



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 12:21 AM UTC

PDB ID : 1JYX / pdb_00001jyx
Title : E. COLI (lacZ) BETA-GALACTOSIDASE IN COMPLEX WITH IPTG
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

<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

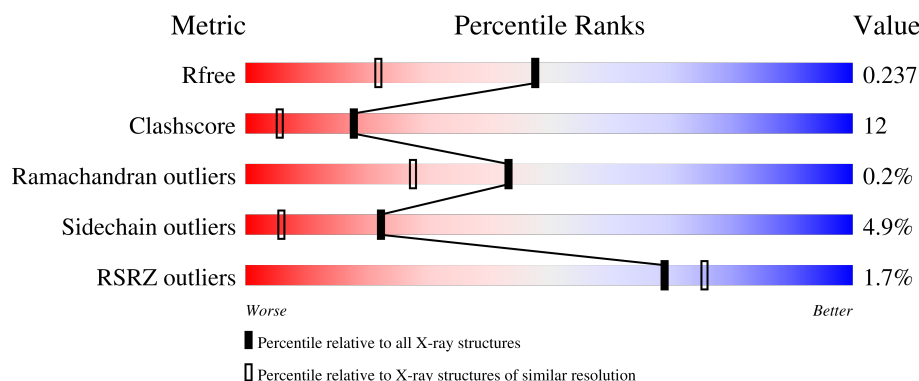
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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}	180053	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (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 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	67% 26% 5% ..
1	B	1023	71% 22% 5% ..
1	C	1023	74% 20% ..
1	D	1023	72% 23% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	A	8420	-	-	X	-
5	DMS	B	8407	-	X	-	-
5	DMS	C	8506	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Beta-Galactosidase.

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

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	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

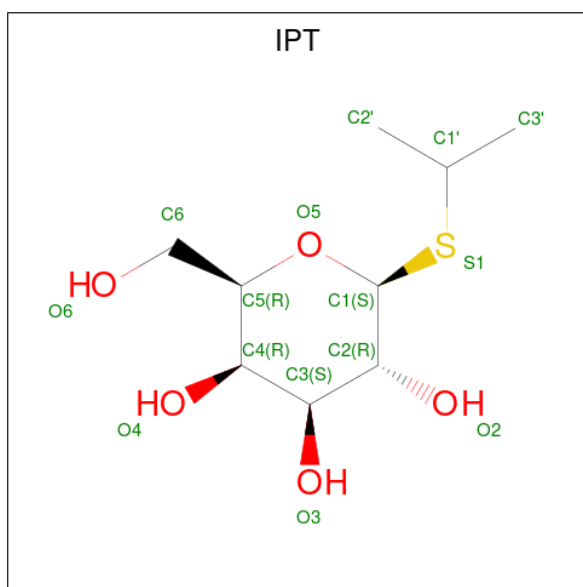
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Na 3 3	0	0
3	B	4	Total Na 4 4	0	0
3	C	4	Total Na 4 4	0	0
3	D	3	Total Na 3 3	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	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		
4	D	1	Total	C	O	S	0	0
			15	9	5	1		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	865	Total	O	0	0
			865	865		

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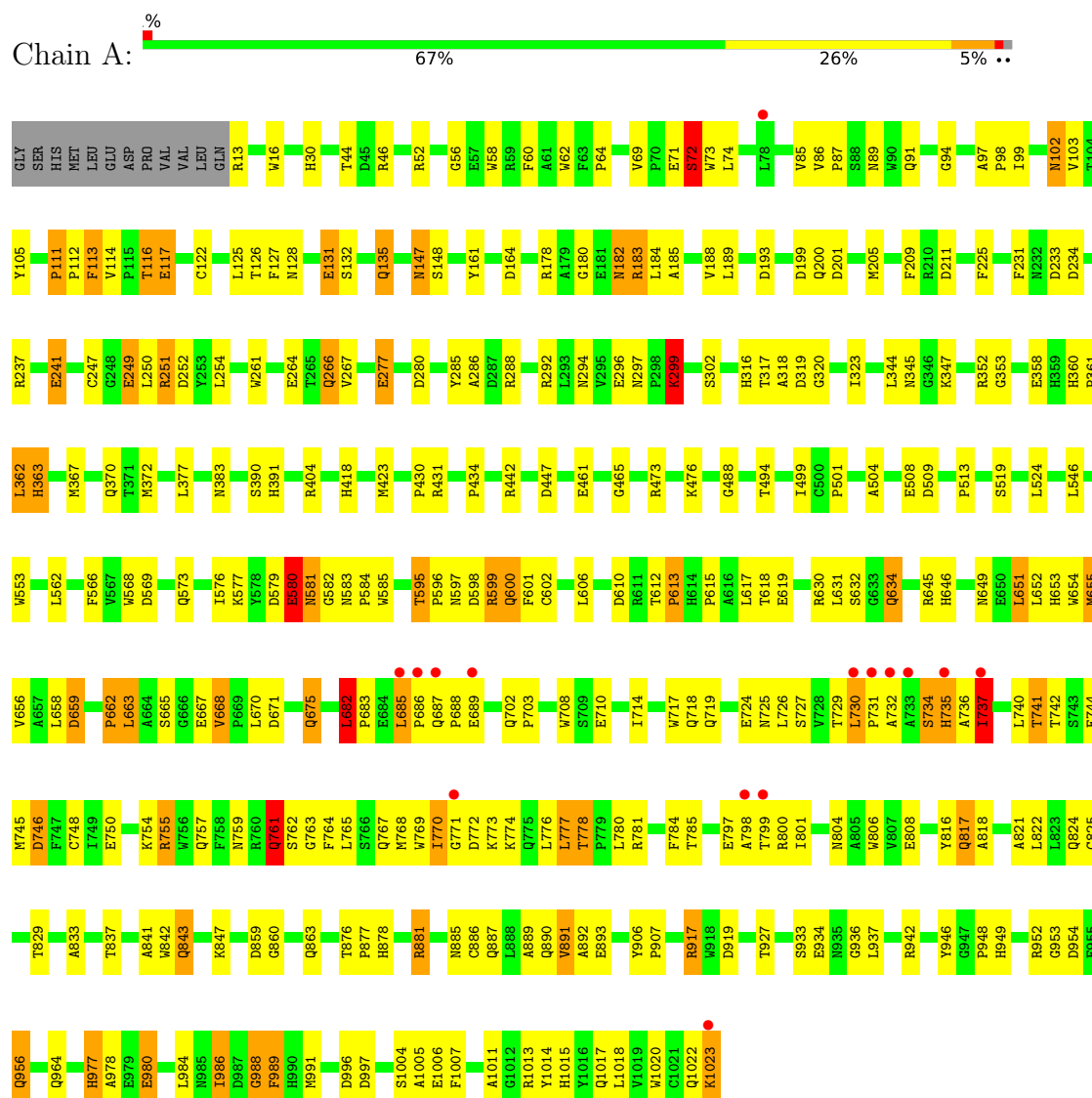
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	935	Total 935	O 935	0	0
6	C	922	Total 922	O 922	0	0
6	D	885	Total 885	O 885	0	0

3 Residue-property plots [i](#)

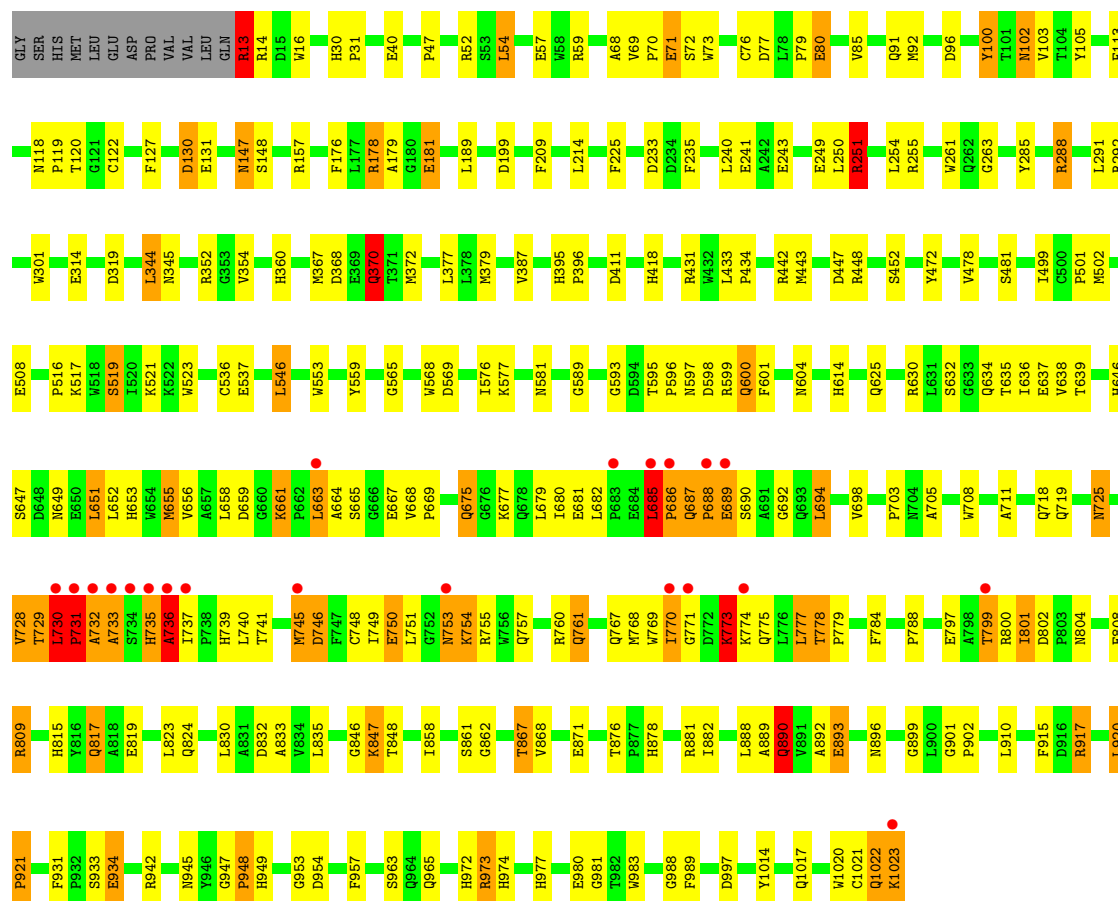
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

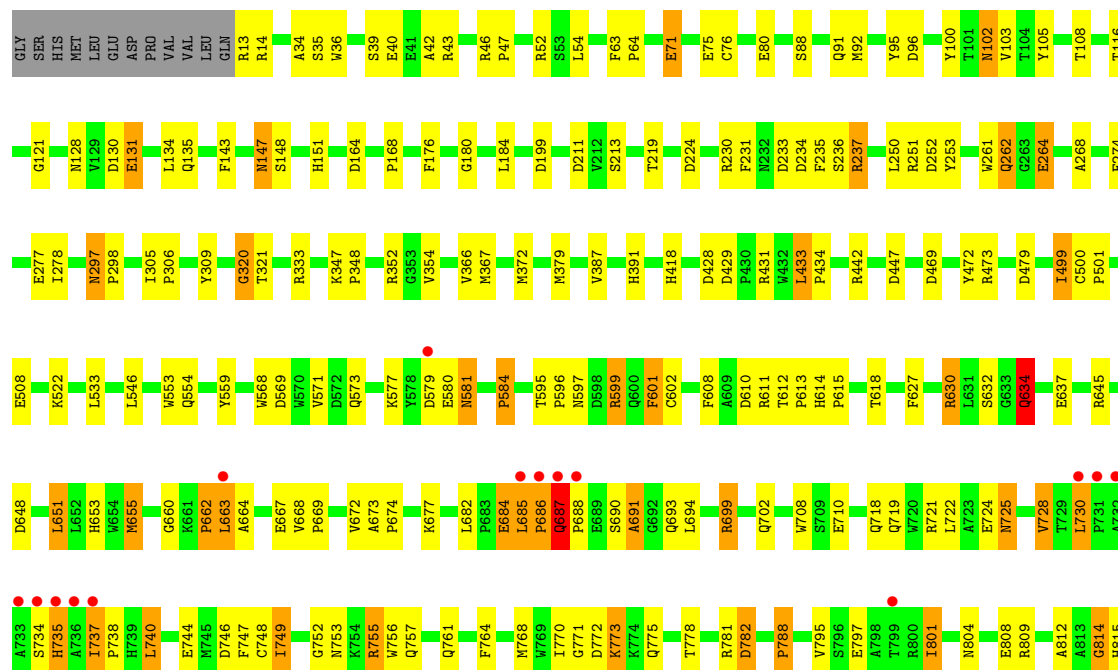
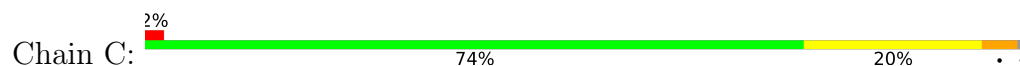


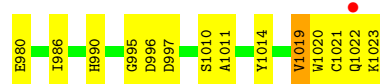
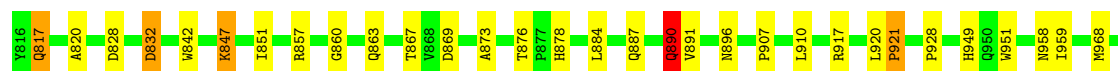
• Molecule 1: Beta-Galactosidase



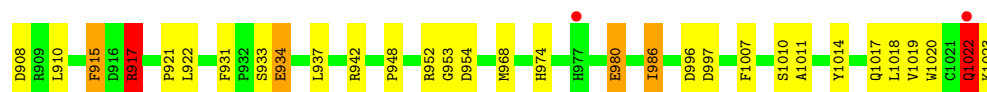
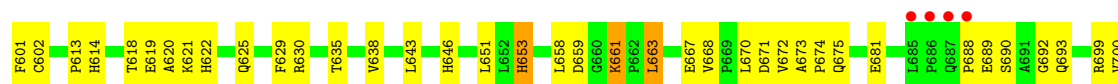
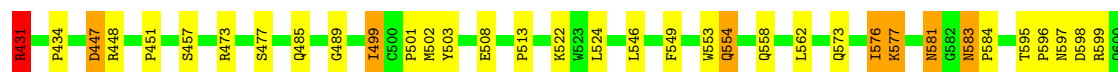


• Molecule 1: Beta-Galactosidase





● Molecule 1: Beta-Galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.77Å 161.19Å 202.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.00 – 1.75 27.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	89.6 (27.00-1.75) 89.5 (27.00-1.75)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.75Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.168 , 0.244 0.172 , 0.237	Depositor DCC
R_{free} test set	6397 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	16.8	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 97.1	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	0.96	EDS
Total number of atoms	36516	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0575e-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: DMS, MG, IPT, NA

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	1.22	4/8367 (0.0%)	1.79	149/11415 (1.3%)
1	B	1.25	3/8367 (0.0%)	1.75	107/11415 (0.9%)
1	C	1.24	9/8367 (0.1%)	1.77	105/11415 (0.9%)
1	D	1.21	4/8367 (0.0%)	1.75	114/11415 (1.0%)
All	All	1.23	20/33468 (0.1%)	1.76	475/45660 (1.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	391	HIS	CE1-NE2	6.63	1.39	1.32
1	C	391	HIS	ND1-CE1	6.10	1.38	1.32
1	C	418	HIS	CG-CD2	5.97	1.42	1.35
1	D	86	VAL	CA-C	5.82	1.56	1.52
1	D	499	ILE	CA-CB	-5.72	1.47	1.54
1	B	973	ARG	N-CA	-5.65	1.39	1.46
1	C	40	GLU	CD-OE2	5.57	1.35	1.25
1	D	348	PRO	CA-C	-5.47	1.47	1.52
1	C	391	HIS	CG-ND1	5.42	1.44	1.38
1	C	990	HIS	CE1-NE2	5.37	1.38	1.32
1	C	347	LYS	C-N	-5.27	1.29	1.33
1	A	418	HIS	CE1-NE2	5.19	1.37	1.32
1	C	151	HIS	ND1-CE1	5.17	1.37	1.32
1	B	118	ASN	C-O	-5.17	1.20	1.24
1	D	40	GLU	CD-OE2	5.17	1.35	1.25
1	B	120	THR	CA-C	-5.15	1.46	1.52
1	C	684	GLU	CD-OE2	5.13	1.35	1.25
1	A	881	ARG	NE-CZ	5.07	1.38	1.33
1	A	358	GLU	CD-OE2	5.01	1.34	1.25
1	A	488	GLY	CA-C	-5.01	1.47	1.52

