4	0.96	0.15	2.39	29,32,44,100	0
6	DMS	B	8405	4/4	0.97	0.12	2.22	27,29,32,32	0
6	DMS	C	8419	4/4	0.86	0.15	2.09	38,51,67,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	DMS	D	8425	4/4	0.95	0.20	2.02	21,31,44,76	4
2	2DG	C	2001	10/11	0.95	0.10	1.86	8,15,17,18	0
6	DMS	A	8506	4/4	0.95	0.12	1.70	35,35,36,38	0
6	DMS	D	8408	4/4	0.98	0.12	1.61	24,31,32,40	0
6	DMS	D	8406	4/4	0.96	0.11	1.61	24,26,26,28	0
6	DMS	C	8417	4/4	0.89	0.13	1.46	27,37,45,68	0
6	DMS	A	8401	4/4	0.99	0.09	1.24	14,15,17,19	0
6	DMS	C	8403	4/4	0.98	0.11	1.08	20,21,24,28	0
6	DMS	C	8411	4/4	0.99	0.10	0.91	24,29,35,45	0
2	2DG	D	2001	10/11	0.97	0.09	0.83	9,11,17,18	0
6	DMS	A	8419	4/4	0.97	0.11	0.75	43,46,51,56	0
5	BTB	C	2002	14/14	0.93	0.10	0.74	14,25,38,98	14
6	DMS	D	8501	4/4	0.94	0.10	0.74	23,35,42,54	0
5	BTB	B	2002	14/14	0.94	0.10	0.73	13,23,30,99	14
5	BTB	D	2002	14/14	0.94	0.11	0.71	15,22,29,95	14
6	DMS	D	8705	4/4	0.93	0.13	0.68	21,33,40,43	0
6	DMS	A	8425	4/4	0.95	0.15	0.64	31,38,42,43	0
4	NA	C	3101	1/1	1.00	0.09	0.62	15,15,15,15	0
6	DMS	A	8502	4/4	0.93	0.14	0.60	23,31,54,67	0
6	DMS	A	8412	4/4	0.97	0.11	0.52	31,33,39,100	0
6	DMS	C	8408	4/4	0.95	0.11	0.45	25,34,39,40	0
2	2DG	B	2001	10/11	0.96	0.10	0.39	5,9,12,13	10
6	DMS	D	8508	4/4	0.93	0.11	0.38	37,39,45,47	0
6	DMS	C	8402	4/4	0.97	0.08	0.35	18,28,30,32	0
4	NA	B	3104	1/1	0.96	0.11	0.33	33,33,33,33	0
6	DMS	B	8506	4/4	0.96	0.12	0.30	31,32,33,47	0
6	DMS	B	8417	4/4	0.96	0.09	0.26	25,34,62,100	0
6	DMS	B	8402	4/4	0.97	0.08	0.25	17,17,23,25	0
6	DMS	C	8404	4/4	0.97	0.08	0.15	19,24,25,31	0
6	DMS	C	8602	4/4	0.95	0.10	0.09	39,45,60,72	0
6	DMS	A	8405	4/4	0.98	0.09	0.02	18,25,28,45	0
6	DMS	C	8412	4/4	0.98	0.09	-0.09	32,35,36,100	0
6	DMS	D	8701	4/4	0.98	0.08	-0.09	14,17,20,31	0
6	DMS	B	8504	4/4	0.94	0.10	-0.12	27,44,46,47	0
6	DMS	D	8401	4/4	0.98	0.08	-0.18	16,18,19,23	0
6	DMS	D	8412	4/4	0.98	0.09	-0.24	27,30,31,37	0
6	DMS	D	8405	4/4	0.98	0.08	-0.33	23,26,31,52	0
4	NA	C	3104	1/1	0.98	0.09	-0.41	30,30,30,30	0
6	DMS	D	8403	4/4	0.98	0.08	-0.43	19,29,29,37	0
6	DMS	A	8408	4/4	0.97	0.08	-0.47	19,31,40,59	0
6	DMS	A	8504	4/4	0.98	0.07	-0.52	18,38,53,89	0
6	DMS	D	8402	4/4	0.98	0.07	-0.61	18,22,23,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NA	A	3104	1/1	0.99	0.08	-0.62	25,25,25,25	0
6	DMS	B	8404	4/4	0.96	0.08	-0.73	22,22,32,36	0
4	NA	B	3101	1/1	0.99	0.07	-0.84	15,15,15,15	0
6	DMS	B	8401	4/4	0.98	0.07	-0.89	15,17,21,21	0
6	DMS	B	8412	4/4	0.98	0.07	-0.91	28,34,34,36	0
6	DMS	C	8405	4/4	0.98	0.07	-0.93	24,24,25,29	0
6	DMS	A	8411	4/4	0.98	0.06	-1.09	28,29,31,45	0
6	DMS	B	8411	4/4	0.98	0.07	-1.12	27,30,30,87	0
4	NA	A	3101	1/1	0.99	0.06	-1.24	16,16,16,16	0
3	MG	A	3002	1/1	0.99	0.07	-1.33	17,17,17,17	0
6	DMS	D	8419	4/4	0.97	0.07	-1.34	23,41,52,62	0
6	DMS	A	8403	4/4	0.99	0.07	-1.35	21,22,25,28	0
6	DMS	D	8411	4/4	0.98	0.07	-1.41	20,27,28,55	0
4	NA	C	3102	1/1	0.99	0.06	-1.43	17,17,17,17	0
4	NA	A	3103	1/1	0.99	0.07	-1.44	28,28,28,28	0
6	DMS	C	8401	4/4	0.99	0.06	-1.45	16,16,21,22	0
