



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:53 PM UTC

PDB ID : 1PX4 / pdb_00001px4
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (G794A) WITH IPTG BOUND
Authors : Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.
Deposited on : 2003-07-02
Resolution : 1.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

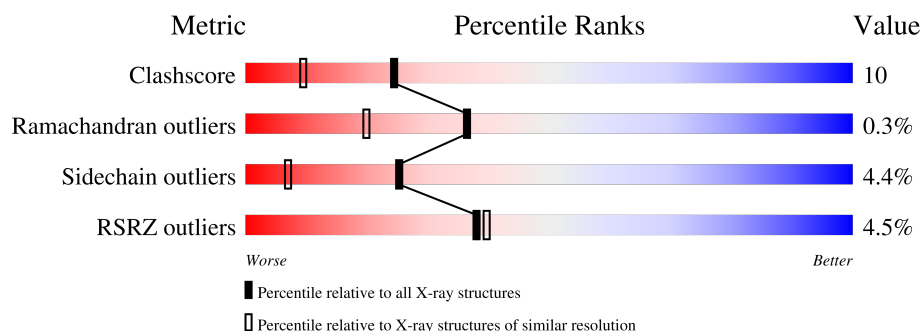
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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))
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	5% 72% 22% • •
1	B	1023	4% 74% 21% • •
1	C	1023	4% 71% 23% 5% •
1	D	1023	5% 74% 20% 5% ••

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	3105	-	-	-	X
5	DMS	A	8404	-	-	X	-
5	DMS	A	8416	-	-	X	-
5	DMS	A	8421	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	C	8506	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36785 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
			8126	5139	1440	1509	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8126	5139	1440	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P00722
A	2	SER	-	cloning artifact	UNP P00722
A	3	HIS	-	cloning artifact	UNP P00722
A	4	MET	-	cloning artifact	UNP P00722
A	5	LEU	-	cloning artifact	UNP P00722
A	6	GLU	-	cloning artifact	UNP P00722
A	7	ASP	-	cloning artifact	UNP P00722
A	8	PRO	-	cloning artifact	UNP P00722
A	794	ALA	GLY	engineered mutation	UNP P00722
B	1	GLY	-	cloning artifact	UNP P00722
B	2	SER	-	cloning artifact	UNP P00722
B	3	HIS	-	cloning artifact	UNP P00722
B	4	MET	-	cloning artifact	UNP P00722
B	5	LEU	-	cloning artifact	UNP P00722
B	6	GLU	-	cloning artifact	UNP P00722
B	7	ASP	-	cloning artifact	UNP P00722
B	8	PRO	-	cloning artifact	UNP P00722
B	794	ALA	GLY	engineered mutation	UNP P00722
C	1	GLY	-	cloning artifact	UNP P00722
C	2	SER	-	cloning artifact	UNP P00722
C	3	HIS	-	cloning artifact	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	cloning artifact	UNP P00722
C	5	LEU	-	cloning artifact	UNP P00722
C	6	GLU	-	cloning artifact	UNP P00722
C	7	ASP	-	cloning artifact	UNP P00722
C	8	PRO	-	cloning artifact	UNP P00722
C	794	ALA	GLY	engineered mutation	UNP P00722
D	1	GLY	-	cloning artifact	UNP P00722
D	2	SER	-	cloning artifact	UNP P00722
D	3	HIS	-	cloning artifact	UNP P00722
D	4	MET	-	cloning artifact	UNP P00722
D	5	LEU	-	cloning artifact	UNP P00722
D	6	GLU	-	cloning artifact	UNP P00722
D	7	ASP	-	cloning artifact	UNP P00722
D	8	PRO	-	cloning artifact	UNP P00722
D	794	ALA	GLY	engineered mutation	UNP P00722

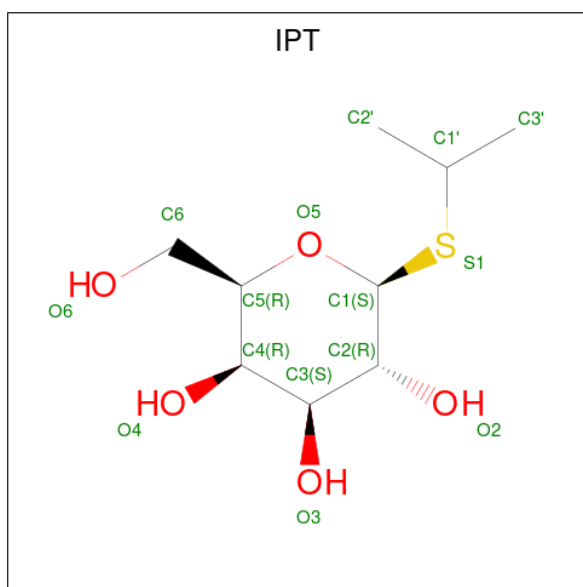
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

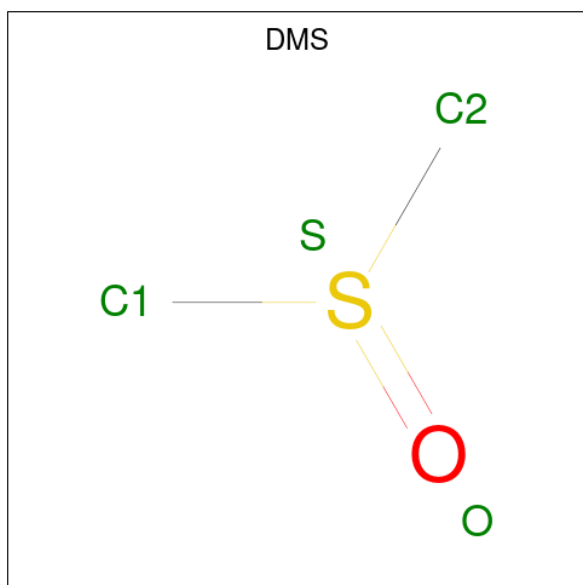
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	4	Total Na 4 4	0	0

- Molecule 4 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: C₉H₁₈O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			15	9	5	1		
4	B	1	Total	C	O	S	0	0
			15	9	5	1		
4	C	1	Total	C	O	S	0	0
			15	9	5	1		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

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

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

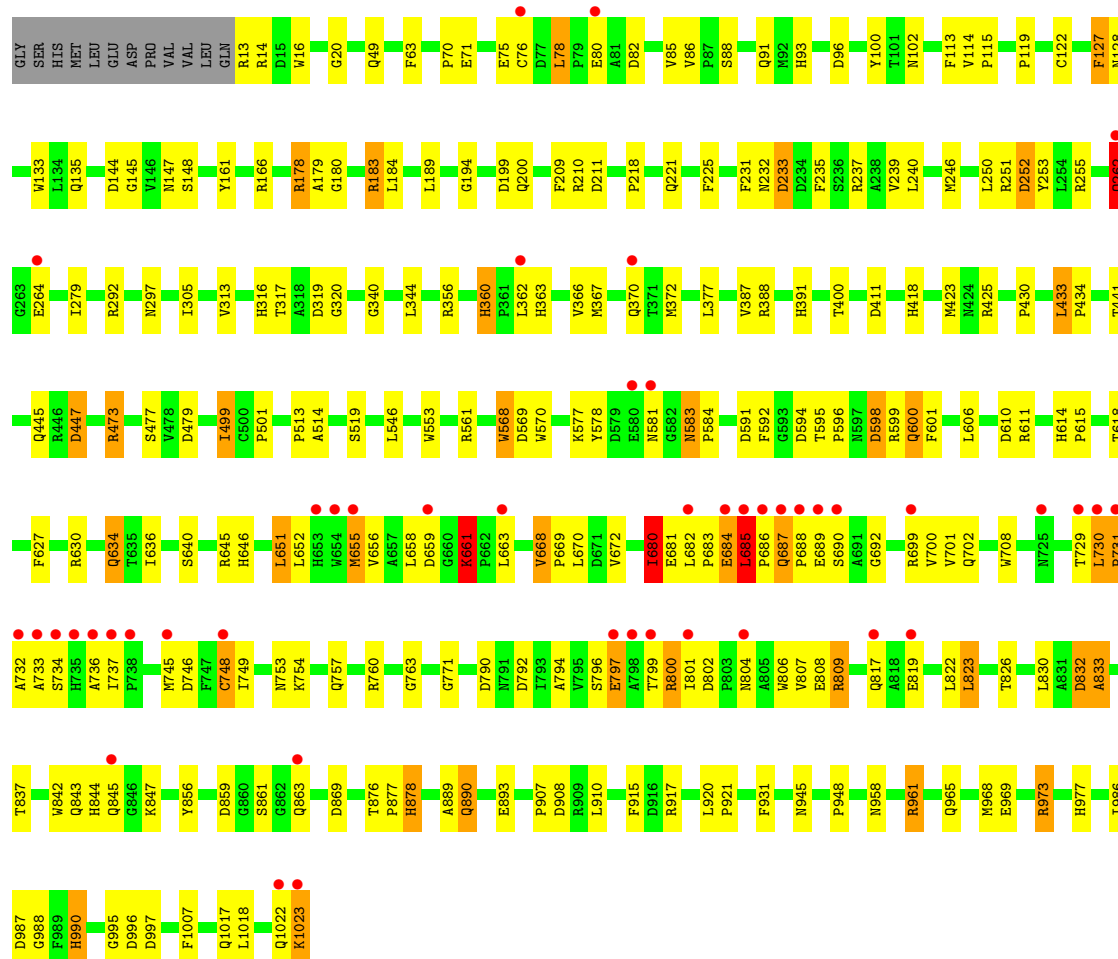
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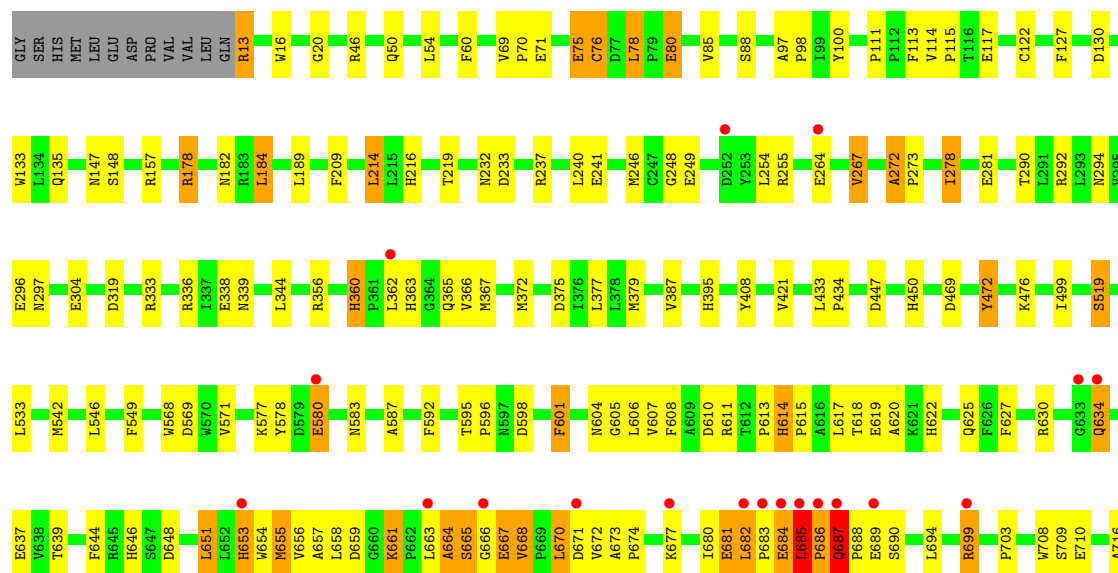
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4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

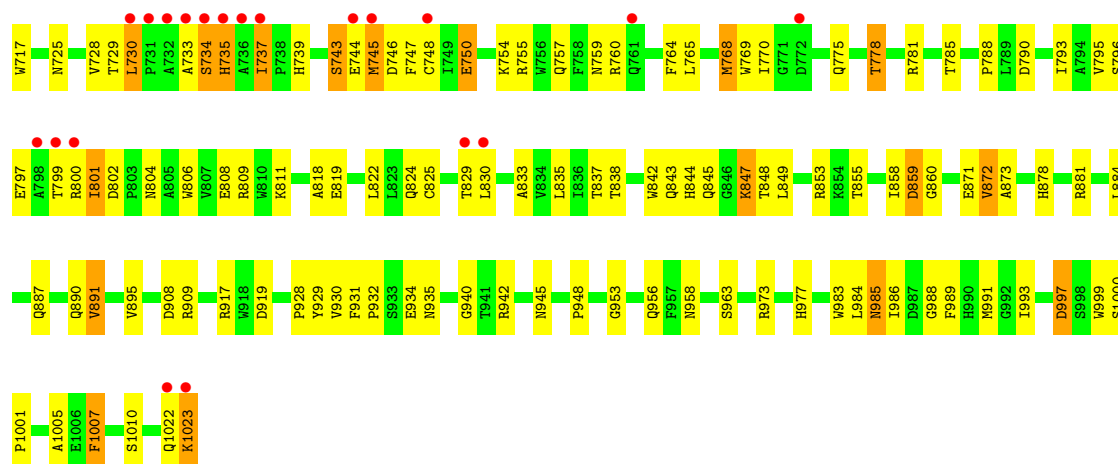
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	950	Total O 950 950	0	0
6	B	971	Total O 971 971	0	0
6	C	943	Total O 943 943	0	0
6	D	949	Total O 949 949	0	0

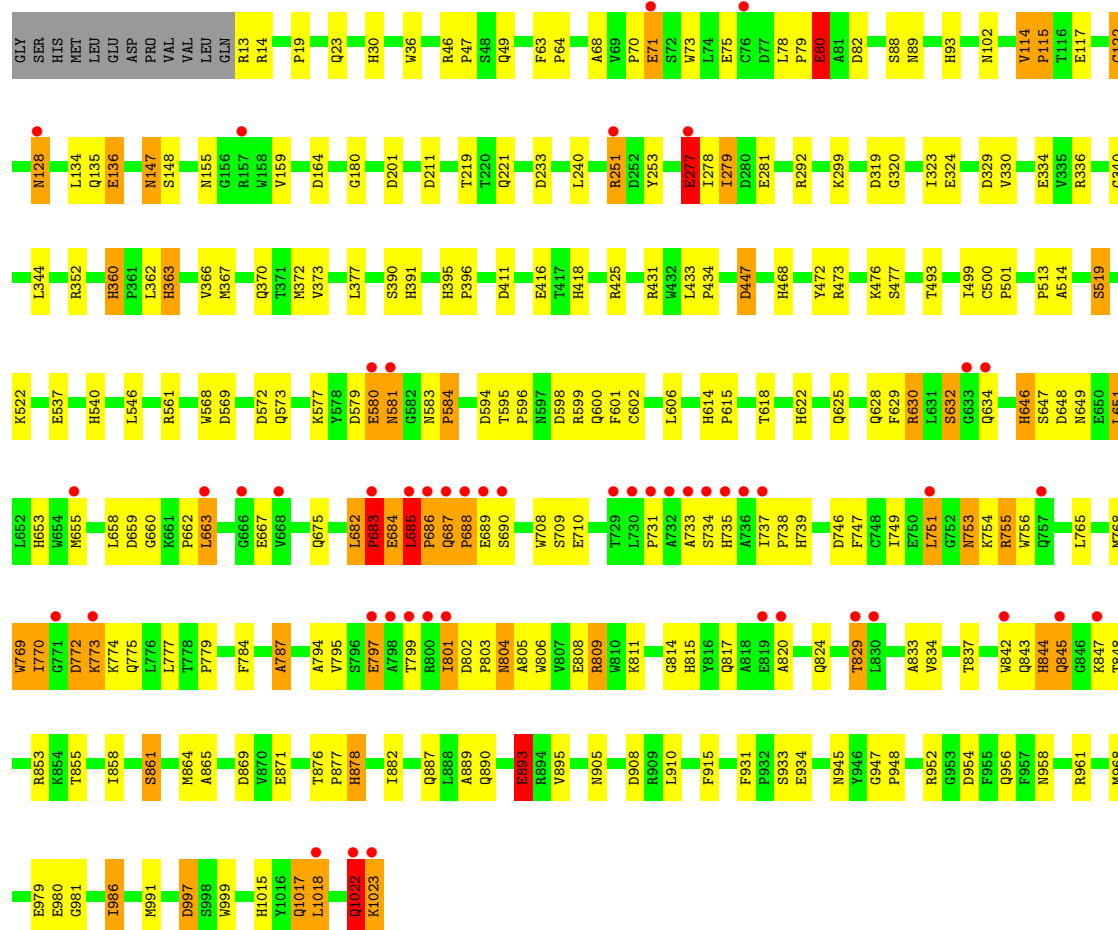


• Molecule 1: beta-galactosidase





• 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	149.49Å 168.29Å 200.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.50 – 1.60 31.50 – 1.60	Depositor EDS
% Data completeness (in resolution range)	94.8 (31.50-1.60) 90.8 (31.50-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.60Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.187 , 0.239 0.177 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtrriage
Anisotropy	0.258	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36785	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.39 % 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 5.0375e-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: IPT, MG, NA, DMS