All (475) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	725	ASN	CA-CB-CG	-12.18	100.42	112.60
1	C	252	ASP	CA-CB-CG	-11.83	100.77	112.60
1	B	733	ALA	N-CA-C	11.71	126.28	110.35
1	A	687	GLN	CA-C-N	11.09	131.81	119.83
1	A	687	GLN	C-N-CA	11.09	131.81	119.83
1	C	130	ASP	CA-CB-CG	9.68	122.28	112.60
1	D	653	HIS	CA-CB-CG	9.12	122.92	113.80
1	D	113	PHE	CA-CB-CG	-9.11	104.69	113.80
1	B	931	PHE	CA-CB-CG	-9.03	104.78	113.80
1	A	771	GLY	N-CA-C	-9.01	95.97	111.47
1	B	954	ASP	CA-CB-CG	-8.57	104.03	112.60
1	A	113	PHE	CA-CB-CG	-8.52	105.28	113.80
1	B	997	ASP	N-CA-CB	8.08	124.33	111.56
1	C	735	HIS	CA-CB-CG	-8.05	105.75	113.80
1	A	320	GLY	CA-C-N	-7.99	110.92	122.19
1	A	320	GLY	C-N-CA	-7.99	110.92	122.19
1	C	584	PRO	CB-CA-C	-7.96	100.55	110.98
1	B	685	LEU	CA-C-N	7.93	129.76	119.84
1	B	685	LEU	C-N-CA	7.93	129.76	119.84
1	D	583	ASN	CA-CB-CG	-7.92	104.67	112.60
1	A	653	HIS	CA-CB-CG	-7.86	105.94	113.80
1	D	613	PRO	CB-CA-C	-7.85	100.69	110.98
1	A	103	VAL	N-CA-C	7.84	117.87	110.74
1	A	989	PHE	CA-CB-CG	-7.83	105.97	113.80
1	A	737	ILE	CB-CA-C	7.80	118.04	110.16
1	B	52	ARG	CB-CA-C	-7.80	95.09	109.37
1	A	771	GLY	CA-C-N	-7.80	110.06	123.25
1	A	771	GLY	C-N-CA	-7.80	110.06	123.25
1	A	209	PHE	N-CA-C	7.77	122.97	113.17
1	A	671	ASP	CA-CB-CG	7.68	120.28	112.60
1	D	779	PRO	CB-CA-C	-7.67	101.23	111.12
1	A	116	THR	CA-C-N	-7.66	112.23	122.42
1	A	116	THR	C-N-CA	-7.66	112.23	122.42
1	A	297	ASN	CA-C-O	7.65	125.75	120.47
1	B	130	ASP	CA-CB-CG	-7.64	104.96	112.60
1	A	581	ASN	N-CA-C	-7.60	103.73	113.16
1	D	74	LEU	CA-C-N	-7.51	110.58	122.29
1	D	74	LEU	C-N-CA	-7.51	110.58	122.29
1	B	761	GLN	N-CA-CB	7.47	122.09	110.44
1	D	917	ARG	CD-NE-CZ	-7.44	113.98	124.40
1	C	997	ASP	N-CA-CB	7.42	123.28	111.56
1	A	319	ASP	CA-CB-CG	7.38	119.98	112.60
1	C	224	ASP	CA-CB-CG	7.35	119.95	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	598	ASP	CA-CB-CG	-7.34	105.26	112.60
1	D	980	GLU	O-C-N	-7.29	113.90	122.87
1	B	113	PHE	CA-CB-CG	-7.14	106.66	113.80
1	A	612	THR	N-CA-C	-7.11	101.11	109.93
1	D	431	ARG	CA-CB-CG	-7.10	99.90	114.10
1	C	702	GLN	CA-C-O	7.08	125.31	119.36
1	D	209	PHE	CA-CB-CG	-7.06	106.74	113.80
1	C	728	VAL	CA-C-O	7.01	125.28	118.98
1	C	553	TRP	CA-CB-CG	-6.99	100.32	113.60
1	B	517	LYS	N-CA-CB	6.98	123.55	110.56
1	C	788	PRO	N-CA-C	6.96	121.74	111.03
1	A	714	ILE	N-CA-CB	-6.96	103.07	111.00
1	B	431	ARG	CA-CB-CG	-6.93	100.23	114.10
1	D	770	ILE	N-CA-CB	6.93	120.54	112.15
1	D	69	VAL	N-CA-C	6.92	115.73	108.95
1	A	917	ARG	CD-NE-CZ	-6.91	114.73	124.40
1	A	601	PHE	CA-CB-CG	-6.90	106.90	113.80
1	A	323	ILE	N-CA-C	-6.88	105.13	111.67
1	C	634	GLN	CB-CA-C	6.87	122.08	111.02
1	A	954	ASP	CA-CB-CG	-6.86	105.74	112.60
1	B	688	PRO	CB-CA-C	-6.85	102.63	111.46
1	A	997	ASP	N-CA-CB	6.84	122.37	111.56
1	C	274	PHE	CA-CB-CG	-6.84	106.96	113.80
1	B	754	LYS	N-CA-C	6.82	120.38	110.28
1	D	770	ILE	CA-CB-CG1	6.82	121.99	110.40
1	B	893	GLU	N-CA-C	6.80	120.06	111.69
1	D	252	ASP	CA-CB-CG	-6.80	105.80	112.60
1	B	846	GLY	CA-C-N	-6.80	112.02	122.09
1	B	846	GLY	C-N-CA	-6.80	112.02	122.09
1	A	891	VAL	N-CA-CB	6.79	120.78	112.10
1	C	722	LEU	CA-C-O	6.78	121.87	117.94
1	A	770	ILE	N-CA-CB	6.77	120.44	111.64
1	C	499	ILE	CA-C-N	-6.75	114.98	123.15
1	C	499	ILE	C-N-CA	-6.75	114.98	123.15
1	A	296	GLU	CA-C-N	-6.73	116.64	123.10
1	A	296	GLU	C-N-CA	-6.73	116.64	123.10
1	B	920	LEU	CA-C-N	6.70	126.62	119.85
1	B	920	LEU	C-N-CA	6.70	126.62	119.85
1	D	997	ASP	N-CA-CB	6.70	122.15	111.56
1	C	433	LEU	CA-C-O	6.67	124.81	118.34
1	A	211	ASP	N-CA-C	6.66	118.89	110.24
1	D	297	ASN	CA-CB-CG	-6.64	105.96	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	ARG	N-CA-C	6.62	118.37	108.31
1	D	451	PRO	N-CA-CB	6.60	110.52	103.39
1	B	948	PRO	CB-CA-C	-6.57	101.11	111.04
1	C	469	ASP	CA-C-N	-6.57	110.96	120.29
1	C	469	ASP	C-N-CA	-6.57	110.96	120.29
1	C	306	PRO	N-CA-CB	6.55	106.83	102.25
1	C	447	ASP	N-CA-C	6.55	121.42	113.17
1	A	30	HIS	CA-CB-CG	-6.52	107.28	113.80
1	A	56	GLY	CA-C-N	-6.52	113.00	122.19
1	A	56	GLY	C-N-CA	-6.52	113.00	122.19
1	A	234	ASP	CA-CB-CG	-6.52	106.08	112.60
1	A	237	ARG	CB-CA-C	-6.52	96.78	109.68
1	B	57	GLU	CA-CB-CG	-6.50	101.10	114.10
1	A	319	ASP	N-CA-CB	6.48	119.87	110.47
1	D	598	ASP	CA-CB-CG	-6.48	106.12	112.60
1	B	13	ARG	CD-NE-CZ	6.46	133.45	124.40
1	D	221	GLN	N-CA-C	6.46	118.77	109.14
1	A	504	ALA	N-CA-C	-6.45	100.94	110.48
1	C	237	ARG	CA-CB-CG	-6.44	101.22	114.10
1	A	613	PRO	CB-CA-C	-6.43	102.56	110.98
1	D	980	GLU	CA-C-N	-6.42	109.83	121.32
1	D	980	GLU	C-N-CA	-6.42	109.83	121.32
1	B	352	ARG	N-CA-C	-6.41	100.67	109.71
1	C	321	THR	CA-CB-OG1	-6.41	99.99	109.60
1	A	741	THR	CA-CB-OG1	-6.40	100.00	109.60
1	A	688	PRO	CB-CA-C	-6.40	103.58	111.64
1	B	233	ASP	N-CA-C	6.39	119.06	111.71
1	C	184	LEU	CB-CA-C	-6.38	98.72	109.50
1	D	893	GLU	N-CA-C	6.38	119.22	111.82
1	A	662	PRO	N-CA-CB	6.35	109.25	103.34
1	D	601	PHE	CA-CB-CG	-6.35	107.45	113.80
1	B	601	PHE	CA-CB-CG	-6.34	107.45	113.80
1	A	988	GLY	N-CA-C	-6.34	104.66	112.77
1	A	843	GLN	CA-C-N	-6.33	111.86	121.86
1	A	843	GLN	C-N-CA	-6.33	111.86	121.86
1	B	746	ASP	N-CA-C	6.33	118.69	109.07
1	C	917	ARG	CD-NE-CZ	-6.31	115.56	124.40
1	A	442	ARG	NE-CZ-NH2	-6.29	113.54	119.20
1	A	147	ASN	N-CA-CB	-6.28	100.85	110.65
1	D	689	GLU	CA-C-N	6.28	130.03	121.05
1	D	689	GLU	C-N-CA	6.28	130.03	121.05
1	A	927	THR	CA-C-O	6.26	126.34	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	634	GLN	N-CA-CB	6.26	120.94	110.92
1	C	627	PHE	CA-CB-CG	-6.26	107.54	113.80
1	C	176	PHE	N-CA-CB	-6.25	101.34	110.53
1	B	731	PRO	N-CA-CB	6.25	109.81	103.25
1	C	662	PRO	CB-CA-C	6.23	119.47	111.56
1	D	220	THR	CA-CB-OG1	-6.22	100.26	109.60
1	A	736	ALA	N-CA-C	6.20	119.64	110.46
1	C	691	ALA	N-CA-C	6.20	118.71	110.53
1	A	1015	HIS	CA-CB-CG	-6.19	107.61	113.80
1	C	599	ARG	N-CA-C	6.19	117.71	108.31
1	C	614	HIS	N-CA-C	-6.15	102.11	110.36
1	A	797	GLU	CB-CG-CD	-6.15	102.14	112.60
1	A	746	ASP	CA-CB-CG	6.14	118.74	112.60
1	B	147	ASN	N-CA-CB	-6.13	101.09	110.65
1	D	770	ILE	N-CA-C	-6.13	96.97	106.72
1	B	472	TYR	N-CA-C	-6.12	104.53	111.07
1	A	13	ARG	CD-NE-CZ	6.11	132.96	124.40
1	A	302	SER	CA-C-O	-6.10	114.92	121.45
1	A	404	ARG	N-CA-C	6.09	118.83	111.40
1	C	352	ARG	N-CA-C	-6.09	101.13	109.71
1	B	735	HIS	N-CA-CB	6.07	119.48	110.49
1	C	740	LEU	N-CA-C	6.07	118.62	108.73
1	D	247	CYS	N-CA-C	-6.07	100.12	109.52
1	C	103	VAL	CB-CA-C	-6.06	104.65	111.80
1	A	209	PHE	CA-CB-CG	-6.05	107.75	113.80
1	D	52	ARG	CB-CA-C	-6.05	98.49	109.38
1	B	890	GLN	N-CA-C	6.04	119.46	110.52
1	D	931	PHE	CA-CB-CG	-6.04	107.76	113.80
1	C	721	ARG	CB-CA-C	-6.03	99.91	109.80
1	A	659	ASP	CB-CA-C	-6.03	102.91	111.95
1	B	103	VAL	N-CA-C	6.03	117.06	111.45
1	C	744	GLU	N-CA-CB	6.03	119.08	110.16
1	C	211	ASP	N-CA-C	6.02	118.54	110.35
1	C	778	THR	CA-C-N	6.02	126.36	119.92
1	C	778	THR	C-N-CA	6.02	126.36	119.92
1	D	231	PHE	N-CA-C	6.01	118.55	109.41
1	D	430	PRO	N-CA-CB	6.01	109.88	103.39
1	A	583	ASN	N-CA-C	-6.01	100.91	109.62
1	D	577	LYS	N-CA-C	-6.00	100.21	109.52
1	D	352	ARG	CA-C-N	-6.00	115.51	122.77
1	D	352	ARG	C-N-CA	-6.00	115.51	122.77
1	C	479	ASP	CA-CB-CG	-5.99	106.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	523	TRP	CA-C-O	5.99	127.10	120.63
1	D	753	ASN	CA-CB-CG	-5.99	106.61	112.60
1	C	869	ASP	CA-CB-CG	-5.99	106.61	112.60
1	B	777	LEU	N-CA-C	-5.99	106.14	113.50
1	A	294	ASN	CA-CB-CG	-5.97	106.63	112.60
1	A	682	LEU	N-CA-CB	5.97	117.25	110.03
1	C	867	THR	CA-CB-OG1	-5.97	100.65	109.60
1	B	519	SER	N-CA-C	-5.96	101.83	110.24
1	D	423	MET	N-CA-C	5.96	118.57	111.71
1	A	646	HIS	N-CA-C	-5.96	101.70	110.52
1	B	521	LYS	CA-CB-CG	-5.96	102.18	114.10
1	C	297	ASN	CA-C-O	5.95	124.58	120.47
1	D	974	HIS	CA-CB-CG	-5.95	107.85	113.80
1	D	554	GLN	OE1-CD-NE2	5.95	128.55	122.60
1	B	668	VAL	CB-CA-C	-5.94	100.55	111.36
1	A	363	HIS	CA-CB-CG	-5.93	107.86	113.80
1	A	837	THR	CA-C-O	-5.93	113.95	120.36
1	C	472	TYR	N-CA-C	-5.93	104.73	111.07
1	C	687	GLN	CA-C-N	5.92	127.24	119.84
1	C	687	GLN	C-N-CA	5.92	127.24	119.84
1	C	917	ARG	NE-CZ-NH2	5.91	124.52	119.20
1	A	447	ASP	N-CA-C	5.89	120.60	113.17
1	C	147	ASN	N-CA-CB	-5.88	101.48	110.65
1	C	116	THR	N-CA-C	-5.87	104.96	111.36
1	D	752	GLY	CA-C-N	-5.87	112.90	122.65
1	D	752	GLY	C-N-CA	-5.87	112.90	122.65
1	A	734	SER	N-CA-C	-5.87	101.79	110.48
1	C	722	LEU	CB-CA-C	-5.87	108.62	117.07
1	C	442	ARG	NE-CZ-NH2	-5.84	113.95	119.20
1	C	890	GLN	CB-CG-CD	-5.84	102.67	112.60
1	A	252	ASP	N-CA-C	5.84	119.50	112.38
1	D	71	GLU	CB-CG-CD	5.83	122.50	112.60
1	D	98	PRO	N-CA-C	-5.81	101.97	111.68
1	D	210	ARG	N-CA-CB	5.81	119.77	111.05
1	D	671	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	37	ARG	NE-CZ-NH1	-5.80	115.70	121.50
1	D	772	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	477	SER	CA-CB-OG	-5.77	99.56	111.10
1	D	829	THR	N-CA-CB	5.77	119.84	110.43
1	D	448	ARG	N-CA-C	5.77	119.42	112.38
1	C	734	SER	N-CA-CB	5.77	119.86	110.17
1	D	921	PRO	CB-CA-C	-5.76	103.55	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	553	TRP	CA-CB-CG	-5.76	102.66	113.60
1	A	188	VAL	N-CA-CB	-5.75	104.08	110.99
1	C	320	GLY	CA-C-N	-5.75	114.08	122.19
1	C	320	GLY	C-N-CA	-5.75	114.08	122.19
1	B	119	PRO	N-CA-CB	5.74	108.36	103.19
1	B	442	ARG	NE-CZ-NH2	-5.74	114.04	119.20
1	D	635	THR	N-CA-C	5.72	118.28	109.07
1	D	1022	GLN	N-CA-CB	5.72	119.89	110.69
1	B	989	PHE	CA-CB-CG	-5.71	108.09	113.80
1	C	752	GLY	CA-C-N	-5.71	110.90	122.31
1	C	752	GLY	C-N-CA	-5.71	110.90	122.31
1	B	481	SER	N-CA-C	5.70	120.08	113.18
1	A	619	GLU	N-CA-C	-5.70	105.07	111.28
1	D	747	PHE	CA-CB-CG	5.70	119.50	113.80
1	B	632	SER	N-CA-CB	5.67	121.77	111.11
1	D	513	PRO	N-CA-CB	5.67	108.36	103.31
1	B	647	SER	CB-CA-C	-5.67	103.30	111.91
1	C	828	ASP	CA-CB-CG	5.66	118.26	112.60
1	D	424	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	B	100	TYR	N-CA-CB	5.64	119.70	110.39
1	C	219	THR	CA-CB-OG1	-5.64	101.13	109.60
1	B	917	ARG	CD-NE-CZ	-5.64	116.50	124.40
1	D	917	ARG	CA-CB-CG	-5.63	102.84	114.10
1	B	685	LEU	N-CA-C	5.63	119.47	108.21
1	C	630	ARG	NE-CZ-NH1	5.62	127.12	121.50
1	C	958	ASN	N-CA-CB	5.62	121.98	111.53
1	B	251	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	B	761	GLN	CB-CG-CD	5.62	122.15	112.60
1	B	448	ARG	N-CA-C	5.61	119.22	112.38
1	A	266	GLN	O-C-N	-5.59	116.50	123.04
1	A	582	GLY	CA-C-O	5.59	126.19	119.82
1	C	771	GLY	N-CA-C	-5.57	101.47	110.95
