



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:52 AM UTC

PDB ID : 1JZ4 / pdb_00001jz4
Title : E. COLI (lacZ) BETA-GALACTOSIDASE-TRAPPED 2-DEOXY-GALACTOSYL-ENZYME INTERMEDIATE (Low Bis-Tris)
Authors : Juers, D.H.; Matthews, B.W.
Deposited on : 2001-09-13
Resolution : 2.10 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

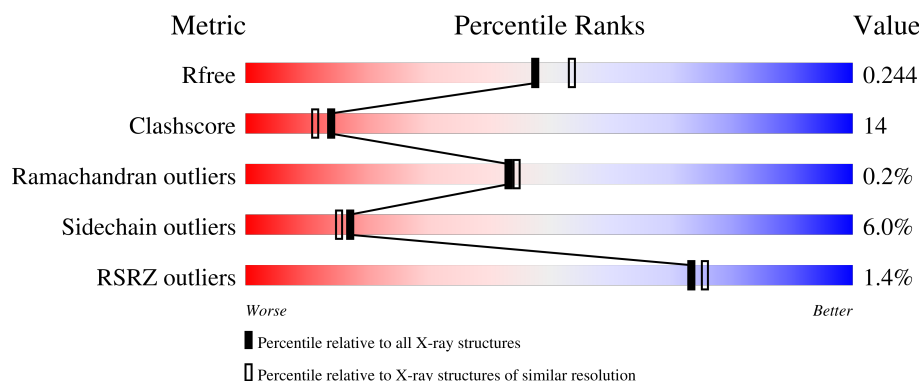
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	2% 65% 27% 6% ..
1	B	1023	2% 61% 30% 6% ..
1	C	1023	2% 59% 32% 7% ..
1	D	1023	2% 63% 28% 7% ..

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	8406	-	-	X	-
5	DMS	B	8504	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	B	8508	-	X	-	-
5	DMS	C	8427	-	-	X	-
5	DMS	C	8503	-	-	X	-
5	DMS	C	8506	-	-	X	-
5	DMS	D	8412	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36890 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:

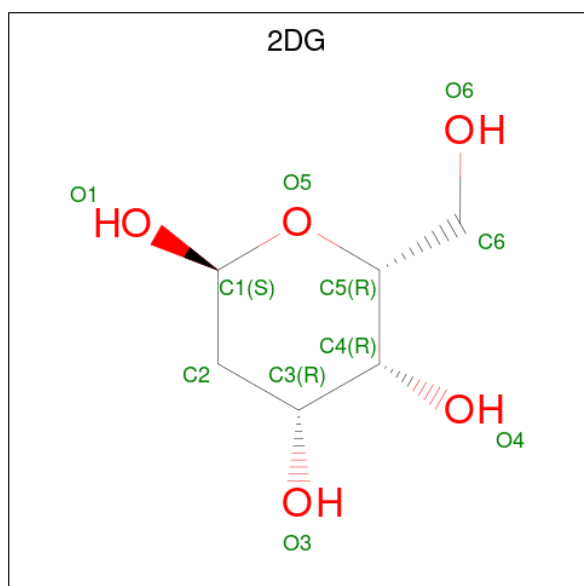
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? 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 2-deoxy-alpha-D-galactopyranose (CCD ID: 2DG) (formula: $C_6H_{12}O_5$).



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

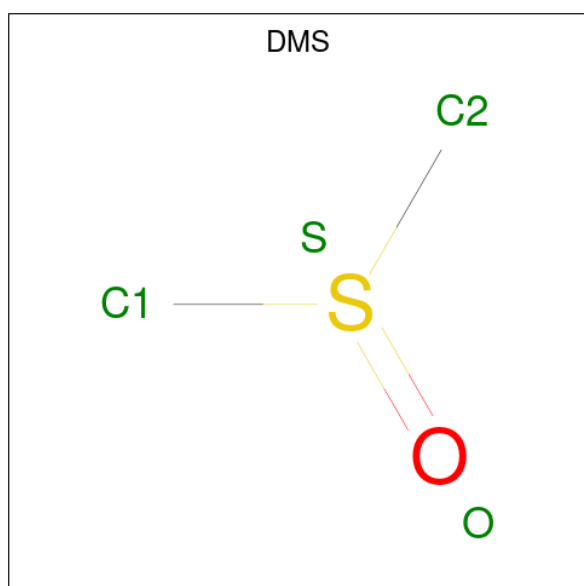
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	992	Total 992	O 992	0	0
6	B	995	Total 995	O 995	0	0