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.30	10/8368 (0.1%)	1.75	122/11417 (1.1%)
1	B	1.30	6/8368 (0.1%)	1.74	115/11417 (1.0%)
1	C	1.27	9/8368 (0.1%)	1.76	121/11417 (1.1%)
1	D	1.32	13/8368 (0.2%)	1.79	111/11417 (1.0%)
All	All	1.30	38/33472 (0.1%)	1.76	469/45668 (1.0%)

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

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

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	737	ILE	CA-CB	-7.24	1.49	1.54
1	A	928	PRO	N-CA	-6.55	1.39	1.47
1	A	909	ARG	NE-CZ	6.12	1.39	1.33
1	A	248	GLY	C-O	-6.11	1.19	1.24
1	A	479	ASP	C-N	-6.08	1.28	1.34
1	C	111	PRO	C-O	-5.91	1.20	1.25
1	B	199	ASP	CG-OD2	5.90	1.36	1.25
1	C	111	PRO	CA-C	-5.76	1.48	1.51
1	A	297	ASN	CA-C	-5.75	1.49	1.53
1	D	30	HIS	CE1-NE2	5.72	1.38	1.32
1	D	540	HIS	CE1-NE2	5.66	1.38	1.32
1	B	360	HIS	CA-C	5.56	1.57	1.52
1	D	418	HIS	CE1-NE2	5.54	1.38	1.32
1	D	122	CYS	CA-C	-5.52	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	537	GLU	CD-OE2	5.46	1.35	1.25
1	D	468	HIS	CE1-NE2	5.41	1.38	1.32
1	C	297	ASN	CA-CB	5.37	1.56	1.52
1	C	940	GLY	C-O	5.32	1.30	1.24
1	C	304	GLU	CD-OE2	5.28	1.35	1.25
1	A	162	GLY	CA-C	5.21	1.57	1.51
1	C	281	GLU	CD-OE2	5.19	1.35	1.25
1	B	792	ASP	CG-OD2	5.19	1.35	1.25
1	D	630	ARG	CA-C	5.19	1.58	1.52
1	D	281	GLU	CD-OE2	5.16	1.35	1.25
1	D	893	GLU	CD-OE2	5.16	1.35	1.25
1	A	501	PRO	N-CA	-5.14	1.40	1.47
1	D	425	ARG	NE-CZ	5.13	1.38	1.33
1	C	819	GLU	CD-OE2	5.13	1.35	1.25
1	A	533	LEU	CA-C	5.11	1.58	1.52
1	B	990	HIS	CG-ND1	5.09	1.43	1.38
1	C	296	GLU	CD-OE2	5.08	1.35	1.25
1	B	418	HIS	CE1-NE2	5.08	1.37	1.32
1	C	499	ILE	N-CA	5.07	1.51	1.46
1	D	908	ASP	CG-OD2	5.05	1.34	1.25
1	A	1015	HIS	CE1-NE2	5.04	1.37	1.32
1	A	725	ASN	CA-C	-5.03	1.46	1.53
1	D	80	GLU	CD-OE2	5.02	1.34	1.25
1	D	159	VAL	CA-CB	-5.00	1.49	1.55