1	D	811	LYS	CB-CA-C	-5.57	102.09	110.90
1	D	263	GLY	CA-C-N	-5.57	112.98	122.56
1	D	263	GLY	C-N-CA	-5.57	112.98	122.56
1	B	679	LEU	CA-C-N	-5.56	115.70	123.10
1	B	679	LEU	C-N-CA	-5.56	115.70	123.10
1	A	316	HIS	N-CA-C	5.56	116.42	108.74
1	C	121	GLY	O-C-N	5.56	126.86	123.35
1	B	730	LEU	N-CA-C	5.56	122.09	109.81
1	C	348	PRO	N-CA-CB	5.56	106.95	103.23
1	D	777	LEU	N-CA-C	-5.56	106.63	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	612	THR	N-CA-C	-5.55	103.04	109.93
1	D	37	ARG	CD-NE-CZ	-5.55	116.62	124.40
1	B	209	PHE	CA-CB-CG	-5.55	108.25	113.80
1	A	580	GLU	O-C-N	5.55	128.00	122.12
1	D	954	ASP	CA-CB-CG	-5.55	107.05	112.60
1	A	829	THR	N-CA-CB	5.54	119.47	110.43
1	B	773	LYS	N-CA-CB	-5.54	100.83	109.87
1	A	323	ILE	N-CA-CB	5.53	118.48	110.68
1	C	921	PRO	CB-CA-C	-5.53	104.33	111.46
1	A	732	ALA	CA-C-N	5.53	131.53	121.97
1	A	732	ALA	C-N-CA	5.53	131.53	121.97
1	B	536	CYS	N-CA-C	-5.53	106.04	112.89
1	D	922	LEU	N-CA-C	5.53	118.02	111.33
1	B	614	HIS	N-CA-C	-5.52	102.96	110.36
1	B	685	LEU	O-C-N	5.52	126.38	121.36
1	B	69	VAL	CA-C-N	5.52	125.70	119.90
1	B	69	VAL	C-N-CA	5.52	125.70	119.90
1	D	363	HIS	N-CA-C	5.52	119.86	113.18
1	B	778	THR	CA-C-N	5.51	125.46	119.78
1	B	778	THR	C-N-CA	5.51	125.46	119.78
1	A	352	ARG	N-CA-C	-5.51	101.94	109.71
1	B	319	ASP	CA-CB-CG	5.50	118.10	112.60
1	C	54	LEU	N-CA-C	-5.50	105.88	112.59
1	A	996	ASP	CA-CB-CG	-5.50	107.10	112.60
1	C	39	SER	N-CA-C	5.50	117.27	111.28
1	A	52	ARG	CB-CA-C	-5.50	100.25	109.48
1	A	193	ASP	N-CA-C	-5.50	105.67	112.38
1	B	581	ASN	CA-CB-CG	-5.50	107.11	112.60
1	B	559	TYR	CB-CA-C	-5.49	103.59	109.85
1	C	832	ASP	N-CA-CB	-5.49	102.16	111.27
1	D	553	TRP	CA-CB-CG	-5.49	103.17	113.60
1	A	727	SER	CB-CA-C	-5.49	100.90	109.84
1	B	261	TRP	N-CA-CB	-5.47	101.73	111.08
1	A	816	TYR	CA-C-N	-5.47	114.02	122.49
1	A	816	TYR	C-N-CA	-5.47	114.02	122.49
1	D	777	LEU	N-CA-CB	5.46	118.45	110.47
1	B	988	GLY	N-CA-C	-5.46	105.67	113.86
1	D	614	HIS	N-CA-C	-5.46	103.05	110.36
1	A	610	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	134	LEU	CA-C-N	5.44	128.58	120.31
1	C	134	LEU	C-N-CA	5.44	128.58	120.31
1	D	324	GLU	N-CA-CB	5.44	119.83	111.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	833	ALA	CB-CA-C	-5.42	101.19	110.95
1	D	207	GLY	CA-C-O	-5.42	117.72	122.16
1	D	209	PHE	N-CA-C	5.42	119.88	113.16
1	B	635	THR	N-CA-C	5.42	117.56	108.73
1	C	686	PRO	N-CA-CB	5.42	106.44	102.81
1	B	235	PHE	CA-CB-CG	-5.41	108.39	113.80
1	B	876	THR	N-CA-C	-5.41	103.31	110.40
1	A	241	GLU	CB-CG-CD	-5.41	103.40	112.60
1	B	263	GLY	CA-C-N	-5.40	113.27	122.56
1	B	263	GLY	C-N-CA	-5.40	113.27	122.56
1	B	735	HIS	CB-CA-C	5.40	120.75	111.68
1	D	224	ASP	CA-CB-CG	5.39	117.99	112.60
1	A	277	GLU	CB-CG-CD	5.39	121.76	112.60
1	C	571	VAL	N-CA-C	5.39	116.49	108.46
1	D	447	ASP	N-CA-C	5.39	119.96	113.17
1	A	69	VAL	CA-C-N	5.39	125.56	119.90
1	A	69	VAL	C-N-CA	5.39	125.56	119.90
1	A	777	LEU	N-CA-C	-5.38	107.26	113.88
1	A	423	MET	N-CA-C	5.38	117.90	111.71
1	C	949	HIS	N-CA-C	5.38	118.87	110.32
1	D	772	ASP	CA-C-N	-5.38	115.62	122.77
1	D	772	ASP	C-N-CA	-5.38	115.62	122.77
1	D	86	VAL	CB-CA-C	5.37	115.34	110.13
1	C	108	THR	CA-CB-OG1	-5.37	101.55	109.60
1	D	447	ASP	N-CA-CB	-5.37	102.55	110.49
1	D	875	ASP	CA-CB-CG	5.37	117.97	112.60
1	B	85	VAL	CB-CA-C	-5.36	103.72	111.34
1	A	383	ASN	N-CA-C	5.36	119.77	113.23
1	B	920	LEU	CB-CA-C	-5.36	101.47	109.56
1	D	42	ALA	CB-CA-C	-5.36	101.74	110.85
1	A	977	HIS	O-C-N	-5.36	117.04	123.31
1	D	788	PRO	N-CA-C	5.36	119.28	111.03
1	B	516	PRO	CB-CA-C	-5.35	104.22	111.12
1	C	863	GLN	CB-CA-C	-5.35	100.50	109.48
1	B	443	MET	N-CA-C	-5.34	105.37	111.14
1	A	98	PRO	N-CA-C	-5.34	102.76	111.68
1	A	465	GLY	O-C-N	-5.34	118.95	123.60
1	A	513	PRO	CB-CA-C	-5.34	103.98	110.98
1	D	336	ARG	CD-NE-CZ	5.34	131.88	124.40
1	D	638	VAL	CB-CA-C	-5.34	102.87	110.83
1	C	907	PRO	N-CA-CB	5.33	108.96	103.15
1	A	111	PRO	N-CA-CB	5.33	108.25	103.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	CB-CG-CD	5.32	123.54	111.30
1	B	47	PRO	CA-C-N	-5.32	115.49	122.99
1	B	47	PRO	C-N-CA	-5.32	115.49	122.99
1	B	757	GLN	N-CA-C	5.32	117.08	108.41
1	A	345	ASN	CA-CB-CG	-5.32	107.28	112.60
1	D	147	ASN	N-CA-CB	-5.32	101.64	110.47
1	D	576	ILE	CB-CA-C	-5.31	104.24	111.15
1	D	352	ARG	N-CA-C	-5.31	102.22	109.71
1	D	996	ASP	CA-CB-CG	-5.31	107.29	112.60
1	A	907	PRO	N-CA-CB	5.30	109.31	103.26
1	D	796	SER	N-CA-CB	5.30	117.84	109.83
1	B	965	GLN	CA-CB-CG	-5.30	103.51	114.10
1	D	739	HIS	CA-CB-CG	-5.30	108.50	113.80
1	B	288	ARG	CD-NE-CZ	-5.29	116.99	124.40
1	B	910	LEU	CA-C-N	-5.29	112.67	120.28
1	B	910	LEU	C-N-CA	-5.29	112.67	120.28
1	B	801	ILE	N-CA-C	5.28	116.40	109.58
1	B	732	ALA	CA-C-N	5.28	128.72	120.75
1	B	732	ALA	C-N-CA	5.28	128.72	120.75
1	A	936	GLY	CA-C-N	-5.28	112.78	120.75
1	A	936	GLY	C-N-CA	-5.28	112.78	120.75
1	A	280	ASP	CA-CB-CG	5.27	117.87	112.60
1	A	949	HIS	N-CA-C	5.26	118.68	110.32
1	A	668	VAL	N-CA-CB	-5.25	103.86	111.21
1	C	1019	VAL	N-CA-CB	5.25	118.39	111.25
1	A	885	ASN	OD1-CG-ND2	5.25	127.85	122.60
1	A	58	TRP	CB-CA-C	-5.25	101.58	112.44
1	A	161	TYR	N-CA-CB	-5.24	101.78	111.53
1	C	814	GLY	CA-C-N	-5.24	113.25	120.28
1	C	814	GLY	C-N-CA	-5.24	113.25	120.28
1	D	14	ARG	N-CA-C	-5.24	102.32	109.71
1	A	231	PHE	CA-CB-CG	-5.24	108.56	113.80
1	C	896	ASN	CA-CB-CG	5.24	117.83	112.60
1	B	565	GLY	CA-C-O	-5.23	116.66	121.63
1	B	728	VAL	CA-C-O	5.23	125.22	120.30
1	A	919	ASP	CA-C-N	-5.22	116.44	123.96
1	A	919	ASP	C-N-CA	-5.22	116.44	123.96
1	B	809	ARG	N-CA-C	-5.22	105.49	111.07
1	C	579	ASP	N-CA-CB	5.22	117.53	110.38
1	C	928	PRO	N-CA-C	5.22	119.52	112.48
1	D	619	GLU	N-CA-C	-5.22	105.50	111.14
1	A	980	GLU	CA-C-N	-5.21	108.94	120.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	980	GLU	C-N-CA	-5.21	108.94	120.99
1	A	977	HIS	CA-C-N	-5.21	113.31	120.71
1	A	977	HIS	C-N-CA	-5.21	113.31	120.71
1	B	931	PHE	CA-C-O	5.20	123.73	119.36
1	B	761	GLN	CB-CA-C	5.20	120.10	109.55
1	C	76	CYS	N-CA-C	5.19	117.90	109.24
1	C	213	SER	CB-CA-C	-5.18	99.11	110.67
1	B	418	HIS	N-CA-C	5.18	117.59	111.33
1	C	747	PHE	N-CA-CB	5.17	118.70	110.57
1	D	934	GLU	N-CA-C	-5.17	102.94	110.24
1	A	964	GLN	CA-C-O	5.17	126.03	120.55
1	A	731	PRO	CB-CA-C	-5.17	104.62	111.23
1	A	89	ASN	N-CA-C	-5.17	100.10	108.52
1	A	553	TRP	CA-CB-CG	-5.16	103.79	113.60
1	B	360	HIS	ND1-CG-CD2	5.16	111.26	106.10
1	A	72	SER	CB-CA-C	-5.16	102.17	110.74
1	C	812	ALA	N-CA-CB	5.16	118.17	110.22
1	D	93	HIS	CA-CB-CG	-5.16	108.64	113.80
1	D	503	TYR	CA-CB-CG	-5.15	104.63	113.90
1	A	99	ILE	CB-CA-C	-5.15	102.94	110.62
1	D	787	ALA	N-CA-C	-5.15	100.12	109.44
1	D	279	ILE	N-CA-CB	-5.15	103.23	111.82
1	A	233	ASP	CA-C-N	-5.14	114.49	122.67
1	A	233	ASP	C-N-CA	-5.14	114.49	122.67
1	C	632	SER	N-CA-CB	5.14	118.92	110.90
1	A	390	SER	CA-C-O	-5.14	114.79	120.60
1	D	418	HIS	CE1-NE2-CD2	5.14	114.14	109.00
1	B	725	ASN	CA-CB-CG	-5.13	107.47	112.60
1	D	834	VAL	O-C-N	-5.13	117.90	123.14
1	C	500	CYS	N-CA-CB	-5.13	102.89	110.99
1	A	725	ASN	CA-CB-CG	-5.13	107.47	112.60
1	D	674	PRO	N-CA-CB	5.13	107.80	103.19
1	B	868	VAL	CA-CB-CG2	5.12	119.11	110.40
1	B	40	GLU	CA-C-N	-5.12	112.53	120.31
1	B	40	GLU	C-N-CA	-5.12	112.53	120.31
1	B	736	ALA	N-CA-CB	5.11	119.12	110.49
1	C	442	ARG	NE-CZ-NH1	5.11	126.61	121.50
1	A	859	ASP	N-CA-C	5.11	117.30	109.95
1	A	798	ALA	N-CA-C	5.10	117.50	111.33
1	C	103	VAL	N-CA-C	5.10	116.51	111.67
1	D	155	ASN	CA-CB-CG	-5.10	107.50	112.60
1	C	890	GLN	N-CA-C	5.09	118.06	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	915	PHE	CA-CB-CG	-5.09	108.70	113.80
1	C	668	VAL	CB-CA-C	-5.09	102.09	111.36
1	D	843	GLN	CA-C-N	-5.08	114.88	122.39
1	D	843	GLN	C-N-CA	-5.08	114.88	122.39
1	D	97	ALA	CB-CA-C	-5.08	101.55	108.86
1	A	842	TRP	CE2-CD2-CE3	5.07	123.87	118.80
1	B	604	ASN	CB-CA-C	-5.07	102.54	110.85
1	A	579	ASP	CA-C-N	5.06	127.07	120.28
1	A	579	ASP	C-N-CA	5.06	127.07	120.28
1	D	489	GLY	CA-C-N	-5.06	114.25	122.30
1	D	489	GLY	C-N-CA	-5.06	114.25	122.30
1	C	233	ASP	N-CA-C	5.06	116.80	111.28
1	A	461	GLU	N-CA-CB	-5.06	104.02	111.71
1	C	770	ILE	N-CA-C	-5.06	98.68	106.72
1	B	54	LEU	N-CA-C	-5.06	106.70	112.92
1	A	606	LEU	N-CA-C	-5.05	106.62	112.89
1	A	889	ALA	CA-C-O	5.05	125.78	119.97
1	B	682	LEU	CA-C-N	5.05	126.16	119.84
1	B	682	LEU	C-N-CA	5.05	126.16	119.84
1	D	688	PRO	N-CA-C	-5.05	102.06	112.47
1	C	608	PHE	N-CA-C	-5.05	103.86	110.53
1	A	727	SER	CA-C-N	-5.05	115.70	122.72
1	A	727	SER	C-N-CA	-5.05	115.70	122.72
1	B	815	HIS	CA-C-N	-5.05	112.30	121.14
1	B	815	HIS	C-N-CA	-5.05	112.30	121.14
1	C	959	ILE	O-C-N	-5.05	117.61	123.07
1	D	395	HIS	CA-C-O	5.05	124.92	120.02
1	D	1022	GLN	CB-CG-CD	5.05	121.19	112.60
1	B	370	GLN	CB-CG-CD	5.05	121.18	112.60
1	C	710	GLU	CB-CA-C	-5.05	99.71	109.76
1	C	725	ASN	CA-CB-CG	-5.05	107.55	112.60
1	A	44	THR	CA-C-N	-5.04	115.75	123.47
1	A	44	THR	C-N-CA	-5.04	115.75	123.47
1	A	494	THR	CA-CB-OG1	-5.04	102.03	109.60
1	B	921	PRO	CB-CA-C	-5.04	104.38	110.98
1	C	648	ASP	N-CA-C	5.04	119.07	113.02
1	A	761	GLN	CB-CG-CD	5.04	121.16	112.60
1	D	137	GLY	O-C-N	5.04	127.70	122.91
1	D	1019	VAL	CB-CA-C	-5.03	103.62	110.77
1	C	613	PRO	CB-CA-C	-5.03	104.39	110.98
1	A	225	PHE	N-CA-CB	5.02	119.88	110.99
1	A	612	THR	CB-CA-C	-5.02	101.88	109.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	601	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	247	CYS	N-CA-C	-5.02	101.57	109.50
1	A	893	GLU	N-CA-C	5.02	118.56	112.23
1	A	97	ALA	N-CA-C	5.02	116.39	110.07
1	D	700	VAL	N-CA-CB	5.01	117.08	111.21
1	D	710	GLU	CB-CA-C	-5.01	101.06	109.83
1	A	299	LYS	N-CA-C	-5.01	101.58	109.25
1	A	509	ASP	CB-CA-C	-5.01	100.24	109.46
1	C	52	ARG	NE-CZ-NH1	-5.01	116.49	121.50
1	C	268	ALA	CA-C-O	-5.01	115.59	121.10
1	A	702	GLN	CA-C-O	5.00	123.76	119.71
1	C	782	ASP	CA-CB-CG	-5.00	107.60	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8125	0	7716	194	0
1	B	8125	0	7716	237	0
1	C	8125	0	7716	185	0
1	D	8125	0	7716	175	0
2	A	2	0	0	0	0
2	B	3	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	3	0	0	0	0
4	A	30	0	35	2	0
4	B	15	0	17	0	0
4	C	15	0	17	0	0
4	D	30	0	35	0	0
5	A	72	0	108	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	72	0	108	7	0
5	C	84	0	126	19	0
5	D	68	0	102	10	0
6	A	865	0	0	26	0
6	B	935	0	0	18	0
6	C	922	0	0	14	0
6	D	885	0	0	21	0
All	All	36516	0	31412	790	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 12.