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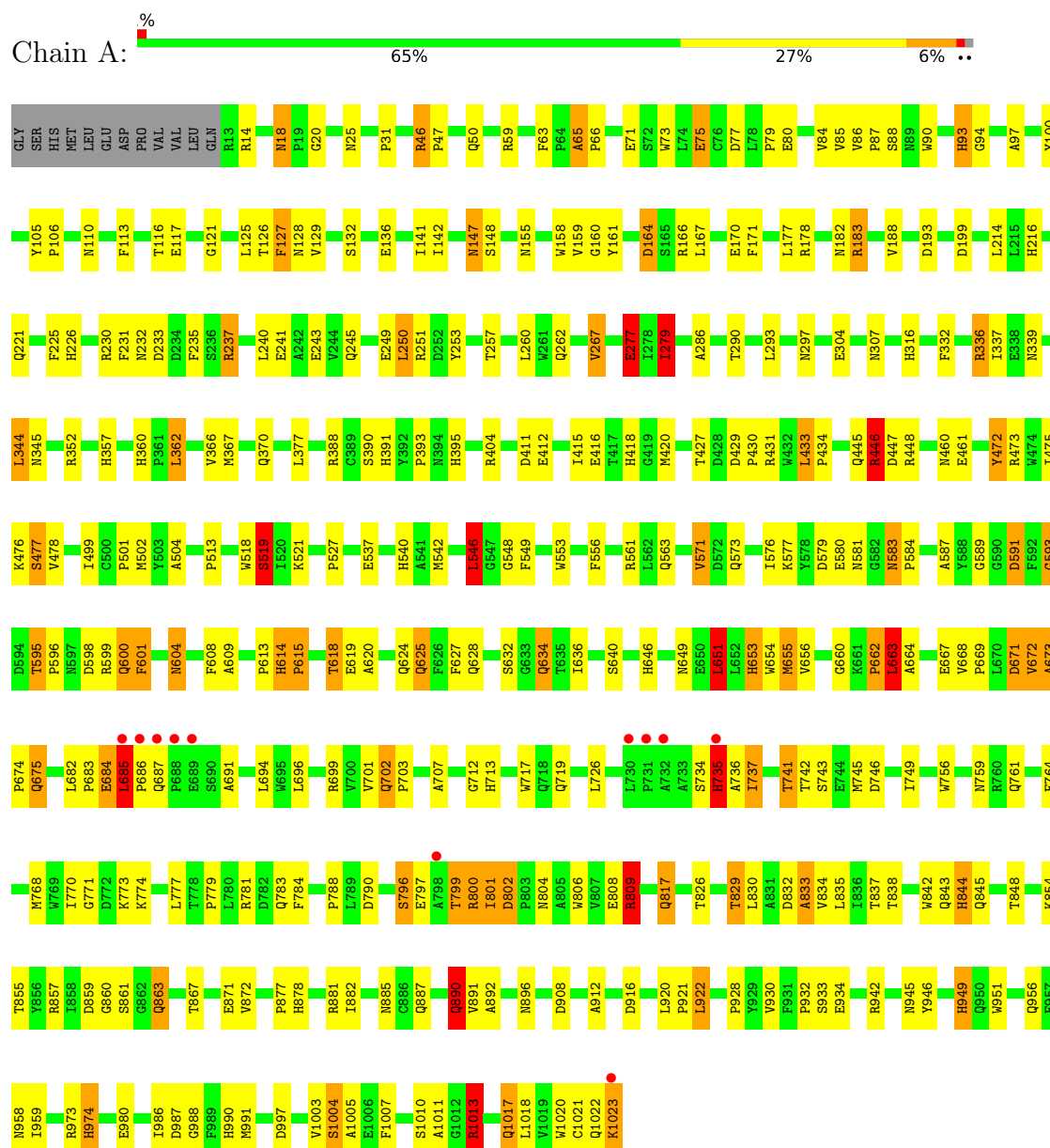
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	946	Total 946	O 946	0	0
6	D	980	Total 980	O 980	0	0