All (469) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	735	HIS	CA-CB-CG	12.55	126.35	113.80
1	B	809	ARG	NE-CZ-NH1	9.31	130.81	121.50
1	C	685	LEU	N-CA-CB	9.30	125.87	110.05
1	A	725	ASN	CA-CB-CG	-8.74	103.86	112.60
1	C	614	HIS	N-CA-C	-8.70	100.12	110.13
1	C	680	ILE	CA-C-N	-8.66	109.75	122.65
1	C	680	ILE	C-N-CA	-8.66	109.75	122.65
1	B	809	ARG	NE-CZ-NH2	-8.56	111.50	119.20
1	C	685	LEU	CA-C-N	8.51	128.55	119.78
1	C	685	LEU	C-N-CA	8.51	128.55	119.78
1	C	249	GLU	N-CA-C	8.43	122.36	108.96
1	D	733	ALA	N-CA-C	8.39	122.06	110.24
1	D	893	GLU	CB-CG-CD	8.21	126.55	112.60
1	D	931	PHE	CA-CB-CG	-8.20	105.60	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	997	ASP	N-CA-CB	8.18	124.48	111.56
1	D	844	HIS	CA-CB-CG	-8.14	105.66	113.80
1	C	113	PHE	CA-CB-CG	-8.09	105.71	113.80
1	C	682	LEU	CA-C-N	8.04	127.99	120.03
1	C	682	LEU	C-N-CA	8.04	127.99	120.03
1	D	687	GLN	N-CA-CB	8.02	119.05	109.74
1	B	363	HIS	CA-CB-CG	-8.00	105.80	113.80
1	A	832	ASP	CA-CB-CG	-7.99	104.61	112.60
1	D	878	HIS	CA-CB-CG	-7.93	105.87	113.80
1	C	130	ASP	CA-CB-CG	-7.90	104.70	112.60
1	A	691	ALA	N-CA-C	7.88	121.07	110.35
1	B	878	HIS	CA-CB-CG	-7.79	106.01	113.80
1	B	1018	LEU	CB-CA-C	-7.77	92.98	110.07
1	C	725	ASN	CA-CB-CG	-7.68	104.92	112.60
1	B	986	ILE	CB-CA-C	7.65	121.64	110.77
1	D	945	ASN	CA-CB-CG	-7.63	104.97	112.60
1	A	996	ASP	N-CA-C	-7.61	102.01	111.75
1	D	277	GLU	CB-CG-CD	7.61	125.53	112.60
1	B	611	ARG	CB-CA-C	7.59	117.34	109.83
1	D	739	HIS	CA-CB-CG	-7.53	106.28	113.80
1	B	809	ARG	CD-NE-CZ	7.51	134.91	124.40
1	A	829	THR	CA-CB-CG2	7.50	123.24	110.50
1	A	954	ASP	CA-CB-CG	-7.50	105.11	112.60
1	B	78	LEU	CA-C-O	7.49	125.23	119.46
1	C	319	ASP	CA-C-N	-7.46	111.92	122.00
1	C	319	ASP	C-N-CA	-7.46	111.92	122.00
1	A	770	ILE	N-CA-CB	7.42	121.25	111.90
1	B	640	SER	CB-CA-C	-7.40	97.67	109.80
1	B	570	TRP	N-CA-C	7.36	118.99	110.97
1	D	751	LEU	CB-CA-C	7.35	121.01	110.79
1	D	746	ASP	N-CA-C	7.33	120.30	109.24
1	B	753	ASN	CA-CB-CG	7.32	119.92	112.60
1	D	319	ASP	CA-CB-CG	-7.31	105.29	112.60
1	B	598	ASP	CA-CB-CG	-7.28	105.32	112.60
1	A	69	VAL	CB-CA-C	-7.27	104.18	110.94
1	D	583	ASN	CA-CB-CG	-7.23	105.37	112.60
1	C	363	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	771	GLY	N-CA-C	-7.14	97.72	110.86
1	C	819	GLU	CB-CG-CD	7.12	124.70	112.60
1	A	878	HIS	CA-CB-CG	-7.05	106.75	113.80
1	D	855	THR	N-CA-CB	7.04	123.74	111.13
1	A	816	TYR	CA-C-N	-7.00	111.68	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	816	TYR	C-N-CA	-7.00	111.68	122.60
1	C	844	HIS	CA-CB-CG	-6.99	106.81	113.80
1	B	592	PHE	CA-CB-CG	-6.95	106.85	113.80
1	D	667	GLU	CB-CA-C	6.93	123.45	109.38
1	C	472	TYR	N-CA-C	-6.92	103.67	111.07
1	C	686	PRO	CB-CA-C	-6.88	102.42	111.23
1	A	996	ASP	CA-CB-CG	-6.86	105.74	112.60
1	C	917	ARG	CD-NE-CZ	-6.82	114.86	124.40
1	B	668	VAL	CB-CA-C	-6.80	98.98	111.36
1	D	363	HIS	CA-CB-CG	-6.79	107.01	113.80
1	D	632	SER	N-CA-CB	6.79	123.72	111.36
1	D	845	GLN	CA-C-N	-6.79	112.65	123.31
1	D	845	GLN	C-N-CA	-6.79	112.65	123.31
1	B	252	ASP	CA-CB-CG	-6.78	105.82	112.60
1	C	728	VAL	CA-C-N	-6.75	114.06	122.84
1	C	728	VAL	C-N-CA	-6.75	114.06	122.84
1	B	832	ASP	N-CA-CB	-6.75	101.76	111.54
1	A	433	LEU	CA-C-O	6.71	124.85	118.34
1	B	479	ASP	CA-CB-CG	-6.71	105.89	112.60
1	D	947	GLY	CA-C-N	6.71	126.33	119.56
1	D	947	GLY	C-N-CA	6.71	126.33	119.56
1	C	233	ASP	N-CA-C	6.68	118.56	111.28
1	B	20	GLY	N-CA-C	-6.67	106.59	115.32
1	B	473	ARG	CD-NE-CZ	6.67	133.73	124.40
1	C	598	ASP	CA-CB-CG	-6.66	105.94	112.60
1	D	663	LEU	CB-CA-C	-6.66	97.30	109.15
1	D	753	ASN	N-CA-C	-6.65	105.14	112.72
1	B	997	ASP	N-CA-CB	6.64	122.05	111.56
1	D	279	ILE	CA-CB-CG2	6.64	121.78	110.50
1	A	997	ASP	N-CA-CB	6.62	121.65	111.46
1	A	614	HIS	N-CA-C	-6.61	101.50	110.36
1	C	842	TRP	CE2-CD2-CE3	6.61	125.41	118.80
1	A	632	SER	N-CA-CB	6.60	121.20	110.90
1	D	770	ILE	N-CA-C	-6.59	96.81	107.28
1	B	239	VAL	N-CA-CB	6.59	120.20	111.64
1	A	601	PHE	CA-CB-CG	-6.58	107.22	113.80
1	D	997	ASP	CA-CB-CG	-6.56	106.04	112.60
1	B	183	ARG	CD-NE-CZ	-6.55	115.22	124.40
1	A	235	PHE	CA-CB-CG	-6.55	107.25	113.80
1	D	155	ASN	CA-CB-CG	-6.54	106.06	112.60
1	D	683	PRO	CB-CA-C	-6.54	100.77	111.56
1	A	14	ARG	N-CA-CB	-6.50	102.61	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	VAL	CA-C-O	-6.47	116.57	119.94
1	B	233	ASP	N-CA-C	6.47	118.34	111.28
1	D	829	THR	N-CA-CB	6.47	120.98	110.43
1	A	977	HIS	CA-CB-CG	6.47	120.27	113.80
1	D	915	PHE	CA-CB-CG	-6.47	107.33	113.80
1	B	113	PHE	CA-CB-CG	-6.46	107.33	113.80
1	D	329	ASP	CA-CB-CG	-6.46	106.14	112.60
1	A	185	ALA	N-CA-CB	6.44	120.88	110.77
1	B	297	ASN	CA-C-O	6.44	124.91	120.47
1	C	958	ASN	N-CA-CB	6.44	123.50	111.53
1	C	842	TRP	N-CA-CB	6.43	120.66	110.57
1	B	430	PRO	N-CA-CB	6.41	110.31	103.39
1	A	103	VAL	N-CA-C	6.40	117.40	111.45
1	C	184	LEU	CB-CA-C	-6.40	98.69	109.50
1	D	221	GLN	N-CA-CB	-6.39	101.46	111.56
1	D	687	GLN	CB-CA-C	6.39	119.53	109.37
1	C	759	ASN	CA-CB-CG	-6.39	106.21	112.60
1	B	661	LYS	CA-C-O	6.38	124.04	119.32
1	B	680	ILE	CA-C-N	-6.37	112.39	121.50
1	B	680	ILE	C-N-CA	-6.37	112.39	121.50
1	D	731	PRO	N-CA-CB	6.37	109.37	103.39
1	D	784	PHE	CA-CB-CG	-6.36	107.44	113.80
1	D	395	HIS	N-CA-CB	-6.36	100.00	109.98
1	C	648	ASP	CA-CB-CG	-6.36	106.24	112.60
1	A	653	HIS	CA-CB-CG	-6.34	107.46	113.80
1	C	997	ASP	N-CA-CB	6.33	121.56	111.56
1	B	433	LEU	CA-C-O	6.32	124.93	118.73
1	A	115	PRO	CA-C-N	-6.32	110.17	120.72
1	A	115	PRO	C-N-CA	-6.32	110.17	120.72
1	D	324	GLU	N-CA-CB	6.31	122.17	111.57
1	A	675	GLN	CB-CG-CD	-6.31	101.88	112.60
1	A	82	ASP	CA-CB-CG	-6.29	106.31	112.60
1	A	989	PHE	CA-CB-CG	-6.28	107.53	113.80
1	D	865	ALA	CA-C-N	-6.27	115.42	123.19
1	D	865	ALA	C-N-CA	-6.27	115.42	123.19
1	D	19	PRO	N-CA-CB	6.27	109.30	103.41
1	B	166	ARG	N-CA-C	6.26	120.96	112.88
1	C	729	THR	N-CA-CB	6.24	120.67	110.37
1	D	277	GLU	N-CA-CB	-6.24	100.87	110.04
1	D	360	HIS	CA-CB-CG	-6.23	107.57	113.80
1	C	182	ASN	OD1-CG-ND2	6.22	128.82	122.60
1	C	733	ALA	N-CA-C	6.21	124.04	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	790	ASP	CA-CB-CG	-6.20	106.40	112.60
1	C	360	HIS	CA-CB-CG	-6.20	107.60	113.80
1	D	584	PRO	CB-CA-C	-6.18	102.07	110.60
1	B	988	GLY	N-CA-C	-6.18	104.86	112.77
1	C	209	PHE	CA-CB-CG	-6.18	107.62	113.80
1	C	917	ARG	NE-CZ-NH1	-6.18	115.32	121.50
1	D	416	GLU	CG-CD-OE1	6.16	132.57	118.40
1	C	272	ALA	CA-C-O	6.16	126.11	120.26
1	D	519	SER	N-CA-C	-6.16	101.56	110.24
1	C	730	LEU	N-CA-CB	-6.16	101.11	110.03
1	D	614	HIS	N-CA-C	-6.16	103.05	110.13
1	A	613	PRO	CB-CA-C	-6.14	102.94	110.98
1	A	360	HIS	CA-CB-CG	-6.12	107.68	113.80
1	D	473	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	728	VAL	CA-C-O	6.10	124.69	119.38
1	D	447	ASP	N-CA-C	6.08	120.83	113.17
1	D	685	LEU	N-CA-C	6.08	118.50	110.36
1	C	931	PHE	N-CA-C	-6.07	99.81	109.04
1	A	646	HIS	CA-CB-CG	-6.06	107.74	113.80
1	C	209	PHE	N-CA-C	6.05	120.80	113.17
1	A	752	GLY	CA-C-N	-6.05	112.15	122.56
1	A	752	GLY	C-N-CA	-6.05	112.15	122.56
1	B	796	SER	N-CA-CB	6.05	118.96	109.83
1	A	771	GLY	CA-C-N	-6.04	112.94	122.79
1	A	771	GLY	C-N-CA	-6.04	112.94	122.79
1	C	644	PHE	N-CA-C	6.04	121.53	114.04
1	B	553	TRP	CA-CB-CG	-6.04	102.13	113.60
1	B	614	HIS	N-CA-CB	6.02	116.72	109.74
1	D	93	HIS	N-CA-C	-6.00	105.54	112.92
1	A	359	HIS	CA-CB-CG	-6.00	107.80	113.80
1	C	46	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	B	893	GLU	N-CA-CB	5.99	119.03	110.16
1	D	804	ASN	CB-CA-C	5.98	120.06	109.65
1	A	1018	LEU	CB-CA-C	-5.96	96.95	110.07
1	C	818	ALA	CA-C-N	5.96	130.94	122.72
1	C	818	ALA	C-N-CA	5.96	130.94	122.72
1	A	784	PHE	CA-CB-CG	-5.96	107.84	113.80
1	C	793	ILE	CB-CA-C	-5.94	104.28	112.24
1	D	431	ARG	NE-CZ-NH2	-5.94	113.86	119.20
1	B	209	PHE	N-CA-C	5.93	120.64	113.17
1	A	113	PHE	CA-CB-CG	-5.91	107.89	113.80
1	D	128	ASN	N-CA-CB	5.90	121.17	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	790	ASP	O-C-N	-5.89	115.87	122.12
1	C	267	VAL	CA-CB-CG2	-5.88	100.40	110.40
1	B	400	THR	CB-CA-C	5.88	120.56	110.79
1	C	333	ARG	NE-CZ-NH1	-5.88	115.62	121.50
1	C	248	GLY	CA-C-N	-5.88	114.36	122.30
1	C	248	GLY	C-N-CA	-5.88	114.36	122.30
1	B	100	TYR	CA-CB-CG	-5.87	103.33	113.90
1	D	1022	GLN	CB-CG-CD	5.86	122.56	112.60
1	D	958	ASN	N-CA-CB	5.86	122.42	111.53
1	A	743	SER	N-CA-C	-5.85	100.24	108.96
1	B	144	ASP	CA-CB-CG	-5.85	106.75	112.60
1	A	730	LEU	CB-CA-C	5.84	117.85	109.26
1	D	473	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	A	97	ALA	N-CA-C	5.83	117.42	110.07
1	B	161	TYR	N-CA-CB	-5.83	101.54	111.69
1	C	76	CYS	CA-C-O	5.83	127.82	121.06
1	D	787	ALA	N-CA-C	-5.82	99.39	109.58
1	B	127	PHE	CA-CB-CG	-5.82	107.98	113.80
1	A	147	ASN	CA-CB-CG	5.81	118.41	112.60
1	B	519	SER	N-CA-C	-5.80	102.06	110.24
1	C	339	ASN	CA-CB-CG	-5.80	106.80	112.60
1	C	113	PHE	CB-CA-C	-5.80	99.68	109.83
1	A	675	GLN	OE1-CD-NE2	5.80	128.40	122.60
1	B	225	PHE	N-CA-CB	5.80	121.62	111.13
1	A	166	ARG	NE-CZ-NH2	-5.76	114.01	119.20
1	C	592	PHE	CA-CB-CG	-5.75	108.05	113.80
1	A	894	ARG	NE-CZ-NH1	-5.74	115.77	121.50
1	C	730	LEU	C-N-CD	-5.73	101.50	125.00
1	A	823	LEU	N-CA-C	-5.73	106.83	113.88
1	B	122	CYS	CA-C-N	-5.73	113.65	122.87
1	B	122	CYS	C-N-CA	-5.73	113.65	122.87
1	B	889	ALA	CA-C-O	5.73	126.55	119.79
1	A	247	CYS	N-CA-C	-5.72	100.46	109.50
1	B	568	TRP	CA-CB-CG	-5.72	102.73	113.60
1	C	219	THR	CA-CB-OG1	-5.72	101.03	109.60
1	C	859	ASP	CA-CB-CG	-5.72	106.88	112.60
1	B	75	GLU	CA-C-N	-5.71	112.95	122.21
1	B	75	GLU	C-N-CA	-5.71	112.95	122.21
1	D	320	GLY	N-CA-C	5.70	123.97	115.64
1	B	843	GLN	OE1-CD-NE2	5.70	128.30	122.60
1	C	699	ARG	NE-CZ-NH1	5.69	127.19	121.50
1	A	833	ALA	N-CA-CB	-5.69	102.70	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	PRO	N-CA-CB	5.68	108.30	103.19
1	D	278	ILE	CA-C-N	-5.67	115.10	121.85
1	D	278	ILE	C-N-CA	-5.67	115.10	121.85
1	D	396	PRO	N-CA-CB	5.66	109.71	103.26
1	A	118	ASN	N-CA-CB	-5.65	101.78	111.39
1	A	477	SER	CB-CA-C	-5.65	100.36	110.70
1	D	769	TRP	CA-C-N	-5.65	115.56	123.13
1	D	769	TRP	C-N-CA	-5.65	115.56	123.13
1	C	294	ASN	CA-CB-CG	-5.65	106.95	112.60
1	A	729	THR	CB-CA-C	5.64	118.92	109.89
1	A	894	ARG	NE-CZ-NH2	5.64	124.28	119.20
1	B	313	VAL	CB-CA-C	-5.63	103.66	110.99
1	D	820	ALA	N-CA-C	5.63	117.92	108.23
1	B	356	ARG	NE-CZ-NH1	5.63	127.13	121.50
1	B	583	ASN	CA-CB-CG	-5.63	106.97	112.60
1	B	790	ASP	CA-CB-CG	-5.62	106.98	112.60
1	B	211	ASP	N-CA-C	5.62	117.55	110.24
1	A	317	THR	O-C-N	-5.61	116.46	122.85
1	A	730	LEU	N-CA-C	5.61	116.88	109.93
1	D	687	GLN	C-N-CD	-5.60	102.04	125.00
1	B	890	GLN	N-CA-C	5.60	119.10	110.42
1	D	882	ILE	CA-CB-CG1	-5.59	100.90	110.40
1	B	610	ASP	CA-C-N	-5.59	118.09	126.86
1	B	610	ASP	C-N-CA	-5.59	118.09	126.86
1	B	931	PHE	CA-CB-CG	-5.58	108.22	113.80
1	B	221	GLN	N-CA-CB	-5.58	102.58	111.62
1	D	601	PHE	CA-CB-CG	-5.58	108.22	113.80
1	C	778	THR	O-C-N	5.58	125.84	121.88
1	A	70	PRO	CB-CA-C	-5.57	103.00	110.85
1	B	614	HIS	N-CA-C	-5.56	102.91	110.36
1	A	116	THR	CA-CB-OG1	-5.56	101.26	109.60
1	A	788	PRO	N-CA-CB	5.56	108.26	103.31
1	B	606	LEU	N-CA-C	-5.56	106.00	112.89
1	D	895	VAL	N-CA-CB	5.55	119.36	111.82
1	D	948	PRO	CB-CA-C	-5.54	103.60	111.68
1	B	917	ARG	CD-NE-CZ	-5.53	116.66	124.40
1	A	915	PHE	CA-C-O	5.52	126.89	120.49
1	B	702	GLN	CA-C-O	5.51	123.99	119.36
1	A	279	ILE	CB-CA-C	5.51	115.91	111.06
1	A	671	ASP	CA-CB-CG	5.51	118.11	112.60
1	D	14	ARG	N-CA-CB	-5.51	104.18	110.35
1	C	687	GLN	N-CA-CB	5.50	118.34	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	830	LEU	N-CA-C	-5.50	102.03	109.95
1	A	671	ASP	CA-C-N	-5.50	115.30	122.94
1	A	671	ASP	C-N-CA	-5.50	115.30	122.94
1	A	100	TYR	N-CA-CB	5.49	119.73	110.46
1	B	447	ASP	N-CA-C	5.48	120.64	113.30
1	C	788	PRO	N-CA-CB	5.47	108.20	103.27
1	D	690	SER	O-C-N	-5.47	116.20	122.93
1	C	578	TYR	CA-CB-CG	-5.46	104.07	113.90
1	C	747	PHE	CA-CB-CG	5.46	119.25	113.80
1	C	233	ASP	CA-C-N	-5.45	114.00	122.67
1	C	233	ASP	C-N-CA	-5.45	114.00	122.67
1	D	89	ASN	N-CA-C	-5.45	100.29	109.07
1	A	913	ALA	CA-C-O	-5.45	115.62	121.56
1	B	135	GLN	OE1-CD-NE2	-5.45	117.15	122.60
1	B	700	VAL	N-CA-CB	5.45	117.58	111.21
1	C	1007	PHE	CA-CB-CG	-5.45	108.35	113.80
1	B	70	PRO	O-C-N	-5.45	116.56	123.10
1	A	140	ARG	CA-C-N	-5.43	116.10	123.10
1	A	140	ARG	C-N-CA	-5.43	116.10	123.10
1	A	395	HIS	N-CA-CB	-5.43	101.46	109.98
1	C	450	HIS	CA-C-O	5.43	123.64	119.46
1	B	63	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	658	LEU	CA-C-N	-5.43	114.66	122.36
1	A	658	LEU	C-N-CA	-5.43	114.66	122.36
1	D	320	GLY	CA-C-N	-5.43	114.54	122.19
1	D	320	GLY	C-N-CA	-5.43	114.54	122.19
1	A	147	ASN	N-CA-CB	-5.42	102.19	110.65
1	D	323	ILE	N-CA-C	-5.42	106.41	111.45
1	A	729	THR	N-CA-CB	5.42	117.92	109.85
1	A	860	GLY	CA-C-N	-5.42	113.60	122.54
1	A	860	GLY	C-N-CA	-5.42	113.60	122.54
1	A	409	VAL	N-CA-C	5.41	116.27	108.48
1	A	570	TRP	N-CA-C	5.41	117.03	111.03
1	B	915	PHE	CA-CB-CG	-5.40	108.40	113.80
1	D	23	GLN	CA-C-O	-5.40	115.16	121.10
1	D	147	ASN	N-CA-CB	-5.40	102.23	110.65
1	D	82	ASP	CA-CB-CG	-5.39	107.21	112.60
1	A	571	VAL	N-CA-C	5.39	115.88	108.12
1	B	235	PHE	CA-CB-CG	-5.38	108.42	113.80
1	C	75	GLU	N-CA-C	5.38	119.97	113.41
1	A	159	VAL	CA-C-N	-5.37	112.93	120.56
1	A	159	VAL	C-N-CA	-5.37	112.93	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	297	ASN	CA-CB-CG	-5.37	107.23	112.60
1	A	917	ARG	NE-CZ-NH1	-5.37	116.13	121.50
1	C	739	HIS	CA-CB-CG	-5.36	108.44	113.80
1	D	493	THR	CA-C-O	-5.36	116.38	122.01
1	C	78	LEU	N-CA-C	-5.35	103.03	109.72
1	A	178	ARG	NE-CZ-NH2	-5.34	114.39	119.20
1	C	671	ASP	CA-CB-CG	-5.34	107.26	112.60
1	C	85	VAL	CA-CB-CG2	-5.34	101.32	110.40
1	D	114	VAL	O-C-N	5.34	127.19	121.10
1	A	753	ASN	CA-CB-CG	-5.34	107.26	112.60
1	D	646	HIS	CA-CB-CG	-5.33	108.47	113.80
1	A	126	THR	N-CA-C	-5.33	100.55	109.24
1	C	670	LEU	CB-CA-C	-5.33	100.95	109.75
1	C	85	VAL	N-CA-CB	-5.33	103.21	110.56
1	B	388	ARG	NE-CZ-NH2	-5.33	114.41	119.20
1	B	833	ALA	CA-C-O	5.32	126.98	121.28
1	C	668	VAL	N-CA-CB	-5.32	103.76	111.21
1	B	863	GLN	CB-CG-CD	5.32	121.64	112.60
1	C	69	VAL	N-CA-C	5.32	113.20	108.63
1	B	423	MET	N-CA-C	5.30	117.81	111.71
1	B	958	ASN	N-CA-CB	5.30	121.38	111.53
1	D	820	ALA	CA-C-O	5.30	126.70	120.98
1	A	790	ASP	CA-C-O	5.29	126.35	120.63
1	B	986	ILE	N-CA-CB	-5.29	104.77	111.64
1	A	127	PHE	CA-CB-CG	-5.29	108.52	113.80
1	A	859	ASP	N-CA-C	5.29	118.15	110.17
1	C	98	PRO	N-CA-C	-5.29	102.85	111.68
1	C	872	VAL	CA-C-N	-5.28	113.21	120.71
1	C	872	VAL	C-N-CA	-5.28	113.21	120.71
1	A	598	ASP	CA-CB-CG	-5.28	107.32	112.60
1	A	1015	HIS	CA-CB-CG	-5.28	108.52	113.80
1	B	194	GLY	CA-C-O	5.28	126.10	120.40
1	C	689	GLU	CB-CG-CD	5.28	121.57	112.60
1	A	553	TRP	CA-CB-CG	-5.27	103.58	113.60
1	A	95	TYR	N-CA-C	5.27	117.94	111.82
1	B	977	HIS	CA-CB-CG	5.27	119.07	113.80
1	A	659	ASP	CB-CA-C	-5.27	104.41	111.89
1	A	857	ARG	CA-C-N	-5.27	116.27	123.12
1	A	857	ARG	C-N-CA	-5.27	116.27	123.12
1	B	844	HIS	CA-CB-CG	-5.27	108.53	113.80
1	A	348	PRO	N-CA-CB	5.26	107.73	103.36
1	B	591	ASP	N-CA-C	5.26	119.32	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	745	MET	N-CA-C	5.26	117.09	111.36
1	D	685	LEU	N-CA-CB	5.25	115.83	109.74
1	B	794	ALA	CA-C-N	-5.25	114.82	122.28
1	B	794	ALA	C-N-CA	-5.25	114.82	122.28
1	A	93	HIS	CA-CB-CG	-5.25	108.55	113.80
1	C	665	SER	O-C-N	-5.25	117.75	123.26
1	C	884	LEU	CA-C-N	-5.25	113.26	121.87
1	C	884	LEU	C-N-CA	-5.25	113.26	121.87
1	A	974	HIS	CA-CB-CG	-5.25	108.55	113.80
1	D	13	ARG	NE-CZ-NH2	-5.25	114.48	119.20
1	D	211	ASP	N-CA-C	5.24	117.30	110.43
1	D	686	PRO	N-CA-C	-5.24	102.93	111.68
1	C	447	ASP	N-CA-C	5.24	120.32	113.30
1	C	743	SER	CA-C-N	-5.24	113.26	120.28
1	C	743	SER	C-N-CA	-5.24	113.26	120.28
1	A	872	VAL	CB-CA-C	-5.24	103.34	110.77
1	D	352	ARG	CA-C-N	-5.24	117.04	122.69
1	D	352	ARG	C-N-CA	-5.24	117.04	122.69
1	A	790	ASP	CA-CB-CG	-5.23	107.37	112.60
1	B	856	TYR	CA-C-N	-5.23	115.63	123.00
1	B	856	TYR	C-N-CA	-5.23	115.63	123.00
1	C	684	GLU	CA-C-N	-5.23	112.75	122.06
1	C	684	GLU	C-N-CA	-5.23	112.75	122.06
1	C	653	HIS	CA-CB-CG	5.23	119.03	113.80
1	D	614	HIS	CB-CA-C	-5.23	101.22	110.47
1	A	829	THR	N-CA-CB	-5.22	101.80	110.47
1	D	606	LEU	N-CA-C	-5.22	106.42	112.89
1	D	753	ASN	CA-CB-CG	-5.22	107.38	112.60
1	B	842	TRP	CE2-CD2-CE3	5.21	124.01	118.80
1	A	179	ALA	N-CA-CB	5.21	117.70	109.83
1	C	811	LYS	CB-CA-C	-5.21	102.70	110.88
1	C	601	PHE	CA-CB-CG	-5.21	108.59	113.80
1	C	664	ALA	CB-CA-C	-5.21	100.77	110.56
1	C	993	ILE	CA-C-O	5.20	124.19	119.20
1	D	817	GLN	CB-CG-CD	-5.20	103.75	112.60
1	C	703	PRO	N-CA-CB	5.20	109.03	103.52
1	B	661	LYS	CA-C-N	5.20	125.49	119.93
1	B	661	LYS	C-N-CA	5.20	125.49	119.93
1	B	425	ARG	CA-CB-CG	-5.19	103.72	114.10
1	C	519	SER	N-CA-C	-5.19	102.92	110.24
1	B	890	GLN	CB-CA-C	-5.19	101.23	109.80
1	B	987	ASP	N-CA-C	5.19	117.95	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	583	ASN	CA-CB-CG	-5.19	107.41	112.60
1	B	499	ILE	N-CA-C	-5.19	101.99	108.84
1	B	627	PHE	CA-CB-CG	-5.18	108.62	113.80
1	D	572	ASP	CB-CA-C	-5.18	101.82	109.90
1	A	685	LEU	O-C-N	5.18	127.28	121.32
1	C	571	VAL	N-CA-C	5.18	116.18	108.46
1	A	363	HIS	N-CA-C	5.17	119.59	113.28
1	C	365	GLN	CA-CB-CG	-5.17	103.75	114.10
1	D	136	GLU	N-CA-C	5.17	116.16	108.60
1	A	917	ARG	CD-NE-CZ	-5.17	117.16	124.40
1	D	772	ASP	CB-CA-C	-5.17	100.28	110.11
1	A	746	ASP	CB-CA-C	-5.17	99.33	110.45
1	D	115	PRO	N-CA-CB	5.16	107.91	103.31
1	B	729	THR	N-CA-CB	5.15	118.40	110.21
1	A	779	PRO	N-CA-CB	5.15	108.23	103.39
1	A	277	GLU	CB-CG-CD	5.14	121.35	112.60
1	C	1005	ALA	N-CA-C	5.14	118.33	111.75
1	D	600	GLN	N-CA-C	5.14	119.42	113.20
1	B	889	ALA	CA-C-N	-5.14	113.39	122.74
1	B	889	ALA	C-N-CA	-5.14	113.39	122.74
1	B	685	LEU	N-CA-CB	5.13	119.51	110.37
1	B	973	ARG	NE-CZ-NH1	-5.13	116.36	121.50
1	C	935	ASN	OD1-CG-ND2	5.13	127.73	122.60
1	C	20	GLY	N-CA-C	-5.13	108.60	115.32
1	C	710	GLU	CB-CA-C	-5.13	99.55	109.76
1	D	890	GLN	N-CA-CB	-5.13	102.50	110.04
1	B	797	GLU	CB-CG-CD	-5.12	103.89	112.60
1	D	477	SER	CB-CA-C	-5.12	102.14	110.85
1	A	64	PRO	CB-CA-C	-5.12	103.31	111.04
1	D	330	VAL	CA-C-O	-5.12	115.01	120.39
1	D	779	PRO	CB-CA-C	-5.12	104.52	111.12
1	B	771	GLY	CA-C-N	-5.11	114.47	122.65
1	B	771	GLY	C-N-CA	-5.11	114.47	122.65
1	C	100	TYR	CA-CB-CG	-5.11	104.70	113.90
1	A	522	LYS	CA-C-O	5.11	125.84	120.42
1	A	980	GLU	N-CA-CB	-5.11	102.82	110.17
1	C	395	HIS	N-CA-CB	-5.11	101.96	109.98
1	C	728	VAL	N-CA-CB	5.11	118.80	112.16
1	B	961	ARG	NE-CZ-NH2	-5.10	114.61	119.20
1	D	954	ASP	CA-CB-CG	-5.10	107.50	112.60
1	C	97	ALA	N-CA-C	5.09	116.48	110.07
1	A	221	GLN	N-CA-CB	-5.09	103.52	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	GLU	N-CA-C	5.09	117.59	109.96
1	A	770	ILE	N-CA-C	-5.09	99.19	107.28
1	C	917	ARG	NE-CZ-NH2	5.08	123.77	119.20
1	B	736	ALA	CA-C-N	5.08	127.27	122.85
1	B	736	ALA	C-N-CA	5.08	127.27	122.85
1	D	747	PHE	N-CA-CB	5.08	118.57	110.65
1	B	218	PRO	N-CA-CB	5.07	108.71	103.38
1	A	593	GLY	CA-C-O	5.07	124.74	119.06
1	A	106	PRO	N-CA-CB	5.07	108.02	103.20
1	A	661	LYS	CA-C-N	5.07	125.31	119.83
1	A	661	LYS	C-N-CA	5.07	125.31	119.83
1	C	606	LEU	N-CA-C	-5.07	106.61	112.89
1	D	809	ARG	CG-CD-NE	5.07	123.14	112.00
1	B	636	ILE	CB-CA-C	-5.06	103.57	110.96
1	C	627	PHE	CA-CB-CG	-5.06	108.74	113.80
1	D	147	ASN	CA-CB-CG	5.05	117.65	112.60
1	B	14	ARG	N-CA-CB	5.05	118.84	111.62
1	A	847	LYS	N-CA-C	5.05	117.47	109.24
1	D	842	TRP	CB-CA-C	-5.05	101.42	109.75
1	B	262	GLN	CB-CA-C	5.04	119.44	111.77
1	C	891	VAL	CB-CA-C	-5.04	104.73	110.73
1	B	823	LEU	N-CA-C	-5.04	107.08	113.43
1	A	794	ALA	CB-CA-C	-5.04	110.75	116.54
1	B	869	ASP	CA-CB-CG	-5.03	107.57	112.60
1	D	648	ASP	N-CA-C	5.03	119.06	113.02
1	A	662	PRO	N-CA-CB	5.03	107.80	103.27
1	D	500	CYS	N-CA-C	5.03	116.79	109.30
1	D	49	GLN	CA-CB-CG	-5.02	104.06	114.10
1	B	82	ASP	CA-CB-CG	-5.02	107.58	112.60
1	C	985	ASN	CA-CB-CG	-5.01	107.59	112.60
1	C	408	TYR	CA-C-N	-5.01	116.14	123.06
1	C	408	TYR	C-N-CA	-5.01	116.14	123.06
1	C	765	LEU	N-CA-C	-5.01	101.94	109.15
1	D	905	ASN	CA-CB-CG	5.00	117.61	112.60
1	C	653	HIS	N-CA-CB	5.00	118.58	110.43