All (790) 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:D:804:ASN:ND2	1:D:809:ARG:HH21	1.40	1.18
1:B:730:LEU:HD12	1:B:731:PRO:HD3	1.24	1.16
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.40	1.15
1:D:581:ASN:ND2	1:D:583:ASN:HD22	1.46	1.12
1:D:863:GLN:HE22	1:D:952:ARG:NH2	1.49	1.10
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.26	1.08
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.29	1.08
1:D:581:ASN:HD22	1:D:583:ASN:ND2	1.50	1.07
1:A:634:GLN:H	1:A:634:GLN:NE2	1.56	1.01
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.60	1.00
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.61	0.97
1:A:597:ASN:HD22	1:A:599:ARG:H	1.14	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	1.14	0.94
1:A:634:GLN:HE21	1:A:634:GLN:N	1.65	0.94
1:D:367:MET:HB3	1:D:372:MET:HE2	1.51	0.92
1:B:730:LEU:HD12	1:B:730:LEU:H	1.33	0.92
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.01	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.06	0.90
1:C:597:ASN:HD22	1:C:599:ARG:H	1.14	0.90
1:D:233:ASP:HA	5:D:8417:DMS:H13	1.53	0.90
1:B:597:ASN:HD22	1:B:599:ARG:H	1.13	0.89
1:A:656:VAL:HG21	1:A:685:LEU:CD2	2.04	0.88
1:A:817:GLN:HE21	1:A:817:GLN:N	1.70	0.87
1:B:251:ARG:HH11	1:B:251:ARG:HB3	1.40	0.87
1:A:651:LEU:HD11	1:A:667:GLU:HB2	1.56	0.86
1:B:1022:GLN:HG2	1:B:1023:LYS:N	1.91	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LEU:HB3	1:A:683:PRO:HD2	1.57	0.85
1:D:597:ASN:HD22	1:D:599:ARG:H	1.21	0.85
1:B:685:LEU:HD23	1:B:686:PRO:HD2	1.58	0.85
1:B:664:ALA:HB3	1:B:685:LEU:HD11	1.59	0.85
1:C:890:GLN:HG3	1:C:891:VAL:N	1.92	0.84
1:D:93:HIS:CD2	5:D:8414:DMS:H23	2.13	0.84
1:B:368:ASP:HB2	1:B:370:GLN:HE22	1.42	0.83
1:D:718:GLN:HE21	1:D:719:GLN:H	1.23	0.83
1:B:687:GLN:HB3	1:B:688:PRO:HD2	1.60	0.83
1:B:730:LEU:CD1	1:B:731:PRO:HD3	2.05	0.83
1:D:643:LEU:HD23	1:D:675:GLN:HE21	1.42	0.83
1:A:599:ARG:HB2	1:A:600:GLN:HE21	1.44	0.83
1:C:601:PHE:CE1	5:C:8506:DMS:H23	2.13	0.83
1:D:863:GLN:NE2	1:D:952:ARG:NH2	2.26	0.83
1:A:662:PRO:C	1:A:663:LEU:HD23	2.03	0.83
1:C:795:VAL:HG12	5:C:8506:DMS:H22	1.58	0.83
1:A:817:GLN:N	1:A:817:GLN:NE2	2.26	0.82
1:A:367:MET:HB3	1:A:372:MET:HE2	1.62	0.82
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.59	0.82
1:D:863:GLN:HE22	1:D:952:ARG:HH22	1.23	0.81
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.60	0.81
1:D:804:ASN:HD22	1:D:809:ARG:HH21	0.86	0.81
1:B:804:ASN:HD22	1:B:809:ARG:HH21	0.82	0.81
1:C:251:ARG:NH1	1:C:251:ARG:HB3	1.97	0.80
1:C:730:LEU:HD12	1:C:730:LEU:H	1.46	0.80
1:B:1022:GLN:HG2	1:B:1023:LYS:H	1.46	0.80
1:A:718:GLN:HE21	1:A:719:GLN:H	1.30	0.80
1:C:634:GLN:H	1:C:634:GLN:HE21	1.30	0.79
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.25	0.79
1:C:601:PHE:CZ	5:C:8506:DMS:H23	2.18	0.79
5:A:8415:DMS:H11	6:A:9366:HOH:O	1.83	0.78
1:B:770:ILE:HG21	1:B:1022:GLN:HE21	1.47	0.78
1:C:277:GLU:HG2	6:C:9299:HOH:O	1.84	0.78
1:A:656:VAL:HG21	1:A:685:LEU:HD22	1.66	0.78
1:B:705:ALA:HB1	6:B:9360:HOH:O	1.84	0.78
1:B:830:LEU:HD11	1:B:835:LEU:HB2	1.66	0.78
1:D:863:GLN:NE2	1:D:952:ARG:HH22	1.82	0.77
1:A:580:GLU:OE2	1:A:580:GLU:HA	1.85	0.77
1:B:777:LEU:HD21	1:B:889:ALA:HA	1.67	0.77
1:D:49:GLN:HG2	6:D:9356:HOH:O	1.84	0.77
5:A:8420:DMS:H22	6:D:8709:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:GLU:HB3	1:B:799:THR:HG23	1.66	0.76
1:A:651:LEU:HG	1:A:652:LEU:N	2.01	0.75
1:B:370:GLN:H	1:B:370:GLN:CD	1.94	0.75
1:C:773:LYS:CD	1:C:775:GLN:HE22	2.00	0.75
1:B:749:ILE:N	1:B:749:ILE:HD12	2.01	0.75
1:D:769:TRP:NE1	1:D:774:LYS:HG3	2.00	0.75
1:B:508:GLU:OE2	5:B:8407:DMS:H11	1.85	0.75
1:B:1017:GLN:HB2	6:B:9309:HOH:O	1.85	0.75
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.17	0.75
1:C:773:LYS:HG2	1:C:775:GLN:NE2	2.02	0.75
1:B:354:VAL:CG1	1:B:379:MET:HE3	2.18	0.74
1:D:768:MET:HE1	1:D:1020:TRP:CH2	2.22	0.74
1:C:630:ARG:HB3	1:C:630:ARG:HH11	1.52	0.74
1:C:95:TYR:CE2	5:C:8421:DMS:H23	2.22	0.74
5:A:8410:DMS:H22	6:A:8864:HOH:O	1.87	0.73
1:D:651:LEU:O	1:D:651:LEU:HD12	1.87	0.73
1:C:795:VAL:CG1	5:C:8506:DMS:H22	2.18	0.73
1:B:778:THR:HG23	1:B:779:PRO:HD2	1.70	0.73
1:C:804:ASN:OD1	1:C:809:ARG:NH2	2.21	0.73
1:A:656:VAL:HG21	1:A:685:LEU:HD21	1.71	0.73
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.19	0.73
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.70	0.72
1:C:685:LEU:HD23	1:C:686:PRO:HD2	1.71	0.72
1:D:878:HIS:HD2	6:D:8809:HOH:O	1.73	0.72
1:D:658:LEU:O	1:D:661:LYS:HG3	1.90	0.71
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.15	0.71
1:C:669:PRO:HA	6:C:9344:HOH:O	1.90	0.71
1:A:817:GLN:NE2	6:A:8941:HOH:O	2.20	0.71
1:C:857:ARG:HG2	1:C:857:ARG:HH11	1.56	0.71
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.25	0.71
1:C:773:LYS:HD3	1:C:775:GLN:HE22	1.55	0.71
1:B:656:VAL:HG21	1:B:685:LEU:HD13	1.73	0.71
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.73	0.70
1:D:71:GLU:H	1:D:71:GLU:CD	1.98	0.70
1:B:949:HIS:O	1:B:1023:LYS:HE2	1.91	0.70
1:B:646:HIS:HB3	6:B:9265:HOH:O	1.90	0.70
1:D:139:THR:OG1	1:D:216:HIS:HD2	1.75	0.70
1:B:653:HIS:HD2	1:B:667:GLU:HG3	1.55	0.70
1:B:730:LEU:H	1:B:730:LEU:CD1	1.97	0.70
1:C:749:ILE:N	1:C:749:ILE:HD12	2.06	0.70
1:B:685:LEU:O	1:B:687:GLN:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HB2	1:A:600:GLN:NE2	2.07	0.69
1:B:753:ASN:N	1:B:753:ASN:OD1	2.25	0.69
1:D:863:GLN:HE22	1:D:952:ARG:HH21	1.39	0.69
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.08	0.69
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.28	0.69
1:C:718:GLN:HE21	1:C:719:GLN:H	1.38	0.69
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.25	0.69
1:C:651:LEU:HD12	1:C:651:LEU:C	2.18	0.68
1:D:675:GLN:HG3	6:D:9443:HOH:O	1.94	0.68
1:C:797:GLU:O	1:C:801:ILE:HD13	1.93	0.68
1:A:597:ASN:ND2	1:A:599:ARG:H	1.90	0.68
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.73	0.68
1:D:581:ASN:HD22	1:D:583:ASN:HD22	0.74	0.68
1:A:183:ARG:HG2	6:A:8905:HOH:O	1.93	0.68
1:A:878:HIS:HD2	6:A:8676:HOH:O	1.76	0.68
1:D:78:LEU:HB3	1:D:80:GLU:OE2	1.93	0.68
1:A:887:GLN:NE2	1:A:980:GLU:O	2.27	0.68
1:C:251:ARG:HB3	1:C:251:ARG:HH11	1.57	0.68
1:C:795:VAL:HG12	5:C:8506:DMS:C2	2.23	0.68
1:A:876:THR:OG1	1:A:877:PRO:HD2	1.94	0.68
1:A:615:PRO:O	1:A:618:THR:HG22	1.94	0.68
1:A:800:ARG:NH1	1:A:800:ARG:HB2	2.09	0.68
1:C:102:ASN:C	1:C:102:ASN:HD22	2.02	0.68
1:B:755:ARG:HD3	6:B:9342:HOH:O	1.92	0.67
1:D:92:MET:HA	1:D:92:MET:HE2	1.76	0.67
1:D:765:LEU:HD21	1:D:768:MET:HE2	1.76	0.67
1:B:241:GLU:HG3	1:B:292:ARG:CG	2.18	0.67
1:A:250:LEU:C	1:A:251:ARG:HG2	2.18	0.67
1:B:653:HIS:HD2	1:B:667:GLU:CG	2.07	0.67
1:C:429:ASP:OD1	1:C:431:ARG:HG3	1.95	0.66
1:C:634:GLN:HE21	1:C:634:GLN:N	1.91	0.66
1:B:251:ARG:HB3	1:B:251:ARG:NH1	2.09	0.66
1:A:663:LEU:HD23	1:A:663:LEU:N	2.08	0.66
1:A:634:GLN:H	1:A:634:GLN:HE21	0.79	0.66
1:B:241:GLU:CD	1:B:292:ARG:HE	2.04	0.66
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.26	0.66
1:A:431:ARG:HB2	6:A:9430:HOH:O	1.94	0.66
1:B:948:PRO:O	1:B:1023:LYS:N	2.27	0.66
1:A:737:ILE:O	1:A:737:ILE:HD13	1.95	0.65
1:D:643:LEU:CD2	1:D:675:GLN:HE21	2.06	0.65
1:D:781:ARG:NH1	6:D:9387:HOH:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:554:GLN:NE2	6:C:8683:HOH:O	2.30	0.65
1:D:887:GLN:NE2	1:D:980:GLU:O	2.29	0.65
1:B:368:ASP:OD1	1:B:370:GLN:NE2	2.29	0.65
1:C:857:ARG:HG2	1:C:857:ARG:NH1	2.09	0.65
1:A:772:ASP:C	1:A:773:LYS:HD3	2.22	0.65
1:A:890:GLN:HG3	1:A:891:VAL:N	2.12	0.65
1:B:777:LEU:CD2	1:B:889:ALA:HA	2.27	0.65
1:A:430:PRO:HD3	5:A:8420:DMS:H21	1.79	0.65
1:C:738:PRO:HD3	1:C:860:GLY:HA2	1.79	0.64
1:C:847:LYS:HE3	6:C:8855:HOH:O	1.96	0.64
1:C:878:HIS:HD2	6:C:8600:HOH:O	1.80	0.64
1:B:685:LEU:CD2	1:B:686:PRO:HD2	2.27	0.64
1:B:974:HIS:HD2	6:B:8610:HOH:O	1.79	0.64
1:B:920:LEU:HB3	1:B:921:PRO:HD2	1.80	0.64
1:C:688:PRO:HG3	1:C:725:ASN:HD21	1.63	0.64
1:B:658:LEU:HD11	1:B:692:GLY:HA3	1.80	0.64
1:D:595:THR:HA	1:D:596:PRO:C	2.23	0.64
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.63	0.64
1:A:724:GLU:O	1:B:847:LYS:NZ	2.28	0.63
1:B:251:ARG:HH11	1:B:251:ARG:CB	2.08	0.63
1:C:687:GLN:HB3	1:C:688:PRO:HD2	1.79	0.63
5:D:8410:DMS:H13	6:D:9305:HOH:O	1.98	0.63
1:D:91:GLN:HG3	1:D:96:ASP:OD1	1.99	0.63
1:D:618:THR:HG21	6:D:9043:HOH:O	1.99	0.63
1:D:948:PRO:HA	1:D:1023:LYS:HG3	1.80	0.63
1:B:13:ARG:HG3	1:C:13:ARG:NH1	2.13	0.63
1:A:685:LEU:CD2	1:A:686:PRO:HD2	2.28	0.63
1:A:655:MET:HG3	1:A:656:VAL:N	2.04	0.63
1:B:847:LYS:HG3	1:B:848:THR:N	2.14	0.63
1:C:13:ARG:O	1:C:14:ARG:C	2.39	0.63
1:B:797:GLU:O	1:B:801:ILE:HD13	1.99	0.62
1:B:13:ARG:NH2	1:C:13:ARG:HB2	2.14	0.62
1:C:730:LEU:HD12	1:C:730:LEU:N	2.13	0.62
1:B:79:PRO:HD2	1:B:80:GLU:OE2	1.99	0.62
1:C:748:CYS:C	1:C:749:ILE:HD12	2.25	0.62
1:C:664:ALA:HB3	1:C:685:LEU:HD21	1.81	0.62
1:C:801:ILE:HD12	1:C:808:GLU:OE2	1.99	0.62
1:A:277:GLU:H	1:A:277:GLU:CD	2.07	0.62
1:A:347:LYS:HE3	6:A:9165:HOH:O	1.99	0.61
1:B:241:GLU:CG	1:B:292:ARG:HG2	2.20	0.61
1:C:473:ARG:NH1	6:C:9190:HOH:O	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:GLU:HG3	1:A:755:ARG:HD3	1.82	0.61
1:C:597:ASN:ND2	1:C:599:ARG:H	1.94	0.61
1:A:117:GLU:HG3	6:A:9006:HOH:O	2.00	0.61
1:A:800:ARG:HB2	1:A:800:ARG:CZ	2.30	0.61
1:C:740:LEU:HD12	1:C:748:CYS:O	2.00	0.61
1:B:718:GLN:HE21	1:B:719:GLN:H	1.47	0.61
1:B:1022:GLN:HB2	6:B:9340:HOH:O	2.00	0.61
1:D:800:ARG:HG3	1:D:800:ARG:HH11	1.64	0.61
1:B:92:MET:HE2	1:B:92:MET:HA	1.82	0.61
1:A:102:ASN:C	1:A:102:ASN:HD22	2.08	0.60
1:A:1017:GLN:O	1:A:1018:LEU:HD23	2.00	0.60
1:B:685:LEU:HD23	1:B:686:PRO:CD	2.30	0.60
1:A:634:GLN:NE2	1:A:634:GLN:N	2.36	0.60
1:D:749:ILE:HD11	1:D:836:ILE:HD11	1.83	0.60
1:B:867:THR:HG22	6:B:8921:HOH:O	2.01	0.60
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.36	0.60
1:B:730:LEU:HD12	1:B:730:LEU:N	2.12	0.60
1:B:770:ILE:HG21	1:B:1022:GLN:NE2	2.15	0.60
1:C:43:ARG:NH1	1:C:264:GLU:OE2	2.30	0.60
1:B:878:HIS:HD2	6:B:8589:HOH:O	1.85	0.59
1:A:817:GLN:NE2	1:A:817:GLN:H	1.99	0.59
1:B:102:ASN:HD22	1:B:102:ASN:C	2.09	0.59
1:A:742:THR:HG21	6:A:9241:HOH:O	2.01	0.59
1:B:599:ARG:HB2	1:B:600:GLN:HE21	1.65	0.59
5:A:8408:DMS:H22	6:A:9247:HOH:O	2.02	0.59
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.02	0.59
1:C:832:ASP:OD1	1:C:832:ASP:N	2.35	0.59
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.37	0.59
1:D:890:GLN:HE21	1:D:892:ALA:HB2	1.67	0.59
1:D:1022:GLN:HE21	1:D:1023:LYS:N	2.01	0.59
1:C:691:ALA:HA	1:C:725:ASN:HB2	1.84	0.59
1:B:708:TRP:CZ2	5:B:8403:DMS:H13	2.38	0.58
1:B:595:THR:HA	1:B:596:PRO:C	2.27	0.58
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.38	0.58
1:A:737:ILE:HD13	1:A:737:ILE:C	2.27	0.58
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.85	0.58
1:D:131:GLU:OE2	1:D:135:GLN:HG2	2.02	0.58
1:C:685:LEU:CD2	1:C:686:PRO:HD2	2.32	0.58
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.38	0.58
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.86	0.58
1:A:577:LYS:NZ	6:A:9249:HOH:O	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LEU:HD21	1:D:217:LYS:HD3	1.86	0.58
1:C:688:PRO:CG	1:C:725:ASN:HD21	2.17	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.90	0.58
1:A:759:ASN:OD1	1:A:762:SER:N	2.30	0.57
1:D:26:ARG:HD2	1:D:169:SER:HA	1.86	0.57
1:D:830:LEU:HD11	1:D:835:LEU:HB2	1.85	0.57
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.86	0.57
1:B:687:GLN:HB3	1:B:688:PRO:CD	2.33	0.57
5:A:8420:DMS:H22	6:A:9462:HOH:O	2.05	0.57
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.84	0.57
1:D:693:GLN:NE2	1:D:721:ARG:HD3	2.20	0.57
1:B:833:ALA:HB1	1:B:858:ILE:O	2.04	0.57
1:D:381:GLN:O	1:D:621:LYS:HE3	2.05	0.57
1:D:651:LEU:HD11	1:D:701:VAL:HB	1.86	0.57
1:C:95:TYR:CZ	5:C:8421:DMS:H23	2.39	0.57
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.03	0.57
1:C:773:LYS:HD3	1:C:775:GLN:NE2	2.20	0.56
1:A:94:GLY:O	5:A:8421:DMS:H21	2.05	0.56
1:A:662:PRO:O	1:A:663:LEU:HD23	2.05	0.56
1:B:675:GLN:HG3	6:B:8773:HOH:O	2.04	0.56
1:C:92:MET:HE2	1:C:92:MET:HA	1.88	0.56
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.40	0.56
1:D:431:ARG:HG3	6:D:9405:HOH:O	2.04	0.56
1:B:367:MET:HB3	1:B:372:MET:HE3	1.85	0.56
1:B:770:ILE:HD12	1:B:1022:GLN:HG3	1.87	0.56
1:D:1022:GLN:HE22	1:D:1023:LYS:HG3	1.68	0.56
1:A:577:LYS:O	1:A:584:PRO:HA	2.06	0.56
1:A:508:GLU:OE1	5:A:8407:DMS:H11	2.06	0.56
1:A:781:ARG:NH1	6:A:9263:HOH:O	2.33	0.56
1:A:71:GLU:O	1:A:74:LEU:N	2.33	0.56
1:A:431:ARG:O	1:A:431:ARG:HG2	2.06	0.56
1:B:663:LEU:HD12	1:B:685:LEU:HD22	1.88	0.56