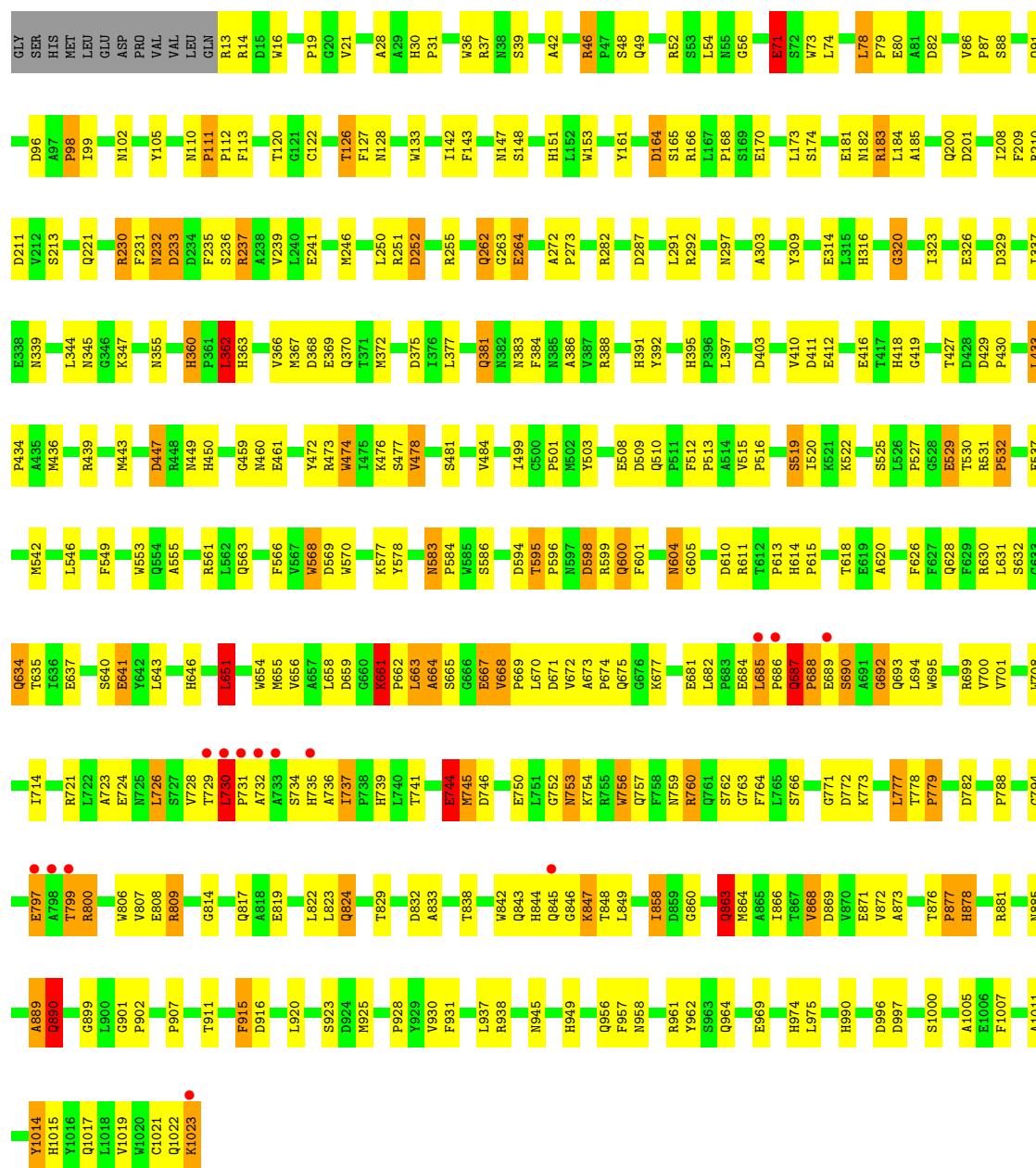
3 Residue-property plots

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.