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	685	LEU	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	8126	0	7718	169	0
1	B	8126	0	7718	133	0
1	C	8126	0	7718	182	0
1	D	8126	0	7718	140	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	5	0	0	0	0
2	D	4	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	15	0	17	1	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	15	0	17	1	0
5	A	96	0	144	30	0
5	B	88	0	132	19	0
5	C	100	0	150	21	0
5	D	92	0	138	13	0
6	A	950	0	0	15	0
6	B	971	0	0	17	0
6	C	943	0	0	20	0
6	D	949	0	0	21	0
All	All	36785	0	31504	640	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (640) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.36	1.06
1:B:102:ASN:HD22	5:B:8506:DMS:H21	1.19	1.01
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:PHE:CG	5:B:8506:DMS:H23	2.01	0.96
1:D:651:LEU:HD11	1:D:653:HIS:CE1	2.01	0.95
1:C:745:MET:HE3	1:C:745:MET:HA	1.50	0.93
1:D:102:ASN:ND2	5:D:8506:DMS:H11	1.83	0.93
1:A:32:PRO:HB2	5:A:8404:DMS:H13	1.52	0.90
1:B:102:ASN:ND2	5:B:8506:DMS:H21	1.86	0.90
1:A:600:GLN:H	1:A:600:GLN:HE21	1.18	0.89
1:A:277:GLU:H	1:A:277:GLU:CD	1.77	0.88
1:D:233:ASP:HA	5:D:8417:DMS:H13	1.55	0.88
1:D:773:LYS:HG2	1:D:775:GLN:HE22	1.39	0.88
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.55	0.88
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.58	0.85
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.10	0.85
1:A:94:GLY:C	5:A:8421:DMS:H21	2.02	0.84
1:B:600:GLN:H	1:B:600:GLN:HE21	1.22	0.84
1:A:473:ARG:NH1	1:A:476:LYS:HB2	1.93	0.84
1:C:651:LEU:HD11	1:C:653:HIS:ND1	1.93	0.83
5:C:8417:DMS:H22	6:C:9205:HOH:O	1.77	0.83
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.58	0.83
1:D:102:ASN:HD22	5:D:8506:DMS:H11	1.43	0.82
1:D:687:GLN:HG3	1:D:688:PRO:HD2	1.62	0.81
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.63	0.80
1:B:634:GLN:HG2	1:B:682:LEU:O	1.82	0.80
1:D:651:LEU:C	1:D:651:LEU:HD12	2.07	0.80
1:B:748:CYS:C	1:B:749:ILE:HD12	2.06	0.80
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.12	0.80
5:D:8413:DMS:H13	6:D:9297:HOH:O	1.81	0.79
1:D:773:LYS:HG2	1:D:775:GLN:NE2	1.96	0.79
1:C:54:LEU:HD21	1:C:214:LEU:CD2	2.13	0.78
1:D:755:ARG:HG3	1:D:769:TRP:HB2	1.66	0.78
1:C:744:GLU:O	1:C:760:ARG:HD3	1.83	0.78
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.64	0.77
5:A:8503:DMS:H22	6:A:9019:HOH:O	1.84	0.77
1:D:135:GLN:C	1:D:136:GLU:HG2	2.09	0.77
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.20	0.77
1:A:797:GLU:O	1:A:801:ILE:HD13	1.84	0.76
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.16	0.76
1:A:686:PRO:C	1:A:688:PRO:HD3	2.12	0.75
1:B:473:ARG:NH2	1:B:477:SER:HB2	2.02	0.75
1:A:251:ARG:HH11	5:A:8416:DMS:C2	2.00	0.75
1:D:128:ASN:HB3	1:D:180:GLY:O	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:O	1:B:661:LYS:HG3	1.86	0.74
1:C:634:GLN:OE1	1:C:681:GLU:HG3	1.87	0.74
1:C:734:SER:CB	1:C:860:GLY:HA3	2.18	0.74
1:C:797:GLU:O	1:C:801:ILE:HD13	1.88	0.74
1:B:102:ASN:HD22	5:B:8506:DMS:C2	1.99	0.73
1:B:651:LEU:O	1:B:651:LEU:HD23	1.87	0.73
1:B:601:PHE:CD2	5:B:8506:DMS:H23	2.22	0.73
1:C:690:SER:HB2	6:C:9322:HOH:O	1.88	0.73
1:C:699:ARG:HH12	5:C:8415:DMS:H11	1.51	0.73
1:A:887:GLN:NE2	1:A:980:GLU:O	2.21	0.73
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.14	0.72
5:C:8601:DMS:H11	6:C:9543:HOH:O	1.88	0.72
1:C:54:LEU:HD21	1:C:214:LEU:HD22	1.71	0.72
1:A:231:PHE:O	5:A:8417:DMS:H23	1.90	0.72
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.71	0.72
1:C:595:THR:HA	1:C:596:PRO:C	2.14	0.72
1:B:655:MET:HE2	1:B:656:VAL:N	2.05	0.72
1:D:299:LYS:NZ	6:D:9381:HOH:O	2.22	0.71
1:D:660:GLY:O	1:D:662:PRO:HD3	1.90	0.71
1:D:663:LEU:HD11	1:D:688:PRO:HG3	1.72	0.71
1:B:13:ARG:HG3	1:C:13:ARG:NH2	2.05	0.71
5:C:8503:DMS:H13	6:C:9040:HOH:O	1.90	0.71
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.73	0.70
1:D:629:PHE:O	1:D:630:ARG:HD3	1.91	0.70
1:A:749:ILE:HD12	1:A:749:ILE:N	2.07	0.70
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.27	0.69
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.74	0.69
6:B:9346:HOH:O	5:C:8420:DMS:H22	1.92	0.69
1:D:201:ASP:OD2	4:D:2001:IPT:H62	1.93	0.69
1:C:601:PHE:CZ	5:C:8506:DMS:H23	2.27	0.69
1:D:579:ASP:O	1:D:580:GLU:C	2.36	0.68
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.23	0.68
1:D:738:PRO:HG3	1:D:751:LEU:HD22	1.75	0.68
1:B:797:GLU:O	1:B:800:ARG:C	2.37	0.68
1:C:699:ARG:NH2	6:C:9411:HOH:O	2.26	0.67
1:D:801:ILE:HD12	1:D:808:GLU:OE2	1.95	0.67
1:A:878:HIS:HD2	6:A:8675:HOH:O	1.78	0.67
1:D:847:LYS:HD3	1:D:848:THR:N	2.10	0.67
1:A:948:PRO:C	1:A:1023:LYS:HE3	2.20	0.67
5:A:8410:DMS:H11	6:A:8942:HOH:O	1.94	0.66
1:A:233:ASP:HA	5:A:8417:DMS:H13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:655:MET:HE2	1:C:664:ALA:O	1.95	0.66
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.31	0.66
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.28	0.66
1:D:795:VAL:HG12	5:D:8506:DMS:H23	1.76	0.66
1:A:650:GLU:N	5:A:8425:DMS:O	2.27	0.65
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.30	0.65
1:D:579:ASP:O	1:D:581:ASN:N	2.29	0.64
1:A:595:THR:HA	1:A:596:PRO:C	2.20	0.64
1:B:878:HIS:HD2	6:B:8689:HOH:O	1.79	0.64
5:B:8410:DMS:H22	6:B:8876:HOH:O	1.98	0.64
1:D:595:THR:HA	1:D:596:PRO:C	2.22	0.64
1:A:634:GLN:HB2	1:A:682:LEU:HB2	1.80	0.64
1:B:797:GLU:O	1:B:800:ARG:N	2.30	0.63
1:D:878:HIS:HD2	6:D:8811:HOH:O	1.80	0.63
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.80	0.63
1:B:231:PHE:O	5:B:8417:DMS:H23	1.98	0.63
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.62	0.63
1:A:84:VAL:HA	5:A:8414:DMS:O	1.99	0.63
1:B:749:ILE:HD12	1:B:749:ILE:N	2.14	0.63
1:C:658:LEU:HG	1:C:661:LYS:NZ	2.12	0.63
1:C:734:SER:HB3	1:C:860:GLY:C	2.24	0.63
1:A:753:ASN:OD1	1:A:753:ASN:N	2.29	0.63
1:A:830:LEU:N	1:A:830:LEU:HD23	2.13	0.63
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.11	0.63
1:C:973:ARG:O	5:C:8423:DMS:H12	1.99	0.63
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.64	0.62
1:C:240:LEU:C	1:C:240:LEU:HD23	2.24	0.62
5:C:8410:DMS:H11	6:C:8970:HOH:O	1.99	0.62
1:A:267:VAL:O	5:A:8602:DMS:H23	2.00	0.62
1:C:878:HIS:HD2	6:C:8699:HOH:O	1.80	0.62
1:B:600:GLN:HE21	1:B:600:GLN:N	1.96	0.62
1:C:853:ARG:NH1	1:C:871:GLU:OE2	2.24	0.61
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.48	0.61
1:A:832:ASP:OD1	1:A:832:ASP:N	2.34	0.61
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.82	0.61
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.19	0.61
1:B:826:THR:OG1	1:B:837:THR:HB	2.00	0.61
5:D:8703:DMS:H21	6:D:9573:HOH:O	1.99	0.61
1:A:370:GLN:HG3	6:A:9095:HOH:O	2.00	0.61
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.61
1:D:802:ASP:OD1	1:D:803:PRO:HD2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:595:THR:HA	1:B:596:PRO:C	2.26	0.60
1:C:658:LEU:O	1:C:661:LYS:HG3	2.00	0.60
1:D:622:HIS:O	1:D:625:GLN:HG3	2.01	0.60
1:D:685:LEU:CD2	1:D:686:PRO:HD2	2.31	0.60
1:A:251:ARG:HD3	5:A:8416:DMS:H22	1.83	0.60
1:A:251:ARG:HH11	5:A:8416:DMS:H22	1.67	0.60
1:B:684:GLU:O	1:B:686:PRO:HD3	2.02	0.60
1:D:615:PRO:O	1:D:618:THR:HG22	2.02	0.60
1:A:93:HIS:O	5:A:8421:DMS:H23	2.02	0.60
1:D:858:ILE:CD1	1:D:864:MET:HB2	2.32	0.60
1:B:655:MET:HE2	1:B:655:MET:C	2.27	0.60
1:D:887:GLN:NE2	1:D:980:GLU:O	2.34	0.60
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.82	0.60
1:A:94:GLY:CA	5:A:8421:DMS:H21	2.31	0.59
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.84	0.59
1:C:601:PHE:CE2	5:C:8506:DMS:H23	2.37	0.59
1:D:277:GLU:CD	1:D:277:GLU:H	1.99	0.59
1:A:178:ARG:HD2	6:A:9398:HOH:O	2.02	0.59
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.84	0.59
1:D:240:LEU:HD23	1:D:240:LEU:C	2.28	0.59
1:C:734:SER:HB3	1:C:860:GLY:CA	2.32	0.59
1:C:634:GLN:H	1:C:634:GLN:NE2	2.01	0.59
1:D:79:PRO:HD2	1:D:80:GLU:OE2	2.03	0.59
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.86	0.58
1:C:601:PHE:CE1	5:C:8506:DMS:H23	2.38	0.58
1:D:522:LYS:NZ	6:D:9159:HOH:O	2.34	0.58
1:C:833:ALA:HB1	1:C:858:ILE:O	2.04	0.58
1:B:651:LEU:HD23	1:B:651:LEU:C	2.29	0.58
1:C:78:LEU:HB3	1:C:80:GLU:HG3	1.85	0.58
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.04	0.58
1:A:32:PRO:HB2	5:A:8404:DMS:C1	2.31	0.58
1:D:649:ASN:HB2	6:D:9342:HOH:O	2.03	0.58
1:C:824:GLN:HG3	1:C:825:CYS:N	2.19	0.57
1:A:252:ASP:H	5:A:8416:DMS:C1	2.17	0.57
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.69	0.57
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.39	0.57
1:C:387:VAL:HG22	6:C:9481:HOH:O	2.04	0.57
1:A:336:ARG:NH2	1:A:338:GLU:OE1	2.29	0.57
1:A:508:GLU:OE2	5:A:8407:DMS:H11	2.04	0.57
1:A:655:MET:HE1	1:A:662:PRO:CB	2.28	0.57
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:593:GLY:O	1:A:595:THR:HG22	2.05	0.57
1:A:829:THR:C	1:A:830:LEU:HD23	2.30	0.57
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.39	0.57
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.39	0.56
1:D:756:TRP:CE2	1:D:858:ILE:HD12	2.39	0.56
1:A:737:ILE:C	1:A:737:ILE:HD13	2.30	0.56
1:C:688:PRO:HG3	1:C:694:LEU:HD11	1.87	0.56
1:D:684:GLU:HG2	1:D:685:LEU:N	2.14	0.56
1:A:580:GLU:O	1:A:580:GLU:OE1	2.22	0.56
1:D:251:ARG:NH2	1:D:253:TYR:OH	2.39	0.56
1:D:579:ASP:O	1:D:579:ASP:OD1	2.24	0.56
1:D:367:MET:HB3	1:D:372:MET:HE2	1.88	0.56
1:A:135:GLN:NE2	6:A:9464:HOH:O	2.39	0.56
1:A:157:ARG:HB2	6:A:9380:HOH:O	2.06	0.56
1:C:945:ASN:OD1	1:C:1023:LYS:HD2	2.06	0.56
1:A:94:GLY:HA3	5:A:8421:DMS:H21	1.86	0.56
1:C:737:ILE:O	1:C:737:ILE:HG13	2.02	0.56
1:C:607:VAL:HG12	1:C:613:PRO:HA	1.88	0.56
1:D:651:LEU:C	1:D:651:LEU:CD1	2.78	0.56
1:A:648:ASP:OD2	6:A:9426:HOH:O	2.18	0.56
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.87	0.55
1:C:687:GLN:HG3	1:C:688:PRO:CD	2.23	0.55
1:D:651:LEU:HD11	1:D:653:HIS:ND1	2.21	0.55
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.87	0.55
5:B:8425:DMS:H22	6:B:9366:HOH:O	2.04	0.55
1:C:178:ARG:O	1:C:178:ARG:HG2	1.90	0.55
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.27	0.55
1:A:262:GLN:HG3	1:A:309:TYR:CE2	2.41	0.55
1:A:653:HIS:CD2	1:A:667:GLU:HG2	2.42	0.55
1:A:634:GLN:HG2	1:A:682:LEU:O	2.05	0.55
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.89	0.55
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.20	0.55
5:D:8406:DMS:O	6:D:9571:HOH:O	2.17	0.55
1:C:654:TRP:O	1:C:665:SER:HB2	2.06	0.55
1:A:600:GLN:HE21	1:A:600:GLN:N	1.95	0.55
1:B:473:ARG:HH21	1:B:477:SER:HB2	1.70	0.55
1:B:615:PRO:O	1:B:618:THR:HG22	2.06	0.55
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.88	0.55
1:C:655:MET:HG3	1:C:655:MET:O	2.07	0.55
1:A:32:PRO:CB	5:A:8404:DMS:H13	2.32	0.54
1:B:685:LEU:O	1:B:686:PRO:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:910:LEU:C	1:B:910:LEU:HD12	2.32	0.54
1:C:367:MET:HB3	1:C:372:MET:HE2	1.89	0.54
1:C:577:LYS:HD3	1:C:587:ALA:HB2	1.88	0.54
1:D:651:LEU:HD12	1:D:651:LEU:O	2.08	0.54
1:B:240:LEU:C	1:B:240:LEU:HD23	2.33	0.54
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.89	0.54
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.26	0.54
1:B:634:GLN:HG2	1:B:682:LEU:HB2	1.89	0.54
1:A:737:ILE:HD13	1:A:737:ILE:O	2.07	0.54
1:C:375:ASP:HB3	1:C:379:MET:HE3	1.90	0.54
1:D:795:VAL:HB	6:D:9340:HOH:O	2.07	0.54
1:B:683:PRO:O	1:B:685:LEU:HG	2.07	0.53
1:C:655:MET:SD	1:C:657:ALA:HB2	2.48	0.53
1:A:58:TRP:CE2	1:A:125:LEU:HD22	2.44	0.53
1:C:54:LEU:CD2	1:C:214:LEU:HD22	2.35	0.53
1:D:749:ILE:HD12	1:D:749:ILE:N	2.24	0.53
1:D:805:ALA:O	1:D:809:ARG:HG3	2.08	0.53
1:A:674:PRO:C	1:A:675:GLN:HG2	2.33	0.53
1:D:858:ILE:HD13	1:D:864:MET:HB2	1.90	0.53
1:C:743:SER:O	1:C:744:GLU:C	2.44	0.53
1:D:804:ASN:O	1:D:809:ARG:NH1	2.42	0.53
1:A:473:ARG:HH12	1:A:477:SER:N	2.07	0.53
1:B:651:LEU:HD22	1:B:701:VAL:O	2.09	0.53
1:B:659:ASP:OD2	1:B:692:GLY:HA3	2.09	0.53
5:B:8421:DMS:H23	6:B:9123:HOH:O	2.09	0.53
1:C:178:ARG:HD3	6:C:9418:HOH:O	2.08	0.53
1:D:765:LEU:HD21	1:D:768:MET:SD	2.48	0.53
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.39	0.52
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.44	0.52
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.52
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.91	0.52
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.24	0.52
1:A:890:GLN:HG3	1:A:891:VAL:N	2.24	0.52
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.09	0.52
1:B:128:ASN:HA	1:B:180:GLY:O	2.09	0.52
1:C:658:LEU:O	1:C:659:ASP:C	2.52	0.52
1:A:88:SER:HA	1:A:366:VAL:HG21	1.91	0.52
1:D:71:GLU:HG2	6:D:9463:HOH:O	2.09	0.52
1:D:685:LEU:CG	1:D:686:PRO:HD2	2.39	0.52
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.25	0.52
1:D:952:ARG:O	1:D:1018:LEU:HD22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:OE1	1:A:634:GLN:N	2.43	0.52
1:D:687:GLN:CG	1:D:688:PRO:HD2	2.36	0.52
1:C:634:GLN:H	1:C:634:GLN:CD	2.17	0.52
1:D:251:ARG:NE	1:D:253:TYR:OH	2.40	0.52
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.09	0.52
1:B:250:LEU:O	1:B:251:ARG:HG2	2.09	0.52
1:A:66:PRO:HG3	1:A:189:LEU:CD2	2.40	0.51
1:B:262:GLN:HG3	6:B:9543:HOH:O	2.08	0.51
1:C:54:LEU:CG	1:C:214:LEU:HD22	2.40	0.51
1:C:806:TRP:CD1	1:C:809:ARG:NH2	2.78	0.51
1:C:785:THR:O	1:C:881:ARG:HD2	2.09	0.51
5:C:8403:DMS:H12	6:C:8702:HOH:O	2.11	0.51
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.79	0.51
1:C:829:THR:C	1:C:830:LEU:HD23	2.36	0.51
1:D:577:LYS:O	1:D:584:PRO:HA	2.10	0.51
1:A:735:HIS:CD2	1:A:735:HIS:N	2.78	0.51
1:B:246:MET:HE3	1:B:250:LEU:HD23	1.93	0.51
1:B:708:TRP:CZ2	5:B:8403:DMS:H13	2.44	0.51
1:B:634:GLN:HG2	1:B:682:LEU:C	2.36	0.51
1:D:797:GLU:O	1:D:801:ILE:HD13	2.10	0.51
1:C:806:TRP:CD1	1:C:809:ARG:HH21	2.27	0.51
1:A:252:ASP:H	5:A:8416:DMS:H12	1.74	0.51
1:C:610:ASP:O	1:C:611:ARG:HB2	2.11	0.51
1:C:806:TRP:CE2	1:C:809:ARG:NH2	2.79	0.51
1:B:806:TRP:CE2	1:B:809:ARG:NH2	2.78	0.51
1:A:608:PHE:CE1	1:A:614:HIS:CD2	2.99	0.51
1:A:685:LEU:HB3	1:A:686:PRO:CD	2.38	0.51
1:A:863:GLN:NE2	1:A:952:ARG:HH22	2.08	0.51
1:B:292:ARG:HH12	5:B:8412:DMS:C2	2.24	0.51
1:B:319:ASP:OD1	1:B:320:GLY:N	2.44	0.51
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.92	0.51
1:C:157:ARG:HD3	6:C:9513:HOH:O	2.10	0.51
1:D:134:LEU:HA	5:D:8705:DMS:H23	1.93	0.51
1:D:773:LYS:HG3	1:D:774:LYS:N	2.19	0.50
1:A:357:HIS:HD2	6:A:9482:HOH:O	1.94	0.50
1:A:1022:GLN:CD	1:A:1023:LYS:H	2.19	0.50
1:C:278:ILE:HD13	1:C:278:ILE:N	2.25	0.50
1:D:513:PRO:O	1:D:514:ALA:HB3	2.10	0.50
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.79	0.50
5:A:8410:DMS:H22	6:A:8861:HOH:O	2.10	0.50
1:C:267:VAL:O	5:C:8601:DMS:H21	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:569:ASP:HB2	6:C:9359:HOH:O	2.10	0.50
1:C:1001:PRO:HD3	6:C:8939:HOH:O	2.11	0.50
1:B:252:ASP:OD2	5:B:8416:DMS:H12	2.10	0.50
1:B:797:GLU:O	1:B:801:ILE:N	2.43	0.50
1:C:745:MET:HA	1:C:745:MET:CE	2.32	0.50
1:B:78:LEU:HD23	6:B:9094:HOH:O	2.11	0.50
1:A:250:LEU:C	1:A:251:ARG:HG2	2.35	0.50
1:C:806:TRP:CG	1:C:809:ARG:HH21	2.29	0.50
5:D:8503:DMS:H22	6:D:9149:HOH:O	2.10	0.50
1:C:608:PHE:CE1	1:C:614:HIS:CD2	2.99	0.50
1:C:806:TRP:HA	1:C:809:ARG:HE	1.75	0.50
1:D:853:ARG:NH1	1:D:871:GLU:OE2	2.38	0.50
1:A:357:HIS:CD2	6:A:9482:HOH:O	2.65	0.50
1:B:655:MET:HE2	1:B:655:MET:CA	2.41	0.50
1:D:646:HIS:CD2	1:D:647:SER:N	2.80	0.49
1:A:890:GLN:CG	1:A:891:VAL:N	2.75	0.49
1:C:254:LEU:C	1:C:255:ARG:HG2	2.36	0.49
1:A:1022:GLN:O	1:A:1023:LYS:HG3	2.13	0.49
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.46	0.49
1:B:890:GLN:OE1	1:B:948:PRO:HD2	2.11	0.49
1:C:601:PHE:CE1	5:C:8506:DMS:C2	2.96	0.49
1:C:615:PRO:O	1:C:618:THR:HG22	2.13	0.49
1:C:843:GLN:HG2	1:C:848:THR:HA	1.95	0.49
1:A:687:GLN:N	1:A:688:PRO:HD3	2.26	0.49
1:A:819:GLU:HA	1:A:819:GLU:OE1	2.12	0.49
1:B:178:ARG:O	1:B:178:ARG:HG2	1.96	0.49
1:C:878:HIS:HE1	6:C:9521:HOH:O	1.94	0.49