1:A:299:LYS:HD2	6:A:9406:HOH:O	2.05	0.56
1:B:593:GLY:O	5:B:8413:DMS:H23	2.06	0.56
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.17	0.56
1:A:201:ASP:OD2	4:A:2001:IPT:H62	2.05	0.55
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.42	0.55
1:C:615:PRO:O	1:C:618:THR:HG22	2.07	0.55
1:D:781:ARG:NH2	6:D:9457:HOH:O	2.39	0.55
1:A:131:GLU:O	1:A:135:GLN:HG2	2.07	0.55
1:C:664:ALA:CB	1:C:685:LEU:HD21	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:651:LEU:HD22	1:B:651:LEU:C	2.31	0.55
1:D:651:LEU:CD1	1:D:701:VAL:HB	2.37	0.55
1:C:46:ARG:HB3	1:C:47:PRO:HD2	1.88	0.55
1:C:688:PRO:HG3	1:C:725:ASN:ND2	2.21	0.55
1:B:847:LYS:HE3	6:B:8840:HOH:O	2.06	0.55
1:B:770:ILE:O	1:B:771:GLY:C	2.49	0.55
1:A:759:ASN:OD1	1:A:761:GLN:N	2.40	0.55
1:B:947:GLY:O	1:B:1023:LYS:NZ	2.28	0.55
1:D:508:GLU:OE2	5:D:8407:DMS:H11	2.06	0.55
1:D:629:PHE:O	1:D:630:ARG:HD2	2.07	0.54
1:C:688:PRO:CG	1:C:725:ASN:ND2	2.70	0.54
1:B:685:LEU:HD23	1:B:685:LEU:C	2.32	0.54
1:A:241:GLU:HG3	1:A:292:ARG:CG	2.37	0.54
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.88	0.54
1:D:75:GLU:CD	1:D:156:GLY:HA3	2.32	0.54
1:D:800:ARG:HG3	1:D:800:ARG:NH1	2.21	0.54
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.42	0.54
1:D:847:LYS:NZ	1:D:875:ASP:OD2	2.34	0.54
1:B:797:GLU:CB	1:B:799:THR:HG23	2.37	0.54
1:C:584:PRO:O	5:C:8411:DMS:H23	2.08	0.54
1:D:581:ASN:ND2	1:D:583:ASN:ND2	2.28	0.54
1:B:739:HIS:O	1:B:750:GLU:OE2	2.24	0.54
1:C:847:LYS:NZ	1:D:724:GLU:O	2.40	0.54
1:D:230:ARG:HB3	6:D:9535:HOH:O	2.07	0.54
1:D:622:HIS:O	1:D:625:GLN:HG3	2.08	0.54
1:D:718:GLN:HE21	1:D:719:GLN:N	1.99	0.54
1:A:984:LEU:HD11	1:A:986:ILE:HG12	1.90	0.54
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.23	0.54
1:B:599:ARG:HB2	1:B:600:GLN:NE2	2.23	0.54
1:D:667:GLU:C	1:D:668:VAL:HG23	2.33	0.54
1:B:778:THR:CG2	1:B:779:PRO:HD2	2.37	0.53
1:C:686:PRO:O	1:C:687:GLN:O	2.26	0.53
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.53
1:D:651:LEU:HD12	1:D:651:LEU:C	2.32	0.53
1:B:181:GLU:HG3	6:B:9314:HOH:O	2.07	0.53
1:C:773:LYS:CG	1:C:775:GLN:HE22	2.22	0.53
1:D:573:GLN:HB2	1:D:602:CYS:O	2.08	0.53
5:A:8410:DMS:H13	6:A:9182:HOH:O	2.07	0.53
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.43	0.53
1:B:291:LEU:N	1:B:291:LEU:HD22	2.24	0.53
1:B:639:THR:OG1	1:B:677:LYS:HE2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:730:LEU:H	1:C:730:LEU:CD1	2.03	0.53
1:B:686:PRO:O	1:B:687:GLN:O	2.26	0.53
1:D:16:TRP:CG	1:D:189:LEU:HD13	2.44	0.53
1:C:431:ARG:HD2	6:C:9247:HOH:O	2.09	0.53
1:C:508:GLU:OE2	5:C:8407:DMS:H11	2.09	0.53
1:D:948:PRO:HB2	1:D:1022:GLN:NE2	2.24	0.53
1:D:861:SER:OG	1:D:863:GLN:HG3	2.09	0.53
1:A:524:LEU:HD11	1:A:562:LEU:HG	1.90	0.52
1:D:770:ILE:HD13	1:D:775:GLN:HG3	1.89	0.52
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.06	0.52
1:B:739:HIS:HB3	1:B:750:GLU:OE2	2.08	0.52
1:B:788:PRO:HD2	6:B:8719:HOH:O	2.08	0.52
1:A:71:GLU:O	1:A:72:SER:C	2.51	0.52
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.74	0.52
1:A:718:GLN:NE2	6:A:9223:HOH:O	2.42	0.52
1:C:653:HIS:NE2	1:C:667:GLU:OE2	2.43	0.52
1:D:737:ILE:HD13	1:D:738:PRO:HD2	1.91	0.52
1:D:890:GLN:HB2	6:D:9434:HOH:O	2.08	0.52
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.22	0.52
1:B:730:LEU:N	1:B:731:PRO:CD	2.73	0.52
1:A:362:LEU:HD12	1:A:363:HIS:CE1	2.44	0.52
1:D:93:HIS:NE2	5:D:8414:DMS:H23	2.25	0.52
1:D:1022:GLN:NE2	1:D:1023:LYS:HB2	2.25	0.52
1:A:717:TRP:CH2	5:A:8415:DMS:H12	2.45	0.52
1:C:262:GLN:HG3	1:C:309:TYR:CE2	2.44	0.52
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.90	0.51
1:B:599:ARG:HD2	1:B:600:GLN:HE22	1.75	0.51
1:C:685:LEU:CG	1:C:686:PRO:HD2	2.39	0.51
1:C:746:ASP:CG	1:C:757:GLN:HE21	2.18	0.51
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.45	0.51
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.23	0.51
1:A:595:THR:HA	1:A:596:PRO:C	2.36	0.51
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.92	0.51
1:D:718:GLN:NE2	6:D:9346:HOH:O	2.43	0.51
1:B:379:MET:HE1	1:B:387:VAL:HB	1.91	0.51
1:B:1020:TRP:CD1	1:B:1020:TRP:C	2.88	0.51
1:B:178:ARG:HG3	1:B:179:ALA:O	2.11	0.51
1:C:920:LEU:HB3	1:C:921:PRO:CD	2.34	0.51
1:D:416:GLU:OE2	1:D:418:HIS:HB2	2.10	0.51
1:B:658:LEU:HD22	1:B:688:PRO:CB	2.40	0.51
1:A:757:GLN:O	1:A:765:LEU:HD12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.10	0.51
1:A:261:TRP:CH2	1:A:266:GLN:HB2	2.46	0.51
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.25	0.51
1:B:395:HIS:ND1	1:B:396:PRO:HD2	2.26	0.51
1:B:655:MET:CE	1:B:665:SER:HB3	2.41	0.51
1:C:773:LYS:CG	1:C:775:GLN:NE2	2.74	0.51
1:C:1020:TRP:HD1	1:C:1021:CYS:N	2.08	0.51
1:A:241:GLU:HG3	1:A:292:ARG:HG3	1.92	0.51
1:A:249:GLU:HG3	1:A:251:ARG:NH1	2.26	0.51
1:B:102:ASN:C	1:B:102:ASN:ND2	2.66	0.51
1:B:658:LEU:HD11	1:B:692:GLY:CA	2.41	0.50
1:B:546:LEU:HA	6:B:8644:HOH:O	2.12	0.50
1:B:739:HIS:CD2	1:B:740:LEU:N	2.79	0.50
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.11	0.50
1:B:368:ASP:CB	1:B:370:GLN:HE22	2.19	0.50
1:B:784:PHE:HA	1:B:881:ARG:O	2.11	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.92	0.50
1:A:573:GLN:HB2	1:A:602:CYS:O	2.11	0.50
1:C:699:ARG:HH11	1:C:699:ARG:HG2	1.77	0.50
1:C:573:GLN:HB2	1:C:602:CYS:O	2.12	0.50
1:C:630:ARG:HH11	1:C:630:ARG:CB	2.24	0.50
1:C:655:MET:SD	1:C:699:ARG:NH2	2.85	0.50
1:D:125:LEU:O	1:D:183:ARG:HA	2.11	0.50
1:D:618:THR:HG23	6:D:9056:HOH:O	2.11	0.50
1:D:778:THR:HG23	1:D:779:PRO:HD2	1.92	0.50
1:A:735:HIS:ND1	1:A:735:HIS:N	2.60	0.50
1:B:749:ILE:C	1:B:750:GLU:HG3	2.36	0.50
1:B:767:GLN:HG3	1:B:768:MET:N	2.27	0.50
1:B:770:ILE:HG13	1:B:775:GLN:NE2	2.26	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:C:820:ALA:HB2	1:C:842:TRP:CE2	2.46	0.50
1:A:824:GLN:HG3	1:A:825:CYS:N	2.27	0.49
1:B:649:ASN:OD1	1:B:703:PRO:HD2	2.12	0.49
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.71	0.49
1:C:236:SER:C	1:C:237:ARG:HG3	2.37	0.49
1:C:367:MET:HE2	1:C:372:MET:HG3	1.93	0.49
1:D:35:SER:HB2	1:D:217:LYS:HD2	1.93	0.49
1:B:777:LEU:HD21	1:B:889:ALA:CA	2.40	0.49
1:D:102:ASN:C	1:D:102:ASN:HD22	2.19	0.49
1:D:643:LEU:HD23	1:D:675:GLN:NE2	2.19	0.49
1:A:655:MET:SD	1:A:662:PRO:HB3	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ASN:HA	1:C:180:GLY:O	2.12	0.49
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.93	0.49
1:A:977:HIS:O	1:A:978:ALA:C	2.50	0.49
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.49
1:B:755:ARG:HG2	1:B:769:TRP:CE3	2.48	0.49
1:B:656:VAL:HG21	1:B:685:LEU:CD1	2.41	0.49
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.43	0.49
1:B:658:LEU:HB2	1:B:694:LEU:CD2	2.42	0.49
1:D:742:THR:HG22	1:D:743:SER:N	2.27	0.49
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.48	0.49
1:D:658:LEU:O	1:D:659:ASP:C	2.56	0.49
1:A:347:LYS:NZ	6:A:9136:HOH:O	2.45	0.49
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.49
1:A:843:GLN:HA	1:A:847:LYS:O	2.13	0.49
1:A:784:PHE:HA	1:A:881:ARG:O	2.13	0.49
1:B:372:MET:HE1	1:B:395:HIS:CG	2.48	0.49
1:A:125:LEU:O	1:A:183:ARG:HA	2.12	0.48
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.48
1:C:46:ARG:HB3	1:C:47:PRO:CD	2.43	0.48
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.48	0.48
1:B:933:SER:O	1:B:934:GLU:C	2.53	0.48
5:B:8410:DMS:H22	6:B:8775:HOH:O	2.12	0.48
1:A:102:ASN:C	1:A:102:ASN:ND2	2.71	0.48
1:B:655:MET:HE2	1:B:664:ALA:O	2.13	0.48
1:A:765:LEU:HD21	1:A:768:MET:HE2	1.95	0.48
1:B:745:MET:SD	1:B:745:MET:N	2.86	0.48
1:C:634:GLN:CA	1:C:634:GLN:NE2	2.77	0.48
1:A:430:PRO:CD	5:A:8420:DMS:H21	2.43	0.48
1:C:431:ARG:HB3	6:C:9335:HOH:O	2.13	0.48
1:D:933:SER:O	1:D:934:GLU:C	2.56	0.48
1:D:948:PRO:CB	1:D:1022:GLN:NE2	2.77	0.48
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.49	0.48
1:B:899:GLY:HA2	1:B:915:PHE:CE1	2.49	0.48
1:C:102:ASN:C	1:C:102:ASN:ND2	2.65	0.48
1:C:320:GLY:HA2	5:C:8406:DMS:O	2.13	0.48
1:B:13:ARG:HH22	1:C:13:ARG:HB2	1.79	0.48
1:B:502:MET:HB2	1:B:537:GLU:HB2	1.96	0.48
1:C:71:GLU:HG2	6:C:9230:HOH:O	2.12	0.48
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.28	0.48
1:C:951:TRP:HA	1:C:1019:VAL:O	2.13	0.48
5:C:8408:DMS:H23	6:C:9206:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:788:PRO:HD2	1:D:968:MET:HG3	1.94	0.48
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.29	0.47
1:B:687:GLN:O	1:B:689:GLU:OE2	2.32	0.47
1:B:974:HIS:CD2	6:B:8610:HOH:O	2.61	0.47
5:B:8420:DMS:H23	6:C:9026:HOH:O	2.14	0.47
1:C:237:ARG:CB	1:C:237:ARG:NH1	2.77	0.47
1:A:767:GLN:HG3	1:A:768:MET:N	2.29	0.47
1:B:625:GLN:NE2	6:B:8717:HOH:O	2.42	0.47
1:C:43:ARG:HD2	1:C:261:TRP:CD2	2.49	0.47
1:C:651:LEU:C	1:C:651:LEU:CD1	2.87	0.47
1:C:663:LEU:HA	1:C:663:LEU:HD22	1.38	0.47
1:D:651:LEU:HD13	1:D:653:HIS:ND1	2.29	0.47
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.45	0.47
1:B:669:PRO:HB3	6:B:9280:HOH:O	2.14	0.47
1:B:741:THR:HB	1:B:748:CYS:HB3	1.97	0.47
1:A:654:TRP:CE3	1:A:665:SER:HA	2.49	0.47
1:B:735:HIS:O	1:B:736:ALA:HB3	2.15	0.47
1:B:801:ILE:HD12	1:B:808:GLU:OE2	2.14	0.47
1:C:851:ILE:HD11	1:D:728:VAL:HG12	1.96	0.47
5:C:8410:DMS:H21	6:C:8873:HOH:O	2.14	0.47
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.95	0.47
1:D:231:PHE:O	5:D:8417:DMS:H23	2.13	0.47
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.48	0.47
1:B:597:ASN:ND2	1:B:599:ARG:H	1.96	0.47
1:A:132:SER:HA	1:A:135:GLN:CG	2.44	0.47
1:A:667:GLU:C	1:A:668:VAL:HG23	2.39	0.47
1:A:778:THR:HG23	1:A:887:GLN:CB	2.37	0.47
1:A:799:THR:OG1	1:A:800:ARG:N	2.47	0.47
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.50	0.47
1:A:948:PRO:CB	1:A:1022:GLN:HE21	2.27	0.47
1:B:733:ALA:HB3	1:B:735:HIS:CE1	2.49	0.47
1:B:733:ALA:CB	1:B:735:HIS:CE1	2.98	0.47
1:D:659:ASP:O	6:D:9261:HOH:O	2.20	0.47
1:D:737:ILE:HD11	1:D:832:ASP:HA	1.97	0.47
1:A:60:PHE:HA	1:A:122:CYS:O	2.15	0.47
1:A:102:ASN:ND2	1:A:201:ASP:HB2	2.29	0.47
1:B:16:TRP:CG	1:B:189:LEU:CD1	2.97	0.47
1:B:655:MET:HE3	1:B:655:MET:HB2	1.79	0.47
1:C:693:GLN:HE22	1:C:724:GLU:HB2	1.79	0.47
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.97	0.47
1:C:581:ASN:OD1	1:C:581:ASN:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:ASN:HA	1:C:148:SER:HA	1.55	0.47
1:D:367:MET:HE1	1:D:371:THR:CG2	2.45	0.47
1:A:734:SER:OG	1:A:860:GLY:HA3	2.15	0.46
1:B:630:ARG:CZ	1:B:637:GLU:OE1	2.63	0.46
1:B:658:LEU:HD22	1:B:688:PRO:HB2	1.98	0.46
1:B:739:HIS:CD2	1:B:740:LEU:H	2.32	0.46
1:D:1022:GLN:NE2	1:D:1023:LYS:CB	2.78	0.46
1:B:249:GLU:HG2	1:B:251:ARG:HD3	1.96	0.46
1:B:942:ARG:HA	1:B:953:GLY:O	2.14	0.46
1:C:601:PHE:CD1	5:C:8506:DMS:H23	2.49	0.46
1:C:749:ILE:O	1:C:755:ARG:HA	2.15	0.46
1:D:131:GLU:HA	1:D:134:LEU:HD12	1.97	0.46
1:B:656:VAL:O	1:B:663:LEU:HB2	2.16	0.46
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.50	0.46
1:B:663:LEU:HD12	1:B:685:LEU:CD2	2.45	0.46
1:A:776:LEU:C	1:A:777:LEU:HD23	2.41	0.46
1:C:660:GLY:O	1:C:662:PRO:HD3	2.15	0.46
1:C:684:GLU:HG2	1:C:685:LEU:N	2.29	0.46
1:D:764:PHE:CE1	1:D:781:ARG:NH1	2.83	0.46
1:A:741:THR:HG22	6:A:9224:HOH:O	2.14	0.46
1:C:788:PRO:HD2	1:C:968:MET:HB2	1.97	0.46
1:C:817:GLN:HE21	1:C:817:GLN:HB3	1.46	0.46
1:A:804:ASN:HB3	6:A:8764:HOH:O	2.15	0.46
1:C:131:GLU:OE1	1:C:135:GLN:NE2	2.49	0.46
1:C:428:ASP:OD2	5:C:8420:DMS:H11	2.16	0.46
1:C:708:TRP:CZ2	5:C:8403:DMS:H13	2.49	0.46
1:A:62:TRP:CH2	1:A:64:PRO:HA	2.51	0.46
1:B:751:LEU:HD23	1:B:862:GLY:HA2	1.98	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.46
1:A:745:MET:HE3	6:A:9319:HOH:O	2.16	0.45
1:C:231:PHE:CD1	1:C:231:PHE:N	2.84	0.45
1:C:693:GLN:NE2	1:C:724:GLU:HB2	2.31	0.45
1:C:804:ASN:HB3	6:C:8686:HOH:O	2.16	0.45
1:D:910:LEU:HD12	1:D:910:LEU:C	2.41	0.45
1:B:131:GLU:HB2	1:B:179:ALA:HB2	1.99	0.45
1:D:102:ASN:C	1:D:102:ASN:ND2	2.74	0.45
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.98	0.45
1:C:637:GLU:OE2	1:C:677:LYS:NZ	2.43	0.45
1:D:730:LEU:H	1:D:730:LEU:HG	1.45	0.45
1:D:742:THR:CG2	1:D:743:SER:N	2.79	0.45
1:A:46:ARG:HH11	1:A:46:ARG:HD3	1.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:948:PRO:HB2	1:A:1022:GLN:HE21	1.81	0.45
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.75	0.45
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.31	0.45
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.43	0.45
1:A:655:MET:HE3	1:A:665:SER:HB3	1.99	0.45
1:C:768:MET:HE1	1:C:1020:TRP:CZ2	2.51	0.45
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.16	0.45
1:C:630:ARG:CB	1:C:630:ARG:NH1	2.80	0.45
1:C:533:LEU:C	1:C:533:LEU:HD23	2.42	0.45