3	MG	C	3002	1/1	0.99	0.07	-1.50	15,15,15,15	0
6	DMS	B	8403	4/4	0.98	0.07	-1.51	18,24,26,26	0
4	NA	D	3104	1/1	0.96	0.07	-1.64	35,35,35,35	0
3	MG	B	3001	1/1	0.99	0.06	-1.72	15,15,15,15	0
3	MG	D	3002	1/1	0.99	0.06	-1.76	17,17,17,17	0
4	NA	C	3103	1/1	0.99	0.06	-1.80	24,24,24,24	0
6	DMS	A	8402	4/4	0.99	0.07	-1.97	16,18,23,29	0
4	NA	D	3103	1/1	0.99	0.06	-1.99	30,30,30,30	0
4	NA	B	3103	1/1	0.99	0.06	-2.06	23,23,23,23	0
4	NA	A	3102	1/1	0.99	0.05	-2.16	14,14,14,14	0
3	MG	D	3001	1/1	0.99	0.06	-2.18	15,15,15,15	0
3	MG	B	3002	1/1	0.99	0.05	-2.38	19,19,19,19	0
4	NA	D	3102	1/1	0.99	0.06	-2.40	15,15,15,15	0
4	NA	D	3101	1/1	1.00	0.06	-2.78	16,16,16,16	0
3	MG	C	3001	1/1	0.99	0.04	-2.95	15,15,15,15	0
4	NA	B	3102	1/1	0.99	0.05	-3.18	16,16,16,16	0
3	MG	A	3001	1/1	0.99	0.05	-5.26	16,16,16,16	0
6	DMS	C	8415	4/4	0.94	0.14	-	26,38,38,46	0
3	MG	C	3006	1/1	0.96	0.19	-	43,43,43,43	0
6	DMS	A	8416	4/4	0.94	0.18	-	23,38,47,100	0
6	DMS	C	8416	4/4	0.95	0.30	-	59,65,71,72	0
6	DMS	C	8601	4/4	0.96	0.17	-	28,47,53,57	0
6	DMS	A	8421	4/4	0.93	0.24	-	54,67,79,94	0
6	DMS	A	8503	4/4	0.95	0.27	-	26,100,100,100	0
6	DMS	B	8427	4/4	0.94	0.09	-	35,38,53,66	0
3	MG	D	3005	1/1	0.98	0.10	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	DMS	A	8414	4/4	0.96	0.12	-	31,43,51,100	0
6	DMS	A	8413	4/4	0.87	0.15	-	36,70,79,100	0
6	DMS	D	8421	4/4	0.96	0.19	-	43,48,50,100	0
3	MG	A	3005	1/1	0.95	0.13	-	30,30,30,30	0
6	DMS	A	8409	4/4	0.96	0.12	-	26,37,45,47	0
6	DMS	D	8416	4/4	0.92	0.19	-	28,30,51,100	0
6	DMS	B	8601	4/4	0.97	0.10	-	29,36,40,48	0
6	DMS	B	8416	4/4	0.92	0.17	-	36,45,53,68	0
6	DMS	C	8506	4/4	0.93	0.12	-	22,30,37,38	0
6	DMS	A	8410	4/4	0.96	0.14	-	25,30,46,55	0
6	DMS	C	8421	4/4	0.96	0.13	-	38,48,94,100	0
6	DMS	C	8409	4/4	0.96	0.12	-	30,32,39,39	0
6	DMS	B	8421	4/4	0.94	0.17	-	28,56,60,67	0
6	DMS	D	8414	4/4	0.98	0.16	-	27,45,89,100	0
3	MG	D	3003	1/1	0.94	0.31	-	30,30,30,30	1
6	DMS	A	8602	4/4	0.96	0.31	-	41,45,100,100	0
6	DMS	B	8409	4/4	0.96	0.12	-	29,31,35,39	0
6	DMS	C	8414	4/4	0.99	0.07	-	21,40,71,100	0
6	DMS	B	8410	4/4	0.92	0.14	-	34,36,57,82	0
3	MG	C	3003	1/1	0.92	0.20	-	24,24,24,24	1
6	DMS	D	8415	4/4	0.86	0.16	-	29,37,68,100	0
6	DMS	D	8503	4/4	0.88	0.20	-	41,57,72,74	0
6	DMS	D	8703	4/4	0.89	0.20	-	31,48,50,51	0
6	DMS	C	8413	4/4	0.94	0.17	-	30,41,52,95	0
6	DMS	C	8410	4/4	0.95	0.18	-	30,37,45,45	0
6	DMS	C	8504	4/4	0.92	0.11	-	30,39,48,58	0
3	MG	A	3003	1/1	0.89	0.36	-	26,26,26,26	1
6	DMS	D	8409	4/4	0.96	0.11	-	30,32,36,36	0
3	MG	B	3003	1/1	0.88	0.17	-	25,25,25,25	1
6	DMS	C	8427	4/4	0.86	0.18	-	42,55,62,70	0
6	DMS	C	8503	4/4	0.94	0.14	-	36,58,65,76	0
3	MG	C	3004	1/1	0.77	0.15	-	51,51,51,51	0
6	DMS	D	8506	4/4	0.96	0.08	-	19,25,31,40	0
6	DMS	B	8413	4/4	0.86	0.16	-	50,55,58,70	0
6	DMS	B	8415	4/4	0.89	0.12	-	27,28,42,56	0
3	MG	C	3105	1/1	0.76	0.34	-	47,47,47,47	1
6	DMS	D	8413	4/4	0.94	0.20	-	39,44,45,83	0
6	DMS	B	8414	4/4	0.96	0.14	-	30,32,51,100	0

6.5 Other polymers

There are no such residues in this entry.