1:A:655:MET:HE2	1:A:656:VAL:O	2.13	0.49
1:A:745:MET:HE1	1:A:761:GLN:NE2	2.27	0.49
1:D:808:GLU:OE1	1:D:811:LYS:NZ	2.36	0.49
1:A:296:GLU:OE1	1:A:296:GLU:HA	2.12	0.49
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.48	0.49
1:D:135:GLN:O	1:D:136:GLU:HG2	2.12	0.49
1:D:847:LYS:HD2	1:D:848:THR:O	2.11	0.49
1:C:847:LYS:HG3	1:C:849:LEU:HD23	1.94	0.49
1:A:433:LEU:N	1:A:434:PRO:CD	2.76	0.49
1:C:699:ARG:NH1	5:C:8415:DMS:H11	2.24	0.49
5:C:8412:DMS:H12	6:C:8962:HOH:O	2.11	0.49
1:D:961:ARG:NH2	1:D:979:GLU:O	2.45	0.49
1:A:232:ASN:C	5:A:8417:DMS:H22	2.38	0.48
1:D:68:ALA:O	1:D:70:PRO:HD3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.94	0.48
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.48
1:B:387:VAL:HG22	6:B:9491:HOH:O	2.12	0.48
1:C:847:LYS:HE2	6:C:9340:HOH:O	2.12	0.48
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.43	0.48
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.49	0.48
1:C:795:VAL:HG12	5:C:8506:DMS:H22	1.94	0.48
1:C:963:SER:HB3	1:C:983:TRP:CE2	2.49	0.48
1:D:933:SER:O	1:D:934:GLU:C	2.57	0.48
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.95	0.48
5:B:8413:DMS:O	6:B:8959:HOH:O	2.20	0.48
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.48	0.48
1:B:1017:GLN:HB2	6:B:9469:HOH:O	2.14	0.48
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.96	0.48
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.38	0.48
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.96	0.48
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.95	0.47
1:B:596:PRO:HB3	6:B:9359:HOH:O	2.15	0.47
1:A:910:LEU:HD12	1:A:910:LEU:C	2.38	0.47
1:D:675:GLN:HG3	6:D:9495:HOH:O	2.14	0.47
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.95	0.47
1:C:768:MET:HE2	1:C:768:MET:HB2	1.80	0.47
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.47
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.49	0.47
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.33	0.47
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.96	0.47
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.49	0.47
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.98	0.47
1:C:802:ASP:O	1:C:808:GLU:HG3	2.14	0.47
1:C:890:GLN:HG2	1:C:891:VAL:N	2.27	0.47
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.50	0.47
1:C:577:LYS:HB3	1:C:577:LYS:HE3	1.69	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.50	0.47
1:A:756:TRP:CD1	1:A:768:MET:HG2	2.49	0.47
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.47
1:B:251:ARG:CZ	1:B:253:TYR:HE2	2.27	0.47
1:B:473:ARG:HE	1:C:469:ASP:HB3	1.80	0.47
5:B:8410:DMS:H11	6:B:9138:HOH:O	2.14	0.47
1:C:54:LEU:HD11	1:C:214:LEU:HD22	1.96	0.47
1:C:577:LYS:HD3	1:C:587:ALA:CB	2.45	0.47
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:832:ASP:O	1:B:833:ALA:HB2	2.14	0.47
1:C:637:GLU:CD	1:C:677:LYS:HD3	2.40	0.47
1:C:655:MET:HE2	1:C:656:VAL:N	2.29	0.47
1:A:742:THR:HG22	1:A:743:SER:N	2.29	0.46
1:A:890:GLN:HG3	1:A:891:VAL:H	1.80	0.46
1:B:583:ASN:HA	1:B:584:PRO:HD3	1.74	0.46
1:C:796:SER:OG	1:C:802:ASP:N	2.36	0.46
1:D:682:LEU:C	1:D:683:PRO:O	2.57	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:A:241:GLU:OE1	1:A:292:ARG:NH2	2.48	0.46
1:A:703:PRO:HG2	5:A:8425:DMS:H12	1.97	0.46
1:A:948:PRO:O	1:A:1023:LYS:HE3	2.15	0.46
1:D:251:ARG:NE	1:D:253:TYR:CE2	2.82	0.46
1:D:1015:HIS:HE2	1:D:1017:GLN:CD	2.23	0.46
1:A:658:LEU:O	1:A:659:ASP:C	2.56	0.46
1:C:687:GLN:HA	1:C:688:PRO:HD3	1.72	0.46
1:B:907:PRO:HG2	1:B:990:HIS:O	2.15	0.46
1:C:830:LEU:HD23	1:C:830:LEU:N	2.31	0.46
1:D:824:GLN:NE2	1:D:837:THR:HG22	2.31	0.46
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.97	0.46
1:C:804:ASN:ND2	1:C:1001:PRO:CD	2.79	0.46
1:C:178:ARG:HG3	6:C:9373:HOH:O	2.15	0.46
1:D:961:ARG:NE	1:D:981:GLY:O	2.45	0.46
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.81	0.46
1:C:745:MET:HE3	1:C:745:MET:CA	2.33	0.46
1:D:336:ARG:HD3	6:D:9324:HOH:O	2.15	0.46
1:A:251:ARG:HH11	5:A:8416:DMS:H21	1.79	0.46
1:B:961:ARG:NH1	6:B:9170:HOH:O	2.30	0.46
1:A:662:PRO:O	1:A:663:LEU:HD23	2.16	0.46
1:C:804:ASN:HD21	1:C:1001:PRO:CD	2.28	0.46
1:D:628:GLN:NE2	6:D:9277:HOH:O	2.48	0.46
1:D:777:LEU:HG	1:D:889:ALA:HA	1.97	0.46
1:A:554:GLN:OE1	6:A:9027:HOH:O	2.21	0.46
1:B:682:LEU:HD23	1:B:682:LEU:HA	1.80	0.46
1:C:88:SER:HA	1:C:366:VAL:HG21	1.98	0.46
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.98	0.46
1:C:890:GLN:OE1	1:C:948:PRO:HD3	2.16	0.46
1:D:893:GLU:O	1:D:893:GLU:HG3	2.12	0.46
1:D:858:ILE:HD11	1:D:864:MET:HB2	1.96	0.45
1:A:521:LYS:HE2	6:A:9027:HOH:O	2.15	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LEU:C	1:A:533:LEU:HD23	2.41	0.45
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.96	0.45
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.97	0.45
1:D:340:GLY:O	1:D:561:ARG:HG2	2.16	0.45
1:B:658:LEU:HD11	1:B:692:GLY:HA3	1.99	0.45
1:D:658:LEU:O	1:D:659:ASP:C	2.59	0.45
1:C:655:MET:HE2	1:C:656:VAL:H	1.81	0.45
1:A:431:ARG:HG3	6:A:9321:HOH:O	2.16	0.45
1:D:36:TRP:HH2	5:D:8404:DMS:H13	1.80	0.45
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.99	0.45
1:D:829:THR:HG21	6:D:9621:HOH:O	2.16	0.45
1:A:94:GLY:O	5:A:8421:DMS:H21	2.17	0.45
1:A:851:ILE:O	1:A:870:VAL:HA	2.17	0.45
1:B:730:LEU:H	1:B:730:LEU:HG	1.28	0.45
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.26	0.45
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.45
1:A:579:ASP:O	1:A:580:GLU:C	2.58	0.45
1:B:232:ASN:C	5:B:8417:DMS:H22	2.42	0.45
1:D:845:GLN:OE1	1:D:845:GLN:N	2.50	0.45
1:B:49:GLN:HG2	6:B:9283:HOH:O	2.17	0.44
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.51	0.44
1:C:988:GLY:C	1:C:989:PHE:CD1	2.95	0.44
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.51	0.44
1:A:1003:VAL:O	5:A:8407:DMS:H23	2.17	0.44
1:C:147:ASN:HA	1:C:148:SER:HA	1.66	0.44
1:C:569:ASP:O	1:C:605:GLY:HA2	2.18	0.44
1:C:942:ARG:HA	1:C:953:GLY:O	2.17	0.44
1:B:13:ARG:CB	1:C:13:ARG:HH22	2.30	0.44
1:B:973:ARG:O	5:B:8423:DMS:H12	2.17	0.44
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.18	0.44
1:D:685:LEU:HG	1:D:686:PRO:CD	2.48	0.44
1:B:600:GLN:H	1:B:600:GLN:NE2	2.03	0.44
1:C:580:GLU:H	1:C:580:GLU:HG3	1.50	0.44
1:A:685:LEU:CB	1:A:686:PRO:CD	2.95	0.44
1:A:730:LEU:HA	1:A:731:PRO:HD3	1.93	0.44
1:A:826:THR:OG1	1:A:837:THR:HB	2.18	0.44
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.42	0.44
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.52	0.44
1:C:601:PHE:CD2	5:C:8506:DMS:H23	2.51	0.44
1:C:843:GLN:CG	1:C:848:THR:HA	2.46	0.44
1:C:1023:LYS:HE2	1:C:1023:LYS:HB3	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:HIS:HD2	6:D:9295:HOH:O	1.99	0.44
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.00	0.44
5:A:8413:DMS:H23	6:A:8966:HOH:O	2.17	0.44
1:B:749:ILE:N	1:B:749:ILE:CD1	2.80	0.44
1:C:13:ARG:NH1	6:C:8624:HOH:O	2.30	0.44
1:C:666:GLY:C	1:C:667:GLU:HG3	2.42	0.44
1:D:794:ALA:CB	6:D:8984:HOH:O	2.66	0.44
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.36	0.44
1:A:843:GLN:HA	1:A:847:LYS:O	2.18	0.44
1:A:950:GLN:OE1	1:A:952:ARG:NE	2.51	0.44
1:C:754:LYS:HZ3	1:C:754:LYS:HG3	1.56	0.44
1:C:757:GLN:OE1	1:C:769:TRP:HH2	2.01	0.44
1:C:930:VAL:O	1:C:932:PRO:HD3	2.17	0.44
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.52	0.44
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.85	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	2.00	0.44
1:C:795:VAL:HG22	6:C:8872:HOH:O	2.17	0.44
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.18	0.44
1:A:201:ASP:OD2	4:A:2001:IPT:H62	2.18	0.43
1:A:251:ARG:HA	5:A:8416:DMS:H13	2.00	0.43
1:A:683:PRO:O	1:A:685:LEU:HG	2.17	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.01	0.43
1:A:608:PHE:CD1	1:A:614:HIS:CD2	3.06	0.43
1:A:738:PRO:HD3	1:A:860:GLY:HA2	2.01	0.43
1:A:773:LYS:HE2	1:A:773:LYS:HB2	1.84	0.43
1:C:232:ASN:ND2	1:C:237:ARG:HG3	2.32	0.43
1:C:619:GLU:HG2	1:C:909:ARG:HG3	1.99	0.43
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.36	0.43
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.54	0.43
1:C:272:ALA:HB1	1:C:273:PRO:HD2	2.01	0.43
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.54	0.43
1:B:807:VAL:CG1	1:B:808:GLU:N	2.81	0.43
1:C:246:MET:SD	1:C:246:MET:C	3.02	0.43
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.52	0.43
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.18	0.43
1:A:802:ASP:OD1	1:A:802:ASP:C	2.61	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.53	0.43
1:C:781:ARG:NH1	1:C:781:ARG:HG2	2.34	0.43
1:D:78:LEU:HD23	1:D:78:LEU:HA	1.84	0.43
1:D:476:LYS:NZ	6:D:8788:HOH:O	2.38	0.43
1:A:506:VAL:CG1	1:A:521:LYS:HE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:GLN:H	1:C:634:GLN:HE21	1.66	0.43
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.79	0.43
1:D:472:TYR:OH	1:D:476:LYS:HE2	2.18	0.43
1:D:1022:GLN:HG3	1:D:1023:LYS:HG2	2.01	0.43
1:A:615:PRO:O	1:A:618:THR:HG22	2.19	0.43
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.74	0.43
1:A:737:ILE:HD13	1:A:738:PRO:O	2.18	0.43
1:A:986:ILE:HD13	1:A:986:ILE:HG23	1.57	0.43
1:C:216:HIS:CG	5:C:8504:DMS:H23	2.54	0.43
1:C:292:ARG:HG3	1:C:292:ARG:NH1	2.33	0.43
1:D:685:LEU:CG	1:D:686:PRO:CD	2.96	0.43
1:B:200:GLN:HG2	1:B:391:HIS:HB2	2.01	0.43
1:C:336:ARG:NH2	1:C:338:GLU:OE1	2.39	0.43
1:A:988:GLY:C	1:A:989:PHE:CD1	2.96	0.43
1:B:93:HIS:CD2	5:B:8414:DMS:H23	2.54	0.43
1:B:699:ARG:NH1	6:B:9545:HOH:O	2.45	0.43
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.82	0.43
1:C:748:CYS:SG	1:C:755:ARG:NH2	2.92	0.43
1:C:822:LEU:HD11	1:C:824:GLN:O	2.19	0.43
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.84	0.42
1:A:290:THR:O	5:A:8412:DMS:H23	2.19	0.42
1:B:178:ARG:HG2	1:B:179:ALA:O	2.19	0.42
1:B:763:GLY:HA3	1:B:822:LEU:HD13	2.01	0.42
1:C:601:PHE:CD1	5:C:8506:DMS:H23	2.54	0.42
1:C:639:THR:OG1	1:C:677:LYS:HG2	2.19	0.42
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.54	0.42
1:B:279:ILE:HD12	1:B:279:ILE:HG23	1.69	0.42
1:C:637:GLU:OE2	1:C:677:LYS:HD3	2.19	0.42
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.55	0.42
1:D:756:TRP:CE2	1:D:858:ILE:CD1	3.02	0.42
1:D:847:LYS:NZ	6:D:9441:HOH:O	2.52	0.42
1:B:661:LYS:HG3	1:B:661:LYS:H	1.64	0.42
1:C:750:GLU:HG3	1:C:754:LYS:O	2.19	0.42
1:C:872:VAL:O	1:C:873:ALA:C	2.57	0.42
1:D:910:LEU:HD12	1:D:910:LEU:C	2.44	0.42
1:C:837:THR:O	1:C:837:THR:HG22	2.13	0.42
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.42
1:D:147:ASN:HA	1:D:148:SER:HA	1.67	0.42
1:A:473:ARG:NH1	1:A:473:ARG:O	2.52	0.42
1:B:807:VAL:HG13	1:B:808:GLU:N	2.34	0.42
1:C:806:TRP:NE1	1:C:809:ARG:NH2	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.00	0.42
1:A:843:GLN:HG3	1:A:847:LYS:C	2.45	0.42
1:B:183:ARG:HD3	6:B:8920:HOH:O	2.19	0.42
1:C:50:GLN:CD	1:C:50:GLN:N	2.76	0.42
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.20	0.42
1:D:219:THR:HG21	6:D:9600:HOH:O	2.19	0.42
1:D:833:ALA:HB1	1:D:858:ILE:O	2.20	0.42
1:A:32:PRO:CB	5:A:8404:DMS:C1	2.97	0.42
1:A:473:ARG:HH12	1:A:476:LYS:C	2.28	0.42
1:B:802:ASP:OD1	1:B:804:ASN:HB3	2.20	0.42
1:C:824:GLN:O	1:C:838:THR:HA	2.19	0.42
1:B:367:MET:CE	1:B:372:MET:HG3	2.50	0.42
1:B:578:TYR:HA	1:B:583:ASN:O	2.20	0.42
1:C:622:HIS:HB2	1:C:717:TRP:CZ2	2.55	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.55	0.42
1:D:753:ASN:N	1:D:753:ASN:OD1	2.45	0.42
1:C:133:TRP:NE1	5:C:8504:DMS:H21	2.35	0.42
1:C:895:VAL:O	1:C:919:ASP:HA	2.19	0.42
1:D:829:THR:HG23	1:D:834:VAL:HG22	2.02	0.42
1:D:861:SER:O	1:D:861:SER:OG	2.38	0.42
1:B:85:VAL:HG12	1:B:86:VAL:N	2.34	0.41
1:C:54:LEU:HD11	1:C:214:LEU:CD2	2.50	0.41
1:D:629:PHE:C	1:D:630:ARG:HD3	2.44	0.41
1:D:685:LEU:HG	1:D:686:PRO:HD3	2.01	0.41
1:A:710:GLU:O	1:A:711:ALA:C	2.61	0.41
1:A:789:LEU:HD11	1:A:993:ILE:HG22	2.00	0.41
1:B:965:GLN:O	1:B:969:GLU:HG3	2.20	0.41
1:C:989:PHE:CD1	1:C:989:PHE:N	2.88	0.41
1:D:708:TRP:CZ3	1:D:709:SER:HB3	2.54	0.41
1:D:869:ASP:OD1	1:D:1015:HIS:ND1	2.53	0.41
1:A:58:TRP:CZ2	1:A:125:LEU:HD22	2.55	0.41
1:B:367:MET:HE2	1:B:372:MET:CG	2.51	0.41
1:B:634:GLN:HG2	1:B:682:LEU:CB	2.51	0.41
1:D:598:ASP:C	1:D:599:ARG:HG2	2.46	0.41
1:A:472:TYR:O	1:A:476:LYS:HG2	2.21	0.41
1:A:635:THR:OG1	1:A:681:GLU:HG3	2.20	0.41
1:A:861:SER:OG	1:A:863:GLN:HG3	2.21	0.41
1:C:542:MET:HA	1:C:604:ASN:HA	2.02	0.41
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.55	0.41
1:D:573:GLN:HB2	1:D:602:CYS:O	2.20	0.41
1:D:847:LYS:HD3	1:D:848:THR:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:808:GLU:CD	1:A:811:LYS:HZ3	2.27	0.41
1:B:577:LYS:O	1:B:584:PRO:HA	2.20	0.41
1:B:668:VAL:HG12	1:B:669:PRO:O	2.20	0.41
1:D:806:TRP:CE2	1:D:991:MET:HE1	2.56	0.41
1:A:696:LEU:HD23	1:A:720:TRP:CE3	2.56	0.41
1:B:340:GLY:O	1:B:561:ARG:HG2	2.21	0.41
1:B:655:MET:HE3	1:B:655:MET:HB2	1.74	0.41
1:B:733:ALA:O	1:B:734:SER:C	2.62	0.41
1:C:667:GLU:C	1:C:668:VAL:HG23	2.46	0.41
1:D:373:VAL:O	1:D:377:LEU:HG	2.21	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.94	0.41
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.41
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.37	0.41
1:A:738:PRO:CD	1:A:751:LEU:HD13	2.51	0.41
1:B:968:MET:HE2	1:B:968:MET:HB3	1.93	0.41
1:C:114:VAL:HB	1:C:115:PRO:CD	2.51	0.41
1:D:794:ALA:HB1	6:D:8984:HOH:O	2.20	0.41
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.87	0.41
1:B:598:ASP:O	1:B:599:ARG:C	2.62	0.41
6:B:9203:HOH:O	5:C:8420:DMS:H12	2.21	0.41
1:C:533:LEU:C	1:C:533:LEU:HD23	2.46	0.41
1:A:636:ILE:HD11	1:A:682:LEU:HD11	2.02	0.41
1:A:660:GLY:O	1:A:662:PRO:HD3	2.21	0.41
1:A:748:CYS:C	1:A:749:ILE:HD12	2.46	0.41
1:A:787:ALA:HA	1:A:968:MET:HG3	2.03	0.41
1:A:836:ILE:HG23	1:A:836:ILE:HD12	1.80	0.41
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.56	0.41
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.56	0.41
1:B:441:THR:O	1:B:445:GLN:HG3	2.20	0.41
1:B:473:ARG:NH2	1:B:477:SER:CB	2.79	0.41
1:B:634:GLN:NE2	1:B:685:LEU:HD12	2.36	0.41
1:B:731:PRO:HB2	1:B:732:ALA:H	1.64	0.41
1:B:806:TRP:CD2	1:B:809:ARG:NH2	2.89	0.41
1:B:995:GLY:O	1:B:996:ASP:C	2.64	0.41
1:C:60:PHE:HA	1:C:122:CYS:O	2.21	0.41
1:C:977:HIS:O	1:C:977:HIS:CD2	2.74	0.41
1:B:668:VAL:HG11	1:B:680:ILE:HG12	2.02	0.41
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.82	0.41
1:C:708:TRP:CE3	1:C:709:SER:HB3	2.56	0.41
1:D:787:ALA:HA	1:D:968:MET:HE2	2.03	0.41
1:D:814:GLY:O	1:D:815:HIS:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:843:GLN:HG3	1:A:847:LYS:O	2.21	0.40
1:A:986:ILE:HG21	1:A:986:ILE:HD12	1.61	0.40
1:B:658:LEU:O	1:B:659:ASP:C	2.62	0.40
1:B:802:ASP:OD1	1:B:802:ASP:C	2.64	0.40
1:C:1000:SER:HA	6:C:8939:HOH:O	2.22	0.40
1:D:770:ILE:HD12	6:D:9560:HOH:O	2.21	0.40
1:A:35:SER:HB2	1:A:217:LYS:HD3	2.02	0.40
1:A:995:GLY:C	1:A:997:ASP:N	2.77	0.40
1:A:50:GLN:N	1:A:50:GLN:CD	2.79	0.40
1:B:145:GLY:HA3	1:B:210:ARG:HB2	2.03	0.40
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.52	0.40
1:C:984:LEU:HD12	1:C:985:ASN:N	2.37	0.40
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.56	0.40
1:B:513:PRO:O	1:B:514:ALA:HB3	2.22	0.40
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.51	0.40
1:C:928:PRO:O	1:C:929:TYR:C	2.64	0.40
1:A:390:SER:HA	1:A:391:HIS:HA	1.90	0.40
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.57	0.40
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.40	0.40
1:C:625:GLN:HG2	1:C:716:ALA:HA	2.03	0.40
1:D:847:LYS:O	1:D:847:LYS:HG3	2.13	0.40
1:D:847:LYS:CD	1:D:848:THR:N	2.82	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	48 27
1	B	1009/1023 (99%)	967 (96%)	35 (4%)	7 (1%)	18 6
1	C	1009/1023 (99%)	962 (95%)	46 (5%)	1 (0%)	48 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	1009/1023 (99%)	969 (96%)	36 (4%)	4 (0%)	30	14
All	All	4036/4092 (99%)	3869 (96%)	154 (4%)	13 (0%)	36	20