1:C:753:ASN:OD1	1:C:753:ASN:N	2.50	0.45
1:D:699:ARG:HH12	5:D:8415:DMS:H11	1.81	0.45
1:A:85:VAL:CG1	1:A:86:VAL:N	2.79	0.45
1:C:688:PRO:HD3	1:C:694:LEU:HD11	1.99	0.45
1:C:749:ILE:N	1:C:749:ILE:CD1	2.79	0.45
1:A:127:PHE:HE2	1:A:184:LEU:HG	1.81	0.45
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.80	0.45
1:B:285:TYR:HB3	1:B:288:ARG:HG3	1.98	0.45
1:B:890:GLN:OE1	1:B:892:ALA:HB2	2.17	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.52	0.45
1:D:1017:GLN:HG2	1:D:1018:LEU:N	2.32	0.45
1:A:147:ASN:HA	1:A:148:SER:HA	1.61	0.45
1:A:292:ARG:NH1	5:A:8412:DMS:C2	2.80	0.45
1:B:354:VAL:HG11	1:B:379:MET:HE3	1.99	0.45
1:B:367:MET:HE2	1:B:367:MET:HA	1.99	0.45
1:B:832:ASP:N	1:B:832:ASP:OD1	2.50	0.45
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.99	0.45
1:A:85:VAL:HG12	1:A:86:VAL:N	2.30	0.44
1:A:127:PHE:CE2	1:A:184:LEU:HG	2.51	0.44
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.98	0.44
1:B:225:PHE:HA	1:B:243:GLU:O	2.17	0.44
1:B:888:LEU:O	1:B:981:GLY:HA3	2.17	0.44
1:C:433:LEU:N	1:C:434:PRO:CD	2.80	0.44
1:D:524:LEU:HD11	1:D:562:LEU:HG	1.99	0.44
1:A:135:GLN:HG2	1:A:135:GLN:H	1.29	0.44
1:A:763:GLY:HA3	1:A:822:LEU:HD13	1.98	0.44
5:A:8502:DMS:O	6:A:9101:HOH:O	2.20	0.44
1:B:754:LYS:HA	1:B:769:TRP:O	2.18	0.44
1:A:377:LEU:HD22	1:A:708:TRP:HA	2.00	0.44
1:A:631:LEU:HG	1:A:632:SER:N	2.32	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.69	0.44
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:737:ILE:HD12	1:C:738:PRO:N	2.32	0.44
1:D:76:CYS:O	6:D:9200:HOH:O	2.21	0.44
1:D:745:MET:HE2	1:D:745:MET:HB2	1.62	0.44
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.99	0.44
1:B:728:VAL:HG23	1:B:729:THR:N	2.31	0.44
1:B:1023:LYS:HB2	1:B:1023:LYS:HE3	1.47	0.44
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.18	0.44
1:C:234:ASP:O	1:C:235:PHE:HB2	2.18	0.44
1:C:1020:TRP:CD1	1:C:1020:TRP:C	2.96	0.44
1:A:264:GLU:HG3	6:A:9345:HOH:O	2.17	0.44
1:A:769:TRP:HA	1:A:773:LYS:O	2.18	0.44
1:B:13:ARG:CG	1:C:13:ARG:NH1	2.80	0.44
1:B:100:TYR:HB3	1:B:589:GLY:HA2	2.00	0.44
1:B:777:LEU:CD1	1:B:980:GLU:HB3	2.47	0.44
1:C:367:MET:HB3	1:C:372:MET:HE2	2.00	0.44
1:A:200:GLN:HG2	1:A:391:HIS:HB2	1.99	0.44
1:A:353:GLY:C	1:A:566:PHE:HA	2.43	0.44
1:A:685:LEU:HB3	1:A:686:PRO:HD2	1.99	0.44
1:C:630:ARG:HB3	1:C:630:ARG:NH1	2.27	0.44
1:C:685:LEU:HG	1:C:686:PRO:HD2	1.98	0.44
1:D:670:LEU:HA	1:D:670:LEU:HD23	1.69	0.44
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.44
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.32	0.44
1:A:654:TRP:O	1:A:665:SER:HB2	2.17	0.44
1:B:127:PHE:CD2	1:B:127:PHE:N	2.85	0.44
1:B:254:LEU:O	1:B:255:ARG:HD3	2.17	0.44
1:B:314:GLU:OE2	5:B:8406:DMS:H21	2.17	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.35	0.44
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.53	0.44
1:A:285:TYR:HB3	1:A:288:ARG:HG3	1.99	0.44
1:A:599:ARG:HB2	1:A:600:GLN:H	1.51	0.44
1:A:780:LEU:HA	1:A:886:CYS:HB3	1.99	0.44
1:D:457:SER:HA	1:D:485:GLN:O	2.18	0.44
1:D:740:LEU:HD12	1:D:741:THR:N	2.32	0.44
1:D:917:ARG:HH11	1:D:917:ARG:HD3	1.39	0.44
1:A:740:LEU:HD12	1:A:748:CYS:O	2.18	0.43
1:C:755:ARG:HG2	1:C:756:TRP:N	2.32	0.43
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.53	0.43
1:A:942:ARG:HA	1:A:953:GLY:O	2.18	0.43
1:B:368:ASP:HB2	1:B:370:GLN:NE2	2.22	0.43
1:B:600:GLN:H	1:B:600:GLN:NE2	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:986:ILE:HG21	1:C:986:ILE:HD13	1.53	0.43
1:A:16:TRP:CD2	1:A:189:LEU:HD13	2.53	0.43
1:A:292:ARG:HH11	5:A:8412:DMS:H23	1.84	0.43
1:B:59:ARG:HE	1:B:77:ASP:CG	2.26	0.43
1:B:68:ALA:O	1:B:70:PRO:HD3	2.18	0.43
1:B:652:LEU:HD22	1:B:680:ILE:HD12	2.00	0.43
1:B:730:LEU:O	1:B:731:PRO:O	2.34	0.43
1:B:890:GLN:HE21	1:B:890:GLN:HB2	1.18	0.43
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.99	0.43
1:C:773:LYS:CD	1:C:775:GLN:NE2	2.77	0.43
1:D:71:GLU:CD	1:D:71:GLU:N	2.70	0.43
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.78	0.43
1:B:770:ILE:CD1	1:B:1022:GLN:HG3	2.47	0.43
1:C:354:VAL:CG1	1:C:379:MET:HE3	2.48	0.43
1:D:240:LEU:HD23	1:D:240:LEU:C	2.43	0.43
1:D:765:LEU:CD2	1:D:768:MET:HE2	2.47	0.43
1:A:128:ASN:HA	1:A:180:GLY:O	2.19	0.43
1:B:250:LEU:O	1:B:251:ARG:HD3	2.18	0.43
1:B:370:GLN:CD	1:B:370:GLN:N	2.71	0.43
1:B:963:SER:HB3	1:B:983:TRP:CE2	2.52	0.43
1:D:30:HIS:HB2	1:D:31:PRO:HD2	1.99	0.43
1:D:145:GLY:N	1:D:210:ARG:HB2	2.33	0.43
1:D:473:ARG:HA	1:D:473:ARG:HD2	1.88	0.43
1:D:737:ILE:HD11	1:D:832:ASP:CA	2.48	0.43
1:D:759:ASN:OD1	1:D:761:GLN:HB3	2.17	0.43
1:C:887:GLN:NE2	1:C:980:GLU:O	2.51	0.43
1:A:986:ILE:HD12	1:A:986:ILE:HG21	1.70	0.43
1:B:595:THR:HG22	5:B:8413:DMS:S	2.58	0.43
1:A:111:PRO:HA	1:A:112:PRO:HA	1.69	0.43
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.68	0.43
1:B:751:LEU:HD23	1:B:862:GLY:CA	2.49	0.43
1:B:777:LEU:CG	1:B:889:ALA:HA	2.49	0.43
1:C:253:TYR:CD1	1:C:253:TYR:C	2.97	0.43
1:C:297:ASN:N	1:C:298:PRO:CD	2.82	0.43
1:D:60:PHE:HA	1:D:122:CYS:O	2.17	0.43
1:D:88:SER:HA	1:D:366:VAL:HG21	2.00	0.43
1:D:692:GLY:N	6:D:9430:HOH:O	2.50	0.43
1:A:817:GLN:O	1:A:818:ALA:C	2.59	0.43
1:B:13:ARG:HG2	1:C:13:ARG:CZ	2.49	0.43
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.00	0.43
1:A:630:ARG:HH11	1:A:630:ARG:HD2	1.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:HD2	1:B:181:GLU:O	2.19	0.43
1:B:251:ARG:NH1	1:B:251:ARG:CG	2.79	0.43
1:B:344:LEU:O	1:B:345:ASN:C	2.59	0.43
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.37	0.43
1:A:770:ILE:HD13	1:A:1022:GLN:HG3	2.01	0.42
1:B:576:ILE:HD12	1:B:576:ILE:HG23	1.67	0.42
1:B:770:ILE:CG2	1:B:1022:GLN:NE2	2.79	0.42
1:B:957:PHE:CD1	1:B:957:PHE:C	2.97	0.42
1:C:584:PRO:HG2	5:C:8411:DMS:H21	2.01	0.42
1:D:942:ARG:HA	1:D:953:GLY:O	2.18	0.42
1:A:254:LEU:HD23	1:A:254:LEU:HA	1.87	0.42
1:A:362:LEU:HD22	1:A:362:LEU:HA	1.81	0.42
1:B:661:LYS:HE3	1:B:661:LYS:HB2	1.57	0.42
1:B:685:LEU:CG	1:B:686:PRO:HD2	2.48	0.42
1:C:577:LYS:O	1:C:584:PRO:HA	2.19	0.42
1:D:829:THR:HG21	6:D:9526:HOH:O	2.19	0.42
1:A:73:TRP:CZ2	1:A:185:ALA:HB1	2.54	0.42
1:B:71:GLU:H	1:B:71:GLU:CD	2.26	0.42
1:B:653:HIS:HD2	1:B:667:GLU:HG2	1.83	0.42
1:D:92:MET:HE2	1:D:92:MET:CA	2.45	0.42
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.19	0.42
1:A:1004:SER:O	1:A:1005:ALA:C	2.61	0.42
1:B:54:LEU:HD11	1:B:214:LEU:HG	2.02	0.42
1:B:368:ASP:CG	1:B:370:GLN:NE2	2.77	0.42
1:B:599:ARG:HD2	1:B:600:GLN:NE2	2.34	0.42
1:B:730:LEU:H	1:B:731:PRO:HD3	1.84	0.42
1:B:890:GLN:O	1:B:890:GLN:HG3	2.12	0.42
1:C:597:ASN:HD22	1:C:599:ARG:N	1.97	0.42
1:C:601:PHE:CE2	5:C:8506:DMS:H23	2.55	0.42
1:C:686:PRO:O	1:C:687:GLN:C	2.63	0.42
1:C:808:GLU:OE1	1:C:808:GLU:HA	2.19	0.42
1:D:859:ASP:OD1	1:D:861:SER:N	2.46	0.42
1:D:906:TYR:CZ	1:D:937:LEU:HB2	2.55	0.42
1:A:126:THR:HA	1:A:182:ASN:O	2.19	0.42
1:A:183:ARG:HG2	1:A:183:ARG:HH11	1.85	0.42
1:B:770:ILE:HD12	1:B:1022:GLN:HE21	1.83	0.42
1:C:595:THR:HA	1:C:596:PRO:C	2.45	0.42
1:A:729:THR:HG23	6:A:9174:HOH:O	2.18	0.42
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.88	0.42
1:A:863:GLN:HE22	1:A:952:ARG:NH2	2.18	0.42
1:B:13:ARG:O	1:B:14:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:658:LEU:HD22	1:B:688:PRO:HB3	2.02	0.42
1:B:730:LEU:N	1:B:731:PRO:HD3	2.34	0.42
1:D:431:ARG:HB3	6:D:9558:HOH:O	2.19	0.42
1:C:634:GLN:HE21	1:C:634:GLN:CA	2.31	0.42
1:C:873:ALA:O	1:C:876:THR:HG22	2.20	0.42
1:D:333:ARG:HA	1:D:345:ASN:OD1	2.20	0.42
1:B:663:LEU:HD22	1:B:663:LEU:HA	1.70	0.42
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.68	0.42
1:D:830:LEU:CD1	1:D:835:LEU:HB2	2.48	0.42
1:A:906:TYR:CZ	1:A:937:LEU:HB2	2.55	0.42
1:A:956:GLN:CD	1:A:956:GLN:N	2.78	0.42
1:B:773:LYS:HA	1:B:773:LYS:HD3	1.74	0.42
1:C:43:ARG:HH22	1:C:264:GLU:CD	2.27	0.42
1:A:754:LYS:NZ	6:A:9351:HOH:O	2.28	0.42
1:A:1006:GLU:HG2	1:A:1007:PHE:CD1	2.55	0.42
1:C:814:GLY:O	1:C:815:HIS:C	2.61	0.42
5:D:8403:DMS:H21	6:D:9017:HOH:O	2.19	0.42
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.55	0.41
1:A:645:ARG:CZ	4:A:2002:IPT:H1'	2.50	0.41
1:A:773:LYS:HD3	1:A:773:LYS:N	2.35	0.41
1:B:687:GLN:CB	1:B:688:PRO:CD	2.94	0.41
1:C:63:PHE:HB3	1:C:64:PRO:HD2	2.01	0.41
1:C:143:PHE:O	1:C:168:PRO:HA	2.20	0.41
1:D:651:LEU:CD1	1:D:651:LEU:C	2.92	0.41
1:A:761:GLN:CD	1:A:762:SER:N	2.78	0.41
1:A:1013:ARG:NH1	6:A:9150:HOH:O	2.40	0.41
1:B:291:LEU:N	1:B:291:LEU:CD2	2.82	0.41
1:B:748:CYS:C	1:B:749:ILE:HD12	2.43	0.41
1:B:817:GLN:OE1	6:B:8928:HOH:O	2.21	0.41
1:C:782:ASP:HA	1:C:884:LEU:HD23	2.03	0.41
1:D:643:LEU:CD2	1:D:675:GLN:NE2	2.79	0.41
1:A:675:GLN:HG3	6:A:8862:HOH:O	2.20	0.41
1:A:785:THR:O	1:A:881:ARG:HD2	2.20	0.41
1:A:801:ILE:HD13	1:A:808:GLU:OE2	2.21	0.41
1:B:882:ILE:CD1	1:B:1014:TYR:CD1	3.03	0.41
1:C:100:TYR:O	1:C:597:ASN:HA	2.21	0.41
1:C:995:GLY:O	1:C:996:ASP:C	2.63	0.41
1:A:613:PRO:HB3	1:A:617:LEU:HD23	2.03	0.41
1:A:988:GLY:C	1:A:989:PHE:CD1	2.98	0.41
1:B:577:LYS:HB3	1:B:577:LYS:HE3	1.95	0.41
1:B:703:PRO:O	1:B:711:ALA:HB1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:8408:DMS:C2	6:C:9206:HOH:O	2.69	0.41
1:D:132:SER:HA	1:D:135:GLN:HG3	2.02	0.41
1:D:133:TRP:N	1:D:133:TRP:CD1	2.87	0.41
1:D:246:MET:SD	1:D:246:MET:C	3.03	0.41
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.56	0.41
1:C:36:TRP:CD2	1:C:42:ALA:HA	2.56	0.41
1:C:682:LEU:HD23	1:C:682:LEU:HA	1.91	0.41
1:D:130:ASP:OD1	1:D:132:SER:N	2.43	0.41
1:D:625:GLN:NE2	6:D:8936:HOH:O	2.47	0.41
1:D:908:ASP:HB3	1:D:1007:PHE:CD1	2.55	0.41
1:A:131:GLU:HG2	1:A:135:GLN:OE1	2.20	0.41
1:B:240:LEU:C	1:B:240:LEU:HD23	2.45	0.41
1:B:749:ILE:N	1:B:749:ILE:CD1	2.77	0.41
1:C:34:ALA:O	1:C:35:SER:C	2.61	0.41
1:C:264:GLU:OE2	1:C:264:GLU:HA	2.21	0.41
1:D:663:LEU:HD22	1:D:663:LEU:HA	1.77	0.41
1:D:824:GLN:HG2	1:D:825:CYS:N	2.33	0.41
1:B:105:TYR:CE2	1:B:199:ASP:HB2	2.56	0.41
1:C:379:MET:HE1	1:C:387:VAL:HB	2.03	0.41
1:C:637:GLU:CD	1:C:677:LYS:NZ	2.79	0.41
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.82	0.41
1:D:111:PRO:HA	1:D:112:PRO:HA	1.82	0.41
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.56	0.41
1:D:130:ASP:O	1:D:131:GLU:C	2.63	0.41
1:D:502:MET:HE1	6:D:9022:HOH:O	2.20	0.41
1:A:726:LEU:HD22	1:B:871:GLU:OE1	2.20	0.41
1:A:933:SER:O	1:A:934:GLU:C	2.63	0.41
1:B:241:GLU:CD	1:B:292:ARG:NE	2.76	0.41
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.95	0.41
1:B:301:TRP:CH2	1:B:452:SER:HA	2.56	0.41
1:B:636:ILE:HD13	1:B:698:VAL:HG11	2.03	0.41
1:C:250:LEU:C	1:C:251:ARG:HG2	2.45	0.41
1:C:910:LEU:HD12	1:C:910:LEU:C	2.46	0.41
1:D:127:PHE:CE2	1:D:184:LEU:HG	2.56	0.41
1:D:915:PHE:CD2	1:D:915:PHE:C	2.99	0.41
1:A:286:ALA:HB2	5:D:8704:DMS:H23	2.03	0.41
1:A:292:ARG:HH11	5:A:8412:DMS:C2	2.34	0.41
1:B:977:HIS:CD2	1:B:977:HIS:O	2.74	0.41
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.83	0.41
1:B:157:ARG:NH1	1:B:176:PHE:HA	2.36	0.40
1:D:576:ILE:HD12	1:D:576:ILE:HG23	1.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:844:HIS:N	1:D:847:LYS:O	2.47	0.40
1:A:250:LEU:HA	1:A:250:LEU:HD23	1.82	0.40
1:A:577:LYS:O	1:A:585:TRP:N	2.54	0.40
1:B:30:HIS:HB2	1:B:31:PRO:CD	2.52	0.40
1:B:598:ASP:O	1:B:599:ARG:C	2.63	0.40
1:B:802:ASP:OD1	1:B:802:ASP:C	2.62	0.40
1:C:688:PRO:HG2	1:C:725:ASN:ND2	2.37	0.40
1:D:241:GLU:CD	1:D:292:ARG:HE	2.29	0.40
1:D:646:HIS:CD2	1:D:673:ALA:HA	2.57	0.40
1:D:777:LEU:HD23	1:D:777:LEU:HA	1.83	0.40
1:A:317:THR:O	1:A:318:ALA:C	2.64	0.40
1:A:658:LEU:O	1:A:659:ASP:C	2.64	0.40
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.03	0.40
1:B:972:HIS:O	1:B:973:ARG:C	2.61	0.40
1:C:522:LYS:HD2	1:D:558:GLN:HG2	2.04	0.40
1:D:800:ARG:HH11	1:D:800:ARG:CG	2.31	0.40
1:A:821:ALA:N	1:A:841:ALA:O	2.53	0.40
1:B:638:VAL:O	1:B:677:LYS:HA	2.22	0.40
1:C:46:ARG:O	5:C:8501:DMS:H22	2.22	0.40
1:C:610:ASP:O	1:C:611:ARG:HB2	2.21	0.40
1:C:653:HIS:CE1	1:C:667:GLU:CD	3.00	0.40
1:B:13:ARG:CG	1:C:13:ARG:CZ	2.99	0.40
1:B:688:PRO:HG2	1:B:725:ASN:ND2	2.36	0.40
1:B:767:GLN:CG	1:B:768:MET:N	2.84	0.40
1:C:559:TYR:CE2	1:D:522:LYS:HA	2.57	0.40
1:D:577:LYS:O	1:D:584:PRO:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	48	32
1	B	1009/1023 (99%)	971 (96%)	33 (3%)	5 (0%)	24	11
1	C	1009/1023 (99%)	968 (96%)	38 (4%)	3 (0%)	36	21
1	D	1009/1023 (99%)	971 (96%)	37 (4%)	1 (0%)	48	32
All	All	4036/4092 (99%)	3881 (96%)	145 (4%)	10 (0%)	43	27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	686	PRO
1	B	687	GLN
1	B	731	PRO
1	C	687	GLN
1	B	732	ALA
1	B	736	ALA
1	C	690	SER
1	A	164	ASP
1	C	164	ASP
1	D	164	ASP

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%)	817 (95%)	47 (5%)	20	5
1	B	864/875 (99%)	813 (94%)	51 (6%)	18	4
1	C	864/875 (99%)	828 (96%)	36 (4%)	26	8
1	D	864/875 (99%)	830 (96%)	34 (4%)	28	9
All	All	3456/3500 (99%)	3288 (95%)	168 (5%)	22	6

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	SER

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	114	VAL
1	A	116	THR
1	A	117	GLU
1	A	131	GLU
1	A	135	GLN
1	A	178	ARG
1	A	182	ASN
1	A	183	ARG
1	A	249	GLU
1	A	251	ARG
1	A	267	VAL
1	A	299	LYS
1	A	344	LEU
1	A	362	LEU
1	A	370	GLN
1	A	519	SER
1	A	546	LEU
1	A	576	ILE
1	A	580	GLU
1	A	581	ASN
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	663	LEU
1	A	675	GLN
1	A	682	LEU
1	A	685	LEU
1	A	689	GLU
1	A	710	GLU
1	A	730	LEU
1	A	735	HIS
1	A	737	ILE
1	A	744	GLU
1	A	746	ASP
1	A	755	ARG
1	A	761	GLN
1	A	774	LYS
1	A	778	THR
1	A	817	GLN

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Mol	Chain	Res	Type
1	A	917	ARG
1	A	956	GLN
1	A	986	ILE
1	A	1023	LYS
1	B	13	ARG
1	B	71	GLU
1	B	72	SER
1	B	76	CYS
1	B	80	GLU
1	B	102	ASN
1	B	130	ASP
1	B	178	ARG
1	B	181	GLU
1	B	251	ARG
1	B	344	LEU
1	B	370	GLN
1	B	478	VAL
1	B	519	SER
1	B	546	LEU
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	655	MET
1	B	661	LYS
1	B	663	LEU
1	B	675	GLN
1	B	681	GLU
1	B	685	LEU
1	B	689	GLU
1	B	690	SER
1	B	694	LEU
1	B	729	THR
1	B	730	LEU
1	B	737	ILE
1	B	745	MET
1	B	750	GLU
1	B	753	ASN
1	B	761	GLN
1	B	770	ILE
1	B	773	LYS
1	B	774	LYS
1	B	799	THR

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Mol	Chain	Res	Type
1	B	800	ARG
1	B	817	GLN
1	B	819	GLU
1	B	824	GLN
1	B	847	LYS
1	B	861	SER
1	B	867	THR
1	B	890	GLN
1	B	893	GLU
1	B	917	ARG
1	B	934	GLU
1	B	1022	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	75	GLU
1	C	80	GLU
1	C	102	ASN
1	C	131	GLU
1	C	230	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	333	ARG
1	C	546	LEU
1	C	580	GLU
1	C	581	ASN
1	C	634	GLN
1	C	651	LEU
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	685	LEU
1	C	687	GLN
1	C	699	ARG
1	C	728	VAL
1	C	730	LEU
1	C	735	HIS
1	C	737	ILE
1	C	749	ILE
1	C	755	ARG
1	C	761	GLN
1	C	772	ASP

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Mol	Chain	Res	Type
1	C	773	LYS
1	C	801	ILE
1	C	817	GLN
1	C	847	LYS
1	C	890	GLN
1	C	1022	GLN
1	C	1023	LYS
1	D	13	ARG
1	D	71	GLU
1	D	75	GLU
1	D	80	GLU
1	D	129	VAL
1	D	135	GLN
1	D	157	ARG
1	D	183	ARG
1	D	217	LYS
1	D	344	LEU
1	D	370	GLN
1	D	431	ARG
1	D	546	LEU
1	D	554	GLN
1	D	581	ASN
1	D	661	LYS
1	D	663	LEU
1	D	672	VAL
1	D	681	GLU
1	D	690	SER
1	D	728	VAL
1	D	730	LEU
1	D	737	ILE
1	D	770	ILE
1	D	799	THR
1	D	800	ARG
1	D	817	GLN
1	D	819	GLU
1	D	824	GLN
1	D	845	GLN
1	D	885	ASN
1	D	917	ARG
1	D	986	ILE
1	D	1022	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	A	128	ASN
1	A	163	GLN
1	A	266	GLN
1	A	363	HIS
1	A	485	GLN
1	A	597	ASN
1	A	600	GLN
1	A	628	GLN
1	A	634	GLN
1	A	675	GLN
1	A	693	GLN
1	A	718	GLN
1	A	817	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1022	GLN
1	B	50	GLN
1	B	102	ASN
1	B	128	ASN
1	B	163	GLN
1	B	266	GLN
1	B	370	GLN
1	B	445	GLN
1	B	485	GLN
1	B	597	ASN
1	B	600	GLN
1	B	653	HIS
1	B	693	GLN
1	B	704	ASN
1	B	718	GLN
1	B	735	HIS
1	B	739	HIS
1	B	757	GLN
1	B	775	GLN
1	B	804	ASN
1	B	824	GLN
1	B	878	HIS
1	B	890	GLN
1	B	974	HIS
1	B	977	HIS
1	B	1022	GLN

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Mol	Chain	Res	Type
1	C	102	ASN
1	C	135	GLN
1	C	485	GLN
1	C	510	GLN
1	C	554	GLN
1	C	581	ASN
1	C	597	ASN
1	C	624	GLN
1	C	634	GLN
1	C	693	GLN
1	C	704	ASN
1	C	718	GLN
1	C	725	ASN
1	C	817	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	102	ASN
1	D	163	GLN
1	D	216	HIS
1	D	245	GLN
1	D	262	GLN
1	D	266	GLN
1	D	485	GLN
1	D	581	ASN
1	D	597	ASN
1	D	646	HIS
1	D	675	GLN
1	D	693	GLN
1	D	718	GLN
1	D	739	HIS
1	D	804	ASN
1	D	817	GLN
1	D	824	GLN
1	D	844	HIS
1	D	863	GLN
1	D	878	HIS
1	D	1022	GLN

5.3.3 RNA ⓘ

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 103 ligands modelled in this entry, 23 are monoatomic - leaving 80 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	B	8501	-	3,3,3	1.92	1 (33%)	3,3,3	0.45	0
5	DMS	B	8420	-	3,3,3	1.67	0	3,3,3	0.29	0
5	DMS	A	8410	-	3,3,3	1.05	0	3,3,3	0.92	0
4	IPT	C	2001	3	15,15,15	0.63	0	18,21,21	1.63	3 (16%)
5	DMS	B	8421	-	3,3,3	0.96	0	3,3,3	0.20	0
5	DMS	D	8417	-	3,3,3	1.29	1 (33%)	3,3,3	0.17	0
5	DMS	B	8404	-	3,3,3	0.30	0	3,3,3	1.03	0
4	IPT	B	2001	3	15,15,15	0.46	0	18,21,21	1.54	2 (11%)
5	DMS	B	8408	-	3,3,3	0.42	0	3,3,3	0.66	0
5	DMS	B	8407	-	3,3,3	2.09	2 (66%)	3,3,3	1.32	1 (33%)
5	DMS	A	8409	-	3,3,3	1.78	1 (33%)	3,3,3	0.32	0
5	DMS	C	8401	-	3,3,3	0.35	0	3,3,3	0.91	0
5	DMS	D	8410	-	3,3,3	1.65	1 (33%)	3,3,3	1.03	0
5	DMS	A	8407	-	3,3,3	1.44	1 (33%)	3,3,3	0.61	0
5	DMS	A	8602	-	3,3,3	0.94	0	3,3,3	0.29	0
4	IPT	D	2001	3	15,15,15	0.50	0	18,21,21	1.79	4 (22%)
5	DMS	C	8403	-	3,3,3	1.24	0	3,3,3	0.49	0
5	DMS	B	8412	-	3,3,3	0.51	0	3,3,3	0.12	0
5	DMS	A	8502	-	3,3,3	1.74	1 (33%)	3,3,3	1.10	0
5	DMS	A	8411	-	3,3,3	1.14	0	3,3,3	0.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8404	-	3,3,3	0.89	0	3,3,3	0.94	0
5	DMS	D	8402	-	3,3,3	0.62	0	3,3,3	0.43	0
5	DMS	D	8409	-	3,3,3	1.82	1 (33%)	3,3,3	1.19	0
5	DMS	B	8409	-	3,3,3	1.78	1 (33%)	3,3,3	0.86	0
5	DMS	C	8408	-	3,3,3	1.82	1 (33%)	3,3,3	0.75	0
5	DMS	C	8405	-	3,3,3	0.59	0	3,3,3	0.60	0
5	DMS	C	8501	-	3,3,3	0.81	0	3,3,3	0.34	0
5	DMS	A	8412	-	3,3,3	1.01	0	3,3,3	0.73	0
5	DMS	B	8406	-	3,3,3	1.67	1 (33%)	3,3,3	0.39	0
5	DMS	C	8402	-	3,3,3	1.45	1 (33%)	3,3,3	1.09	0
5	DMS	A	8403	-	3,3,3	1.61	1 (33%)	3,3,3	0.45	0
5	DMS	A	8413	-	3,3,3	1.35	0	3,3,3	0.35	0
5	DMS	C	8409	-	3,3,3	2.10	1 (33%)	3,3,3	0.56	0
5	DMS	D	8401	-	3,3,3	0.89	0	3,3,3	0.49	0
5	DMS	D	8405	-	3,3,3	0.41	0	3,3,3	0.28	0
5	DMS	A	8401	-	3,3,3	0.74	0	3,3,3	0.37	0
5	DMS	B	8425	3	3,3,3	0.66	0	3,3,3	0.23	0
5	DMS	D	8501	-	3,3,3	1.09	0	3,3,3	0.45	0
5	DMS	B	8410	-	3,3,3	1.22	0	3,3,3	0.22	0
5	DMS	C	8503	-	3,3,3	0.98	0	3,3,3	0.65	0
5	DMS	D	8413	-	3,3,3	1.48	0	3,3,3	0.51	0
5	DMS	C	8506	-	3,3,3	1.48	1 (33%)	3,3,3	0.29	0
4	IPT	A	2002	-	15,15,15	0.69	0	18,21,21	1.11	1 (5%)
5	DMS	A	8415	-	3,3,3	1.58	1 (33%)	3,3,3	0.51	0
5	DMS	B	8502	-	3,3,3	1.50	1 (33%)	3,3,3	0.49	0
5	DMS	B	8403	-	3,3,3	2.06	2 (66%)	3,3,3	0.19	0
5	DMS	C	8420	-	3,3,3	1.83	1 (33%)	3,3,3	0.56	0
5	DMS	D	8704	-	3,3,3	0.46	0	3,3,3	0.10	0
5	DMS	B	8405	-	3,3,3	1.16	0	3,3,3	0.82	0
5	DMS	C	8406	-	3,3,3	1.25	0	3,3,3	0.91	0
5	DMS	D	8404	-	3,3,3	1.68	1 (33%)	3,3,3	0.40	0
4	IPT	A	2001	3	15,15,15	0.48	0	18,21,21	1.30	2 (11%)
5	DMS	A	8501	-	3,3,3	1.10	0	3,3,3	0.43	0
5	DMS	C	8407	-	3,3,3	1.71	1 (33%)	3,3,3	0.77	0
5	DMS	A	8402	-	3,3,3	1.14	0	3,3,3	0.13	0
5	DMS	C	8414	-	3,3,3	0.29	0	3,3,3	0.31	0
5	DMS	C	8411	-	3,3,3	1.83	1 (33%)	3,3,3	0.61	0
5	DMS	D	8403	-	3,3,3	1.62	0	3,3,3	0.57	0
4	IPT	D	2002	-	15,15,15	0.53	0	18,21,21	1.64	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8411	-	3,3,3	0.73	0	3,3,3	0.33	0
5	DMS	A	8408	-	3,3,3	0.31	0	3,3,3	0.51	0
5	DMS	B	8402	-	3,3,3	1.10	0	3,3,3	0.26	0
5	DMS	C	8421	-	3,3,3	0.68	0	3,3,3	0.21	0
5	DMS	A	8420	-	3,3,3	0.96	0	3,3,3	0.38	0
5	DMS	D	8411	-	3,3,3	0.56	0	3,3,3	0.29	0
5	DMS	D	8408	-	3,3,3	0.95	0	3,3,3	0.46	0
5	DMS	D	8407	-	3,3,3	1.75	1 (33%)	3,3,3	0.97	0
5	DMS	D	8412	-	3,3,3	0.37	0	3,3,3	0.43	0
5	DMS	A	8405	-	3,3,3	0.15	0	3,3,3	0.63	0
5	DMS	B	8413	-	3,3,3	1.92	1 (33%)	3,3,3	0.08	0
5	DMS	C	8412	-	3,3,3	0.86	0	3,3,3	0.47	0
5	DMS	C	8422	-	3,3,3	1.24	0	3,3,3	0.33	0
5	DMS	C	8410	-	3,3,3	0.61	0	3,3,3	0.26	0
5	DMS	C	8415	-	3,3,3	1.46	1 (33%)	3,3,3	0.36	0
5	DMS	A	8421	-	3,3,3	0.70	0	3,3,3	0.17	0
5	DMS	D	8415	-	3,3,3	1.24	0	3,3,3	0.58	0
5	DMS	A	8404	-	3,3,3	1.27	1 (33%)	3,3,3	1.59	1 (33%)
5	DMS	D	8414	-	3,3,3	0.43	0	3,3,3	0.18	0
5	DMS	B	8401	-	3,3,3	0.23	0	3,3,3	0.67	0
5	DMS	C	8425	3	3,3,3	1.96	1 (33%)	3,3,3	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IPT	A	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	1/6/26/26	0/1/1/1
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	D	2002	-	-	0/6/26/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8413	DMS	O-S	3.32	1.72	1.50
5	C	8425	DMS	O-S	3.31	1.72	1.50
5	C	8409	DMS	O-S	3.16	1.71	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8409	DMS	O-S	3.07	1.70	1.50
5	B	8403	DMS	O-S	2.90	1.69	1.50
5	C	8420	DMS	C2-S	2.72	1.95	1.76
5	B	8407	DMS	O-S	2.69	1.68	1.50
5	A	8409	DMS	O-S	2.65	1.67	1.50
5	A	8502	DMS	C1-S	2.64	1.94	1.76
5	D	8410	DMS	O-S	2.63	1.67	1.50
5	B	8406	DMS	C2-S	2.58	1.94	1.76
5	B	8501	DMS	C1-S	2.56	1.94	1.76
5	A	8415	DMS	O-S	2.56	1.67	1.50
5	B	8409	DMS	O-S	2.53	1.66	1.50
5	B	8407	DMS	C2-S	2.42	1.93	1.76
5	C	8411	DMS	C1-S	2.38	1.93	1.76
5	C	8408	DMS	O-S	2.35	1.65	1.50
5	C	8506	DMS	O-S	2.29	1.65	1.50
5	C	8402	DMS	O-S	2.26	1.65	1.50
5	A	8407	DMS	O-S	2.19	1.64	1.50
5	A	8403	DMS	C1-S	-2.17	1.60	1.76
5	B	8502	DMS	C1-S	2.13	1.91	1.76
5	D	8404	DMS	O-S	-2.07	1.36	1.50
5	A	8404	DMS	C2-S	2.07	1.90	1.76
5	D	8417	DMS	O-S	2.07	1.63	1.50
5	B	8403	DMS	C2-S	2.06	1.90	1.76
5	C	8415	DMS	O-S	2.03	1.63	1.50
5	D	8407	DMS	C2-S	2.02	1.90	1.76
5	C	8407	DMS	O-S	2.00	1.63	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2001	IPT	C6-C5-C4	4.16	123.24	113.02
4	D	2002	IPT	C6-C5-C4	4.05	122.97	113.02
4	B	2001	IPT	C6-C5-C4	3.91	122.63	113.02
4	D	2002	IPT	O6-C6-C5	3.69	123.89	111.33
4	C	2001	IPT	O2-C2-C1	-3.60	103.90	110.30
4	D	2001	IPT	O5-C5-C6	-3.25	98.37	106.44
4	D	2001	IPT	O6-C6-C5	-3.16	100.59	111.33
4	D	2001	IPT	O2-C2-C1	-2.82	105.29	110.30
4	B	2001	IPT	O6-C6-C5	-2.74	101.99	111.33
4	C	2001	IPT	O5-C5-C6	-2.73	99.67	106.44
5	A	8404	DMS	C2-S-C1	2.71	112.30	98.42
4	A	2001	IPT	O2-C2-C3	-2.38	104.77	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	8407	DMS	C2-S-C1	2.28	110.10	98.42
4	D	2002	IPT	O5-C5-C6	-2.26	100.83	106.44
4	D	2002	IPT	C3'-C1'-C2'	-2.25	103.42	111.61
4	A	2001	IPT	C1-C2-C3	-2.21	106.22	110.55
4	C	2001	IPT	C6-C5-C4	2.09	118.15	113.02
4	A	2002	IPT	O3-C3-C2	2.08	115.28	110.38