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	688	PRO
1	B	690	SER
1	B	731	PRO
1	C	1022	GLN
1	D	580	GLU
1	D	688	PRO
1	B	685	LEU
1	B	687	GLN
1	B	800	ARG
1	D	164	ASP
1	A	164	ASP
1	D	683	PRO
1	B	684	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	829 (96%)	35 (4%)	27	8
1	B	864/875 (99%)	828 (96%)	36 (4%)	26	7
1	C	864/875 (99%)	821 (95%)	43 (5%)	22	5
1	D	864/875 (99%)	825 (96%)	39 (4%)	24	7
All	All	3456/3500 (99%)	3303 (96%)	153 (4%)	25	7

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN

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Mol	Chain	Res	Type
1	A	71	GLU
1	A	85	VAL
1	A	213	SER
1	A	250	LEU
1	A	262	GLN
1	A	277	GLU
1	A	279	ILE
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	667	GLU
1	A	675	GLN
1	A	687	GLN
1	A	689	GLU
1	A	730	LEU
1	A	734	SER
1	A	735	HIS
1	A	737	ILE
1	A	796	SER
1	A	799	THR
1	A	801	ILE
1	A	817	GLN
1	A	819	GLU
1	A	829	THR
1	A	843	GLN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	71	GLU
1	B	76	CYS
1	B	80	GLU
1	B	178	ARG
1	B	262	GLN
1	B	264	GLU
1	B	344	LEU
1	B	370	GLN

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Mol	Chain	Res	Type
1	B	546	LEU
1	B	581	ASN
1	B	594	ASP
1	B	600	GLN
1	B	630	ARG
1	B	634	GLN
1	B	646	HIS
1	B	651	LEU
1	B	652	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	672	VAL
1	B	680	ILE
1	B	681	GLU
1	B	687	GLN
1	B	689	GLU
1	B	730	LEU
1	B	745	MET
1	B	748	CYS
1	B	754	LYS
1	B	799	THR
1	B	817	GLN
1	B	819	GLU
1	B	845	GLN
1	B	847	LYS
1	B	1022	GLN
1	B	1023	LYS
1	C	13	ARG
1	C	71	GLU
1	C	75	GLU
1	C	76	CYS
1	C	80	GLU
1	C	117	GLU
1	C	135	GLN
1	C	178	ARG
1	C	214	LEU
1	C	264	GLU
1	C	278	ILE
1	C	344	LEU
1	C	519	SER
1	C	546	LEU

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Mol	Chain	Res	Type
1	C	580	GLU
1	C	630	ARG
1	C	634	GLN
1	C	651	LEU
1	C	655	MET
1	C	661	LYS
1	C	663	LEU
1	C	667	GLU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	750	GLU
1	C	768	MET
1	C	799	THR
1	C	800	ARG
1	C	801	ILE
1	C	845	GLN
1	C	847	LYS
1	C	859	ASP
1	C	934	GLU
1	C	956	GLN
1	C	986	ILE
1	C	1023	LYS
1	D	71	GLU
1	D	75	GLU
1	D	80	GLU
1	D	117	GLU
1	D	251	ARG
1	D	277	GLU
1	D	279	ILE
1	D	344	LEU
1	D	370	GLN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP

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Mol	Chain	Res	Type
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	682	LEU
1	D	684	GLU
1	D	685	LEU
1	D	689	GLU
1	D	710	GLU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	754	LYS
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	801	ILE
1	D	861	SER
1	D	893	GLU
1	D	956	GLN
1	D	986	ILE
1	D	1017	GLN
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	135	GLN
1	A	266	GLN
1	A	363	HIS
1	A	370	GLN
1	A	445	GLN
1	A	600	GLN
1	A	624	GLN
1	A	675	GLN
1	A	735	HIS
1	A	757	GLN
1	A	761	GLN

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Mol	Chain	Res	Type
1	A	844	HIS
1	A	863	GLN
1	A	878	HIS
1	A	903	GLN
1	A	977	HIS
1	A	1017	GLN
1	B	49	GLN
1	B	163	GLN
1	B	262	GLN
1	B	363	HIS
1	B	365	GLN
1	B	485	GLN
1	B	554	GLN
1	B	600	GLN
1	B	624	GLN
1	B	653	HIS
1	B	704	ASN
1	B	753	ASN
1	B	844	HIS
1	B	878	HIS
1	B	977	HIS
1	C	128	ASN
1	C	163	GLN
1	C	262	GLN
1	C	266	GLN
1	C	363	HIS
1	C	445	GLN
1	C	485	GLN
1	C	614	HIS
1	C	624	GLN
1	C	646	HIS
1	C	653	HIS
1	C	735	HIS
1	C	804	ASN
1	C	843	GLN
1	C	878	HIS
1	C	903	GLN
1	D	135	GLN
1	D	163	GLN
1	D	262	GLN
1	D	363	HIS
1	D	628	GLN

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Mol	Chain	Res	Type
1	D	634	GLN
1	D	739	HIS
1	D	761	GLN
1	D	804	ASN
1	D	824	GLN
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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 130 ligands modelled in this entry, 32 are monoatomic - leaving 98 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	$\# Z > 2$
5	DMS	C	8403	-	3,3,3	0.72	0	3,3,3	0.77	0
5	DMS	A	8401	-	3,3,3	0.89	0	3,3,3	0.56	0
5	DMS	A	8504	-	3,3,3	1.01	0	3,3,3	0.87	0
4	IPT	C	2001	3	15,15,15	0.59	0	18,21,21	1.21	2 (11%)
5	DMS	B	8410	-	3,3,3	1.10	0	3,3,3	0.78	0
5	DMS	A	8421	-	3,3,3	1.17	0	3,3,3	0.13	0
5	DMS	C	8410	-	3,3,3	0.53	0	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8409	-	3,3,3	2.12	1 (33%)	3,3,3	0.24	0
5	DMS	D	8701	-	3,3,3	2.30	2 (66%)	3,3,3	0.82	0
5	DMS	A	8410	-	3,3,3	0.76	0	3,3,3	0.66	0
5	DMS	A	8413	-	3,3,3	2.02	2 (66%)	3,3,3	0.40	0
5	DMS	D	8414	-	3,3,3	0.20	0	3,3,3	0.42	0
5	DMS	C	8423	-	3,3,3	0.48	0	3,3,3	0.37	0
5	DMS	A	8405	-	3,3,3	1.43	1 (33%)	3,3,3	0.36	0
5	DMS	C	8401	-	3,3,3	1.61	1 (33%)	3,3,3	0.73	0
5	DMS	B	8413	-	3,3,3	0.97	0	3,3,3	0.30	0
5	DMS	C	8407	-	3,3,3	0.88	0	3,3,3	0.11	0
5	DMS	D	8409	-	3,3,3	1.91	1 (33%)	3,3,3	0.74	0
5	DMS	D	8406	-	3,3,3	0.98	0	3,3,3	0.50	0
5	DMS	B	8404	-	3,3,3	0.92	0	3,3,3	0.40	0
5	DMS	C	8421	-	3,3,3	0.46	0	3,3,3	0.97	0
5	DMS	D	8404	-	3,3,3	0.66	0	3,3,3	0.72	0
5	DMS	C	8409	-	3,3,3	2.19	1 (33%)	3,3,3	0.27	0
5	DMS	C	8501	-	3,3,3	1.74	1 (33%)	3,3,3	0.66	0
5	DMS	B	8504	-	3,3,3	1.07	0	3,3,3	0.04	0
5	DMS	C	8405	-	3,3,3	1.65	1 (33%)	3,3,3	0.91	0
5	DMS	A	8414	-	3,3,3	0.98	0	3,3,3	0.17	0
5	DMS	C	8415	-	3,3,3	1.91	1 (33%)	3,3,3	0.42	0
5	DMS	B	8502	-	3,3,3	1.33	0	3,3,3	0.99	0
5	DMS	D	8401	-	3,3,3	1.81	1 (33%)	3,3,3	0.37	0
5	DMS	C	8414	-	3,3,3	1.11	0	3,3,3	0.67	0
5	DMS	B	8508	-	3,3,3	1.88	1 (33%)	3,3,3	0.53	0
5	DMS	B	8411	-	3,3,3	1.35	0	3,3,3	0.52	0
5	DMS	B	8403	-	3,3,3	0.70	0	3,3,3	0.55	0
5	DMS	C	8411	-	3,3,3	0.48	0	3,3,3	0.27	0
5	DMS	C	8402	-	3,3,3	1.93	1 (33%)	3,3,3	0.39	0
5	DMS	A	8417	-	3,3,3	0.73	0	3,3,3	0.66	0
5	DMS	D	8421	-	3,3,3	0.64	0	3,3,3	0.95	0
5	DMS	A	8501	-	3,3,3	1.33	0	3,3,3	0.43	0
4	IPT	B	2001	3	15,15,15	0.57	0	18,21,21	1.52	2 (11%)
5	DMS	D	8506	-	3,3,3	0.59	0	3,3,3	0.35	0
5	DMS	A	8406	-	3,3,3	1.42	1 (33%)	3,3,3	0.44	0
5	DMS	B	8425	3	3,3,3	1.26	0	3,3,3	0.41	0
5	DMS	C	8413	-	3,3,3	1.14	0	3,3,3	0.62	0
5	DMS	C	8417	-	3,3,3	0.42	0	3,3,3	0.78	0
5	DMS	B	8416	-	3,3,3	0.62	0	3,3,3	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	IPT	A	2001	3	15,15,15	0.61	0	18,21,21	1.50	4 (22%)
5	DMS	C	8404	-	3,3,3	1.43	0	3,3,3	1.64	1 (33%)
5	DMS	C	8504	-	3,3,3	0.67	0	3,3,3	0.75	0
5	DMS	A	8408	-	3,3,3	0.94	0	3,3,3	0.51	0
5	DMS	B	8409	-	3,3,3	2.56	1 (33%)	3,3,3	0.48	0
5	DMS	A	8407	-	3,3,3	1.32	0	3,3,3	0.33	0
5	DMS	D	8416	-	3,3,3	0.98	0	3,3,3	0.22	0
5	DMS	B	8417	-	3,3,3	0.47	0	3,3,3	0.64	0
5	DMS	D	8402	-	3,3,3	1.85	1 (33%)	3,3,3	0.26	0
5	DMS	D	8503	-	3,3,3	0.98	0	3,3,3	0.39	0
5	DMS	C	8420	-	3,3,3	0.69	0	3,3,3	0.20	0
5	DMS	B	8412	-	3,3,3	1.08	0	3,3,3	0.24	0
5	DMS	B	8405	-	3,3,3	2.08	2 (66%)	3,3,3	0.49	0
5	DMS	B	8408	-	3,3,3	1.52	1 (33%)	3,3,3	0.30	0
5	DMS	C	8506	-	3,3,3	1.50	1 (33%)	3,3,3	0.67	0
5	DMS	A	8412	-	3,3,3	1.14	0	3,3,3	0.40	0
5	DMS	B	8601	-	3,3,3	1.47	0	3,3,3	0.91	0
5	DMS	D	8405	-	3,3,3	1.17	0	3,3,3	0.96	0
5	DMS	C	8602	-	3,3,3	0.91	0	3,3,3	0.56	0
5	DMS	A	8502	-	3,3,3	1.94	1 (33%)	3,3,3	1.08	0
5	DMS	A	8425	3	3,3,3	1.23	0	3,3,3	0.59	0
5	DMS	C	8601	-	3,3,3	1.32	1 (33%)	3,3,3	0.62	0
5	DMS	D	8508	-	3,3,3	1.94	2 (66%)	3,3,3	0.38	0
5	DMS	C	8412	-	3,3,3	1.19	0	3,3,3	0.10	0
5	DMS	D	8705	-	3,3,3	2.14	1 (33%)	3,3,3	0.86	0
5	DMS	A	8602	-	3,3,3	0.89	0	3,3,3	0.18	0
5	DMS	B	8414	-	3,3,3	0.61	0	3,3,3	0.59	0
5	DMS	D	8408	-	3,3,3	1.19	0	3,3,3	0.35	0
5	DMS	C	8408	-	3,3,3	0.43	0	3,3,3	1.42	1 (33%)
5	DMS	B	8421	-	3,3,3	1.17	0	3,3,3	0.63	0
5	DMS	A	8416	-	3,3,3	3.17	1 (33%)	3,3,3	0.47	0
5	DMS	D	8412	-	3,3,3	1.41	0	3,3,3	0.74	0
5	DMS	D	8411	-	3,3,3	1.01	0	3,3,3	0.24	0
5	DMS	D	8403	-	3,3,3	1.45	0	3,3,3	0.85	0
5	DMS	B	8423	-	3,3,3	0.35	0	3,3,3	0.15	0
5	DMS	A	8420	-	3,3,3	0.68	0	3,3,3	0.27	0
5	DMS	A	8403	-	3,3,3	1.63	1 (33%)	3,3,3	0.63	0
5	DMS	D	8413	-	3,3,3	1.27	1 (33%)	3,3,3	0.42	0
4	IPT	D	2001	3	15,15,15	0.82	0	18,21,21	1.83	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8501	-	3,3,3	0.94	0	3,3,3	0.61	0
5	DMS	A	8411	-	3,3,3	0.45	0	3,3,3	0.39	0
5	DMS	A	8402	-	3,3,3	1.56	0	3,3,3	0.34	0
5	DMS	B	8402	-	3,3,3	1.74	1 (33%)	3,3,3	0.53	0
5	DMS	B	8401	-	3,3,3	0.62	0	3,3,3	0.39	0
5	DMS	B	8506	-	3,3,3	1.01	0	3,3,3	1.21	1 (33%)
5	DMS	C	8425	3	3,3,3	1.11	0	3,3,3	0.53	0
5	DMS	D	8703	-	3,3,3	0.99	0	3,3,3	0.39	0
5	DMS	A	8404	-	3,3,3	1.33	0	3,3,3	0.42	0
5	DMS	D	8410	-	3,3,3	1.15	0	3,3,3	0.55	0
5	DMS	A	8503	-	3,3,3	1.74	1 (33%)	3,3,3	0.42	0
5	DMS	C	8503	-	3,3,3	0.35	0	3,3,3	0.80	0
5	DMS	D	8417	-	3,3,3	0.44	0	3,3,3	1.20	1 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IPT	A	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	D	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	B	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	1/6/26/26	0/1/1/1

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8416	DMS	C1-S	-5.19	1.38	1.76
5	B	8409	DMS	O-S	4.06	1.77	1.50
5	C	8409	DMS	O-S	3.60	1.74	1.50
5	A	8409	DMS	O-S	3.51	1.73	1.50
5	D	8705	DMS	O-S	3.42	1.72	1.50
5	C	8402	DMS	C2-S	3.22	1.99	1.76
5	C	8415	DMS	C1-S	3.03	1.97	1.76
5	A	8502	DMS	C1-S	2.98	1.97	1.76
5	A	8503	DMS	C2-S	2.96	1.97	1.76
5	B	8402	DMS	C2-S	2.84	1.96	1.76
5	D	8701	DMS	O-S	2.83	1.68	1.50
5	D	8409	DMS	O-S	2.79	1.68	1.50
5	D	8701	DMS	C2-S	2.68	1.95	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8508	DMS	C1-S	2.62	1.94	1.76
5	D	8402	DMS	C2-S	2.61	1.94	1.76
5	D	8508	DMS	O-S	2.57	1.67	1.50
5	C	8501	DMS	C1-S	-2.50	1.58	1.76
5	B	8405	DMS	C2-S	2.47	1.93	1.76
5	C	8506	DMS	C1-S	2.29	1.92	1.76
5	C	8601	DMS	C2-S	2.27	1.92	1.76
5	B	8408	DMS	C1-S	2.26	1.92	1.76
5	A	8405	DMS	O-S	2.23	1.64	1.50
5	A	8413	DMS	C2-S	2.20	1.91	1.76
5	A	8413	DMS	O-S	2.19	1.64	1.50
5	D	8413	DMS	O-S	2.18	1.64	1.50
5	B	8405	DMS	O-S	2.17	1.64	1.50
5	D	8508	DMS	C1-S	2.15	1.91	1.76
5	C	8405	DMS	O-S	2.12	1.64	1.50
5	C	8401	DMS	C2-S	2.04	1.90	1.76
5	A	8406	DMS	C2-S	-2.03	1.61	1.76
5	A	8403	DMS	C2-S	2.03	1.90	1.76
5	D	8401	DMS	O-S	2.02	1.63	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	IPT	C6-C5-C4	4.81	124.82	113.02
4	A	2001	IPT	O5-C5-C6	-4.30	95.77	106.44
4	D	2001	IPT	O5-C5-C6	-4.29	95.81	106.44
4	D	2001	IPT	C1-O5-C5	-3.14	106.92	112.56
4	D	2001	IPT	O6-C6-C5	-2.89	101.48	111.33
5	C	8404	DMS	C2-S-C1	2.77	112.64	98.42
4	C	2001	IPT	O2-C2-C1	-2.71	105.48	110.30
4	A	2001	IPT	C3-C4-C5	-2.60	105.52	110.23
4	A	2001	IPT	O6-C6-C5	-2.43	103.04	111.33
4	B	2001	IPT	O3-C3-C2	-2.39	104.74	110.38
5	C	8408	DMS	C2-S-C1	2.34	110.39	98.42
4	C	2001	IPT	O3-C3-C4	2.25	115.68	110.38
4	D	2001	IPT	O2-C2-C1	-2.23	106.33	110.30
4	D	2001	IPT	C6-C5-C4	-2.19	107.65	113.02
4	D	2001	IPT	C3-C4-C5	-2.16	106.32	110.23
4	D	2001	IPT	C3'-C1'-C2'	-2.11	103.92	111.61
5	B	8506	DMS	C2-S-C1	2.09	109.14	98.42
5	D	8417	DMS	C2-S-C1	2.04	108.89	98.42
4	A	2001	IPT	C1-O5-C5	-2.01	108.95	112.56

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2001	IPT	O5-C5-C6-O6
4	C	2001	IPT	O5-C5-C6-O6
4	D	2001	IPT	O5-C5-C6-O6
4	B	2001	IPT	O5-C5-C6-O6

There are no ring outliers.