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

33 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8420	DMS	1	0
5	A	8410	DMS	2	0
5	D	8417	DMS	2	0
5	B	8407	DMS	1	0
5	D	8410	DMS	1	0
5	A	8407	DMS	1	0
5	C	8403	DMS	1	0
5	A	8502	DMS	1	0
5	C	8408	DMS	2	0
5	C	8501	DMS	1	0
5	A	8412	DMS	3	0
5	B	8406	DMS	1	0
5	B	8410	DMS	1	0
5	C	8506	DMS	7	0
4	A	2002	IPT	1	0
5	A	8415	DMS	2	0
5	B	8403	DMS	1	0
5	C	8420	DMS	1	0
5	D	8704	DMS	1	0
5	C	8406	DMS	1	0
4	A	2001	IPT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8407	DMS	1	0
5	C	8411	DMS	2	0
5	D	8403	DMS	2	0
5	A	8408	DMS	1	0
5	C	8421	DMS	2	0
5	A	8420	DMS	4	0
5	D	8407	DMS	1	0
5	B	8413	DMS	2	0
5	C	8410	DMS	1	0
5	A	8421	DMS	1	0
5	D	8415	DMS	1	0
5	D	8414	DMS	2	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%)	-0.36	15 (1%) 72 78	11, 22, 50, 98	0
1	B	1011/1023 (98%)	-0.40	21 (2%) 63 70	11, 20, 51, 100	0
1	C	1011/1023 (98%)	-0.48	16 (1%) 70 77	11, 19, 50, 99	0
1	D	1011/1023 (98%)	-0.36	17 (1%) 69 75	12, 23, 52, 96	0
All	All	4044/4092 (98%)	-0.40	69 (1%) 69 75	11, 21, 51, 100	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	733	ALA	5.6
1	A	686	PRO	4.6
1	D	737	ILE	4.5
1	D	733	ALA	4.4
1	A	685	LEU	4.3
1	B	733	ALA	4.1
1	D	686	PRO	4.1
1	C	685	LEU	3.9
1	B	770	ILE	3.7
1	B	731	PRO	3.6
1	C	686	PRO	3.6
1	B	735	HIS	3.5
1	A	798	ALA	3.5
1	D	735	HIS	3.4
1	A	1023	LYS	3.3
1	A	735	HIS	3.3
1	B	732	ALA	3.3
1	D	799	THR	3.2
1	C	737	ILE	3.2
1	C	732	ALA	3.2
1	A	799	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	685	LEU	3.1
1	B	686	PRO	3.1
1	D	1022	GLN	3.0
1	B	1023	LYS	3.0
1	C	731	PRO	2.9
1	C	730	LEU	2.9
1	B	799	THR	2.9
1	A	732	ALA	2.8
1	B	663	LEU	2.8
1	A	733	ALA	2.8
1	A	730	LEU	2.8
1	A	771	GLY	2.8
1	B	688	PRO	2.7
1	C	1022	GLN	2.7
1	A	731	PRO	2.7
1	D	732	ALA	2.7
1	D	688	PRO	2.6
1	C	687	GLN	2.6
1	D	731	PRO	2.6
1	B	771	GLY	2.6
1	B	753	ASN	2.5
1	D	730	LEU	2.5
1	C	688	PRO	2.5
1	B	737	ILE	2.5
1	B	734	SER	2.5
1	C	735	HIS	2.4
1	D	977	HIS	2.4
1	B	745	MET	2.4
1	B	689	GLU	2.4
1	D	770	ILE	2.4
1	C	663	LEU	2.3
1	C	579	ASP	2.3
1	A	78	LEU	2.3
1	C	799	THR	2.2
1	C	734	SER	2.2
1	D	319	ASP	2.2
1	D	687	GLN	2.2
1	A	737	ILE	2.2
1	C	736	ALA	2.2
1	B	685	LEU	2.1
1	B	730	LEU	2.1
1	B	774	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	741	THR	2.1
1	B	683	PRO	2.1
1	A	689	GLU	2.0
1	A	687	GLN	2.0
1	B	736	ALA	2.0
1	D	773	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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($\text{\AA}^2$)	Q<0.9
5	DMS	A	8420	4/4	0.87	0.16	39,40,51,84	0
5	DMS	A	8421	4/4	0.88	0.09	43,59,69,79	0
5	DMS	C	8422	4/4	0.88	0.14	34,42,54,66	0
5	DMS	C	8421	4/4	0.89	0.15	48,57,64,83	0
5	DMS	D	8415	4/4	0.89	0.12	39,41,58,66	0
5	DMS	C	8503	4/4	0.90	0.12	35,41,54,64	0
5	DMS	C	8420	4/4	0.90	0.19	51,51,62,94	0
5	DMS	A	8602	4/4	0.91	0.13	42,52,61,79	0
5	DMS	B	8420	4/4	0.91	0.16	41,44,49,100	0
5	DMS	C	8415	4/4	0.91	0.13	29,55,67,77	0
5	DMS	C	8506	4/4	0.91	0.18	46,50,76,100	0
5	DMS	A	8502	4/4	0.91	0.12	40,41,45,54	0
5	DMS	D	8417	4/4	0.91	0.15	26,28,64,100	0
5	DMS	D	8410	4/4	0.92	0.10	25,39,50,55	0
5	DMS	D	8413	4/4	0.92	0.09	27,40,43,54	0
5	DMS	B	8413	4/4	0.92	0.13	38,54,55,100	0
5	DMS	A	8415	4/4	0.92	0.12	30,37,54,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8410	4/4	0.93	0.13	26,45,47,100	0
5	DMS	A	8409	4/4	0.93	0.13	36,38,45,46	0
5	DMS	B	8406	4/4	0.93	0.18	43,44,100,100	0
5	DMS	D	8704	4/4	0.93	0.17	32,55,100,100	0
5	DMS	B	8502	4/4	0.94	0.13	28,29,46,100	0
5	DMS	C	8410	4/4	0.94	0.10	29,36,44,45	0
5	DMS	D	8408	4/4	0.94	0.08	35,42,49,50	0
5	DMS	B	8425	4/4	0.94	0.13	43,54,64,100	0
5	DMS	B	8409	4/4	0.95	0.09	22,39,41,41	0
5	DMS	C	8404	4/4	0.95	0.08	26,29,35,40	0
5	DMS	D	8414	4/4	0.95	0.13	31,61,100,100	0
3	NA	B	3104	1/1	0.95	0.08	28,28,28,28	0
5	DMS	A	8408	4/4	0.95	0.10	35,47,48,100	0
5	DMS	A	8413	4/4	0.95	0.12	37,52,80,94	0
5	DMS	A	8407	4/4	0.96	0.09	32,34,38,40	0
5	DMS	C	8425	4/4	0.96	0.11	38,40,44,100	0
5	DMS	C	8501	4/4	0.96	0.09	21,42,47,48	0
5	DMS	B	8410	4/4	0.96	0.08	37,39,40,42	0
5	DMS	C	8406	4/4	0.96	0.10	22,46,49,55	0
5	DMS	C	8407	4/4	0.96	0.07	28,28,31,39	0
5	DMS	D	8409	4/4	0.96	0.08	34,34,35,42	0
3	NA	B	3103	1/1	0.96	0.08	35,35,35,35	0
5	DMS	C	8411	4/4	0.96	0.13	24,30,33,100	0
5	DMS	C	8414	4/4	0.96	0.10	27,46,60,76	0
5	DMS	A	8501	4/4	0.96	0.10	22,41,53,58	0
5	DMS	B	8421	4/4	0.96	0.07	28,38,52,53	0
5	DMS	B	8407	4/4	0.96	0.07	22,33,38,45	0
4	IPT	D	2002	15/15	0.97	0.08	19,26,33,100	0
3	NA	C	3104	1/1	0.97	0.07	31,31,31,31	0
5	DMS	C	8408	4/4	0.97	0.08	16,38,39,40	0
5	DMS	B	8408	4/4	0.97	0.09	40,41,54,100	0
3	NA	D	3103	1/1	0.97	0.07	34,34,34,34	0
5	DMS	B	8404	4/4	0.97	0.06	21,23,27,35	0
5	DMS	B	8411	4/4	0.97	0.11	34,38,49,100	0
5	DMS	D	8501	4/4	0.97	0.08	25,40,41,47	0
5	DMS	D	8407	4/4	0.97	0.06	26,31,33,40	0
4	IPT	D	2001	15/15	0.98	0.05	14,18,31,33	0
2	MG	D	3002	1/1	0.98	0.05	23,23,23,23	0
5	DMS	A	8403	4/4	0.98	0.05	20,24,25,28	0
5	DMS	A	8404	4/4	0.98	0.05	21,23,32,36	0
5	DMS	A	8405	4/4	0.98	0.07	26,28,31,34	0
4	IPT	A	2001	15/15	0.98	0.05	14,18,23,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	IPT	A	2002	15/15	0.98	0.06	13,21,26,28	15
5	DMS	B	8402	4/4	0.98	0.06	21,28,30,31	0
5	DMS	C	8402	4/4	0.98	0.06	21,25,27,28	0
5	DMS	D	8402	4/4	0.98	0.07	17,26,28,29	0
5	DMS	D	8403	4/4	0.98	0.08	28,28,31,38	0
5	DMS	D	8404	4/4	0.98	0.06	18,27,31,34	0
5	DMS	C	8403	4/4	0.98	0.06	21,23,29,30	0
5	DMS	B	8403	4/4	0.98	0.07	26,28,30,42	0
5	DMS	C	8405	4/4	0.98	0.05	23,25,26,29	0
4	IPT	B	2001	15/15	0.98	0.05	10,18,24,25	0
5	DMS	B	8405	4/4	0.98	0.05	23,25,28,31	0
4	IPT	C	2001	15/15	0.98	0.05	15,17,26,26	0
5	DMS	C	8409	4/4	0.98	0.07	24,37,39,57	0
5	DMS	A	8411	4/4	0.98	0.09	28,32,36,100	0
5	DMS	A	8412	4/4	0.98	0.08	29,34,41,100	0
5	DMS	C	8412	4/4	0.98	0.06	24,31,39,43	0
3	NA	A	3101	1/1	0.99	0.04	18,18,18,18	0
3	NA	A	3102	1/1	0.99	0.02	16,16,16,16	0
5	DMS	B	8501	4/4	0.99	0.05	18,19,25,25	0
3	NA	A	3103	1/1	0.99	0.04	29,29,29,29	0
5	DMS	C	8401	4/4	0.99	0.03	16,18,22,22	0
5	DMS	A	8402	4/4	0.99	0.06	18,23,24,28	0
5	DMS	D	8401	4/4	0.99	0.05	17,19,21,22	0
3	NA	B	3102	1/1	0.99	0.02	16,16,16,16	0
2	MG	A	3002	1/1	0.99	0.04	21,21,21,21	0
2	MG	B	3001	1/1	0.99	0.02	18,18,18,18	0
5	DMS	D	8405	4/4	0.99	0.06	23,23,26,27	0
3	NA	C	3102	1/1	0.99	0.03	16,16,16,16	0
3	NA	C	3103	1/1	0.99	0.05	30,30,30,30	0
2	MG	B	3002	1/1	0.99	0.07	22,22,22,22	0
3	NA	D	3101	1/1	0.99	0.02	20,20,20,20	0
5	DMS	D	8411	4/4	0.99	0.06	25,28,37,48	0
5	DMS	D	8412	4/4	0.99	0.05	23,26,32,39	0
3	NA	D	3102	1/1	0.99	0.03	16,16,16,16	0
2	MG	B	3007	1/1	0.99	0.07	24,24,24,24	0
2	MG	C	3001	1/1	0.99	0.02	17,17,17,17	0
5	DMS	B	8412	4/4	0.99	0.05	22,29,30,34	0
2	MG	C	3002	1/1	0.99	0.07	17,17,17,17	0
2	MG	A	3001	1/1	0.99	0.02	18,18,18,18	0
2	MG	D	3001	1/1	1.00	0.02	17,17,17,17	0
3	NA	C	3101	1/1	1.00	0.02	17,17,17,17	0
5	DMS	A	8401	4/4	1.00	0.03	16,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	B	3101	1/1	1.00	0.03	17,17,17,17	0
5	DMS	B	8401	4/4	1.00	0.03	15,16,16,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.