47 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8403	DMS	1	0
5	B	8410	DMS	2	0
5	A	8421	DMS	5	0
5	C	8410	DMS	1	0
5	A	8410	DMS	2	0
5	A	8413	DMS	1	0
5	C	8423	DMS	1	0
5	B	8413	DMS	1	0
5	D	8406	DMS	1	0
5	D	8404	DMS	1	0
5	B	8504	DMS	1	0
5	A	8414	DMS	1	0
5	C	8415	DMS	2	0
5	B	8403	DMS	1	0
5	A	8417	DMS	3	0
5	D	8506	DMS	3	0
5	B	8425	DMS	1	0
5	C	8417	DMS	1	0
5	B	8416	DMS	1	0
4	A	2001	IPT	1	0
5	C	8504	DMS	2	0
5	A	8407	DMS	2	0
5	B	8417	DMS	3	0
5	D	8503	DMS	1	0
5	C	8420	DMS	2	0
5	B	8412	DMS	1	0
5	C	8506	DMS	7	0
5	A	8412	DMS	1	0
5	A	8425	DMS	2	0
5	C	8601	DMS	2	0
5	C	8412	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	8705	DMS	1	0
5	A	8602	DMS	1	0
5	B	8414	DMS	1	0
5	B	8421	DMS	1	0
5	A	8416	DMS	7	0
5	D	8412	DMS	2	0
5	D	8403	DMS	1	0
5	B	8423	DMS	1	0
5	D	8413	DMS	1	0
4	D	2001	IPT	1	0
5	B	8506	DMS	5	0
5	D	8703	DMS	1	0
5	A	8404	DMS	4	0
5	A	8503	DMS	1	0
5	C	8503	DMS	1	0
5	D	8417	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.13	48 (4%)	36	38	9, 17, 46, 98	0
1	B	1011/1023 (98%)	-0.12	46 (4%)	38	40	8, 17, 43, 100	0
1	C	1011/1023 (98%)	-0.11	39 (3%)	43	45	10, 17, 48, 98	0
1	D	1011/1023 (98%)	-0.07	49 (4%)	35	37	9, 17, 49, 98	0
All	All	4044/4092 (98%)	-0.11	182 (4%)	38	40	8, 17, 47, 100	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	7.4
1	A	798	ALA	6.1
1	B	730	LEU	5.9
1	A	730	LEU	5.8
1	B	733	ALA	5.2
1	B	685	LEU	5.1
1	C	730	LEU	5.1
1	A	737	ILE	5.0
1	D	733	ALA	4.8
1	B	732	ALA	4.7
1	C	685	LEU	4.6
1	D	686	PRO	4.6
1	B	798	ALA	4.6
1	A	688	PRO	4.5
1	A	1023	LYS	4.5
1	C	737	ILE	4.5
1	D	799	THR	4.5
1	D	735	HIS	4.4
1	C	733	ALA	4.4
1	B	731	PRO	4.4
1	C	1022	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	798	ALA	4.3
1	A	735	HIS	4.3
1	D	685	LEU	4.2
1	A	729	THR	4.1
1	B	663	LEU	4.1
1	B	845	GLN	4.0
1	D	734	SER	4.0
1	C	735	HIS	3.9
1	D	732	ALA	3.9
1	A	733	ALA	3.9
1	B	801	ILE	3.8
1	A	687	GLN	3.8
1	B	686	PRO	3.7
1	C	731	PRO	3.7
1	D	798	ALA	3.7
1	A	771	GLY	3.7
1	B	736	ALA	3.7
1	D	737	ILE	3.7
1	D	634	GLN	3.7
1	A	732	ALA	3.6
1	D	683	PRO	3.6
1	D	688	PRO	3.6
1	D	1023	LYS	3.6
1	B	729	THR	3.5
1	A	689	GLU	3.5
1	D	797	GLU	3.5
1	A	736	ALA	3.5
1	C	663	LEU	3.5
1	C	772	ASP	3.5
1	C	736	ALA	3.4
1	B	799	THR	3.4
1	D	581	ASN	3.4
1	A	800	ARG	3.4
1	D	730	LEU	3.4
1	D	736	ALA	3.3
1	B	735	HIS	3.3
1	D	729	THR	3.2
1	D	751	LEU	3.2
1	B	684	GLU	3.2
1	C	761	GLN	3.2
1	A	663	LEU	3.2
1	A	683	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	1022	GLN	3.1
1	A	646	HIS	3.1
1	C	732	ALA	3.1
1	A	634	GLN	3.1
1	C	677	LYS	3.1
1	A	731	PRO	3.1
1	C	687	GLN	3.1
1	D	801	ILE	3.1
1	C	686	PRO	3.0
1	B	737	ILE	3.0
1	B	1023	LYS	3.0
1	C	684	GLU	3.0
1	C	734	SER	3.0
1	B	581	ASN	2.9
1	D	76	CYS	2.9
1	A	1022	GLN	2.9
1	B	687	GLN	2.9
1	C	580	GLU	2.9
1	D	128	ASN	2.9
1	B	80	GLU	2.9
1	A	829	THR	2.8
1	C	799	THR	2.8
1	C	699	ARG	2.8
1	D	800	ARG	2.8
1	D	687	GLN	2.8
1	C	633	GLY	2.8
1	A	79	PRO	2.8
1	A	651	LEU	2.8
1	C	682	LEU	2.8
1	D	731	PRO	2.8
1	D	773	LYS	2.8
1	A	734	SER	2.8
1	D	771	GLY	2.8
1	D	157	ARG	2.7
1	D	663	LEU	2.7
1	B	682	LEU	2.7
1	B	725	ASN	2.7
1	A	669	PRO	2.7
1	D	277	GLU	2.7
1	A	799	THR	2.7
1	D	829	THR	2.7
1	D	666	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1023	LYS	2.7
1	D	71	GLU	2.6
1	B	817	GLN	2.6
1	A	76	CYS	2.6
1	C	830	LEU	2.6
1	C	829	THR	2.6
1	A	653	HIS	2.6
1	B	653	HIS	2.6
1	A	250	LEU	2.5
1	A	682	LEU	2.5
1	A	684	GLU	2.5
1	C	689	GLU	2.5
1	B	699	ARG	2.5
1	D	1018	LEU	2.5
1	A	668	VAL	2.5
1	B	580	GLU	2.4
1	C	800	ARG	2.4
1	A	801	ILE	2.4
1	D	580	GLU	2.4
1	A	655	MET	2.4
1	D	633	GLY	2.4
1	D	820	ALA	2.4
1	A	772	ASP	2.4
1	B	748	CYS	2.4
1	B	804	ASN	2.4
1	C	671	ASP	2.4
1	A	77	ASP	2.3
1	A	685	LEU	2.3
1	B	362	LEU	2.3
1	B	655	MET	2.3
1	A	739	HIS	2.3
1	B	734	SER	2.3
1	B	688	PRO	2.3
1	D	830	LEU	2.3
1	B	797	GLU	2.3
1	D	689	GLU	2.3
1	A	370	GLN	2.3
1	B	262	GLN	2.3
1	C	362	LEU	2.3
1	C	745	MET	2.3
1	A	845	GLN	2.2
1	D	757	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	249	GLU	2.2
1	B	690	SER	2.2
1	D	847	LYS	2.2
1	D	655	MET	2.2
1	A	130	ASP	2.2
1	B	659	ASP	2.2
1	C	252	ASP	2.2
1	B	76	CYS	2.2
1	D	845	GLN	2.2
1	B	264	GLU	2.2
1	B	689	GLU	2.2
1	C	666	GLY	2.2
1	C	683	PRO	2.2
1	D	668	VAL	2.1
1	B	863	GLN	2.1
1	D	251	ARG	2.1
1	D	690	SER	2.1
1	A	131	GLU	2.1
1	C	264	GLU	2.1
1	D	819	GLU	2.1
1	A	820	ALA	2.1
1	A	817	GLN	2.1
1	B	745	MET	2.1
1	B	819	GLU	2.1
1	C	748	CYS	2.1
1	B	370	GLN	2.1
1	C	634	GLN	2.1
1	A	116	THR	2.0
1	C	653	HIS	2.0
1	B	738	PRO	2.0
1	C	744	GLU	2.0
1	B	654	TRP	2.0
1	D	842	TRP	2.0
1	D	1022	GLN	2.0
1	A	664	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
2	MG	A	3105	1/1	0.45	0.45	97,97,97,97	1
5	DMS	C	8407	4/4	0.66	0.35	51,100,100,100	0
5	DMS	C	8504	4/4	0.78	0.24	39,52,72,76	0
5	DMS	A	8407	4/4	0.79	0.18	29,50,51,89	0
3	NA	D	3104	1/1	0.80	0.22	44,44,44,44	0
5	DMS	A	8425	4/4	0.81	0.27	37,55,76,100	0
5	DMS	A	8421	4/4	0.82	0.22	45,52,72,81	0
5	DMS	D	8417	4/4	0.83	0.20	23,27,70,75	0
5	DMS	B	8421	4/4	0.84	0.17	26,42,54,55	0
2	MG	C	3006	1/1	0.84	0.24	53,53,53,53	0
2	MG	D	3105	1/1	0.84	0.15	38,38,38,38	1
5	DMS	A	8503	4/4	0.84	0.23	36,51,55,100	0
5	DMS	D	8503	4/4	0.84	0.18	28,58,59,61	0
5	DMS	A	8417	4/4	0.85	0.20	26,29,59,100	0
5	DMS	C	8413	4/4	0.85	0.23	49,59,61,97	0
5	DMS	B	8413	4/4	0.85	0.18	33,40,53,58	0
5	DMS	A	8420	4/4	0.85	0.26	47,53,82,100	0
5	DMS	D	8421	4/4	0.85	0.27	40,48,96,100	0
5	DMS	B	8506	4/4	0.85	0.33	44,100,100,100	0
5	DMS	D	8703	4/4	0.85	0.23	37,48,53,98	0
5	DMS	C	8417	4/4	0.86	0.14	30,31,51,69	0
5	DMS	D	8416	4/4	0.86	0.17	32,43,61,100	0
5	DMS	C	8415	4/4	0.87	0.22	25,36,60,100	0
5	DMS	B	8508	4/4	0.87	0.16	36,41,54,56	0
5	DMS	C	8503	4/4	0.87	0.14	25,32,50,52	0
5	DMS	D	8413	4/4	0.88	0.22	46,49,51,100	0
5	DMS	A	8406	4/4	0.88	0.22	15,52,66,83	0
5	DMS	B	8410	4/4	0.88	0.13	28,33,34,70	0
5	DMS	C	8423	4/4	0.88	0.16	32,34,67,76	0
2	MG	C	3004	1/1	0.88	0.16	53,53,53,53	0
5	DMS	A	8502	4/4	0.88	0.15	29,29,52,61	0
5	DMS	C	8420	4/4	0.89	0.19	38,50,61,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8506	4/4	0.89	0.23	42,45,48,100	0
5	DMS	A	8416	4/4	0.89	0.12	13,32,46,66	0
5	DMS	A	8414	4/4	0.89	0.18	24,47,55,91	0
5	DMS	B	8423	4/4	0.90	0.19	46,55,57,100	0
5	DMS	C	8601	4/4	0.90	0.17	34,44,46,100	0
5	DMS	D	8506	4/4	0.90	0.20	42,52,59,100	0
5	DMS	D	8404	4/4	0.90	0.13	26,27,54,57	0
5	DMS	B	8417	4/4	0.91	0.14	24,30,61,69	0
5	DMS	C	8602	4/4	0.91	0.16	21,61,62,71	0
5	DMS	D	8501	4/4	0.91	0.12	22,29,41,50	0
5	DMS	B	8425	4/4	0.91	0.12	23,37,39,46	0
5	DMS	B	8416	4/4	0.91	0.14	37,43,47,100	0
5	DMS	C	8421	4/4	0.91	0.14	35,46,47,62	0
5	DMS	B	8409	4/4	0.92	0.13	22,26,44,51	0
5	DMS	A	8409	4/4	0.92	0.12	27,29,29,54	0
5	DMS	A	8504	4/4	0.92	0.18	25,38,42,100	0
5	DMS	B	8414	4/4	0.92	0.17	29,54,62,88	0
5	DMS	D	8705	4/4	0.92	0.13	30,42,42,44	0
5	DMS	D	8414	4/4	0.93	0.19	26,42,83,100	0
5	DMS	C	8425	4/4	0.93	0.12	34,41,43,45	0
5	DMS	A	8404	4/4	0.93	0.13	17,30,39,41	0
5	DMS	A	8412	4/4	0.93	0.17	31,36,40,100	0
3	NA	B	3104	1/1	0.93	0.13	32,32,32,32	0
5	DMS	B	8504	4/4	0.93	0.13	26,38,43,54	0
5	DMS	A	8602	4/4	0.93	0.18	31,53,100,100	0
5	DMS	D	8508	4/4	0.93	0.18	37,42,52,100	0
3	NA	A	3104	1/1	0.93	0.10	30,30,30,30	0
5	DMS	B	8601	4/4	0.93	0.13	34,36,44,49	0
5	DMS	A	8501	4/4	0.94	0.10	20,25,31,36	0
5	DMS	C	8501	4/4	0.94	0.12	22,25,38,53	0
5	DMS	D	8409	4/4	0.94	0.11	27,29,31,37	0
2	MG	C	3105	1/1	0.94	0.12	28,28,28,28	1
2	MG	B	3105	1/1	0.94	0.10	28,28,28,28	1
5	DMS	C	8412	4/4	0.94	0.20	34,37,75,100	0
5	DMS	A	8413	4/4	0.94	0.12	34,36,42,47	0
3	NA	C	3104	1/1	0.95	0.11	29,29,29,29	0
5	DMS	C	8409	4/4	0.95	0.10	26,38,39,40	0
5	DMS	C	8410	4/4	0.95	0.14	24,36,40,80	0
5	DMS	A	8410	4/4	0.95	0.14	33,37,47,61	0
5	DMS	B	8502	4/4	0.95	0.10	26,29,36,42	0
5	DMS	C	8414	4/4	0.95	0.10	20,35,36,43	0
3	NA	D	3103	1/1	0.95	0.10	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8405	4/4	0.95	0.11	23,30,31,32	0
5	DMS	B	8408	4/4	0.95	0.13	27,28,35,59	0
5	DMS	D	8406	4/4	0.95	0.10	22,25,25,30	0
5	DMS	A	8408	4/4	0.95	0.16	17,35,41,100	0
5	DMS	B	8411	4/4	0.96	0.11	28,32,38,43	0
5	DMS	C	8411	4/4	0.96	0.13	24,28,32,100	0
5	DMS	D	8411	4/4	0.96	0.14	29,30,34,100	0
2	MG	A	3005	1/1	0.96	0.07	30,30,30,30	0
5	DMS	A	8411	4/4	0.96	0.15	26,27,30,100	0
3	NA	A	3103	1/1	0.96	0.10	32,32,32,32	0
5	DMS	B	8404	4/4	0.96	0.10	23,25,35,55	0
5	DMS	B	8412	4/4	0.97	0.08	25,29,33,35	0
5	DMS	C	8402	4/4	0.97	0.08	18,18,26,30	0
5	DMS	C	8404	4/4	0.97	0.08	20,22,32,35	0
5	DMS	D	8403	4/4	0.97	0.08	20,26,28,36	0
5	DMS	C	8405	4/4	0.97	0.08	21,26,27,28	0
2	MG	D	3005	1/1	0.97	0.05	25,25,25,25	0
5	DMS	D	8408	4/4	0.97	0.08	19,29,31,38	0
5	DMS	C	8408	4/4	0.97	0.08	26,28,30,33	0
5	DMS	D	8410	4/4	0.97	0.08	23,33,34,37	0
5	DMS	D	8701	4/4	0.97	0.11	16,18,20,41	0
5	DMS	A	8403	4/4	0.97	0.09	22,26,29,32	0
5	DMS	D	8412	4/4	0.97	0.11	20,20,30,92	0
5	DMS	D	8402	4/4	0.98	0.07	17,20,21,22	0
4	IPT	D	2001	15/15	0.98	0.05	13,17,22,22	0
3	NA	B	3103	1/1	0.98	0.04	25,25,25,25	0
5	DMS	D	8405	4/4	0.98	0.09	25,26,30,35	0
5	DMS	C	8401	4/4	0.98	0.07	16,20,20,27	0
5	DMS	B	8402	4/4	0.98	0.06	14,15,20,21	0
5	DMS	C	8403	4/4	0.98	0.06	21,22,26,29	0
5	DMS	B	8403	4/4	0.98	0.07	22,25,28,30	0
4	IPT	A	2001	15/15	0.98	0.06	11,16,24,28	0
4	IPT	B	2001	15/15	0.98	0.06	14,16,23,27	0
4	IPT	C	2001	15/15	0.98	0.07	14,17,28,28	0
2	MG	A	3002	1/1	0.99	0.03	16,16,16,16	0
2	MG	B	3001	1/1	0.99	0.02	12,12,12,12	0
5	DMS	A	8401	4/4	0.99	0.05	13,14,15,16	0
5	DMS	A	8402	4/4	0.99	0.07	15,18,21,25	0
3	NA	B	3101	1/1	0.99	0.06	15,15,15,15	0
2	MG	B	3002	1/1	0.99	0.05	15,15,15,15	0
5	DMS	A	8405	4/4	0.99	0.06	24,25,25,29	0
2	MG	D	3001	1/1	0.99	0.03	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	8401	4/4	0.99	0.06	18,19,20,20	0
3	NA	C	3101	1/1	0.99	0.03	15,15,15,15	0
3	NA	C	3102	1/1	0.99	0.08	14,14,14,14	0
3	NA	C	3103	1/1	0.99	0.08	25,25,25,25	0
2	MG	D	3002	1/1	0.99	0.04	14,14,14,14	0
3	NA	D	3101	1/1	0.99	0.05	17,17,17,17	0
3	NA	D	3102	1/1	0.99	0.04	12,12,12,12	0
2	MG	A	3001	1/1	0.99	0.03	15,15,15,15	0
2	MG	C	3002	1/1	0.99	0.03	14,14,14,14	0
5	DMS	D	8401	4/4	0.99	0.05	13,14,18,19	0
3	NA	A	3101	1/1	0.99	0.05	16,16,16,16	0
3	NA	A	3102	1/1	0.99	0.04	12,12,12,12	0
2	MG	C	3001	1/1	1.00	0.05	14,14,14,14	0
3	NA	B	3102	1/1	1.00	0.05	12,12,12,12	0

6.5 Other polymers [i](#)

There are no such residues in this entry.