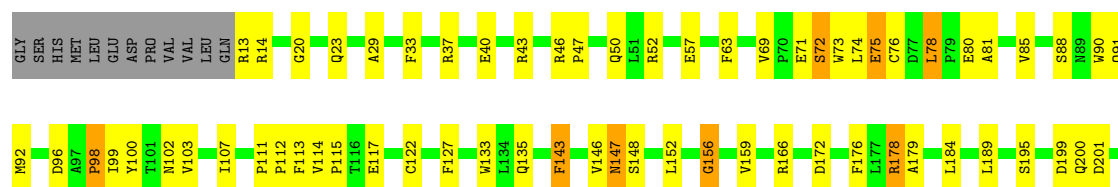
• Molecule 1: Beta-Galactosidase

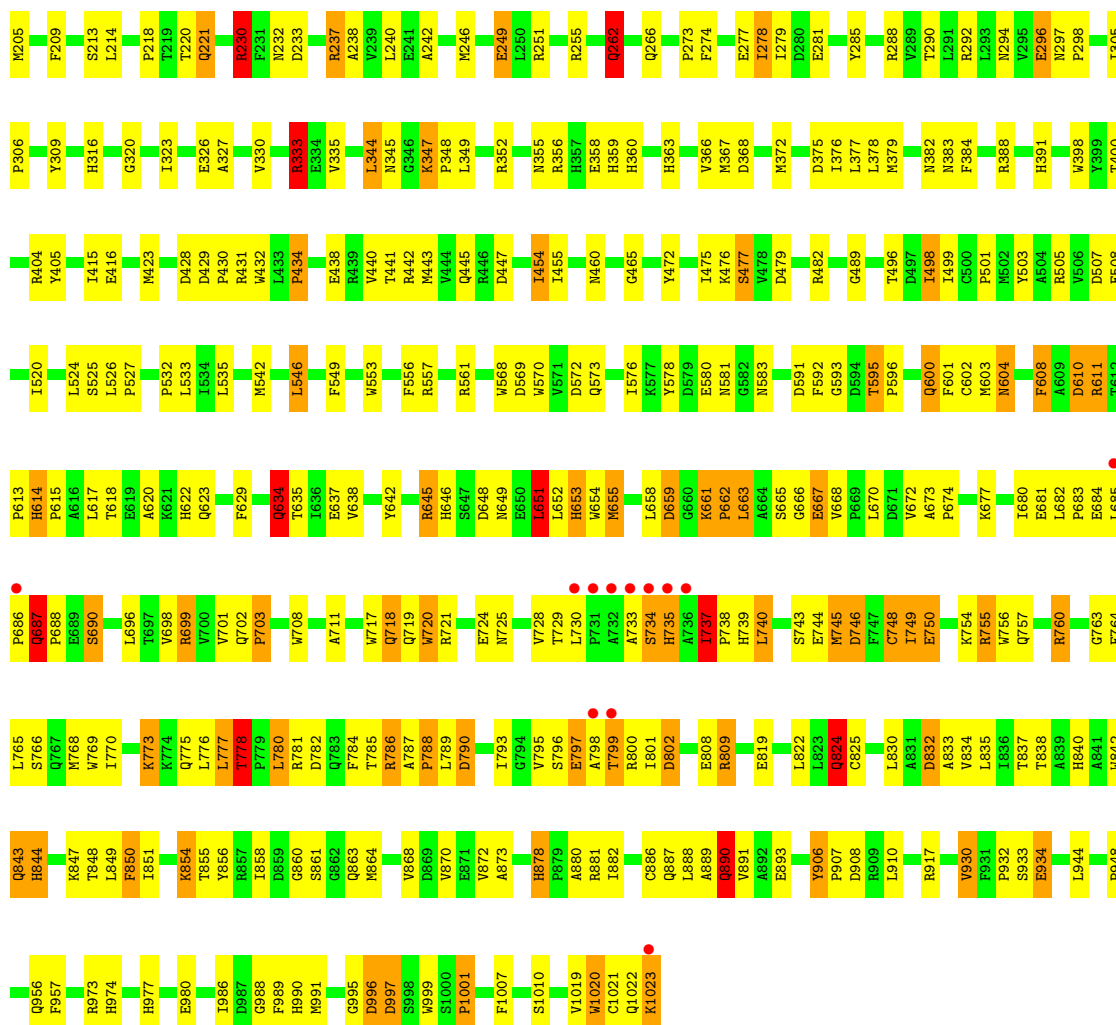


• Molecule 1: Beta-Galactosidase

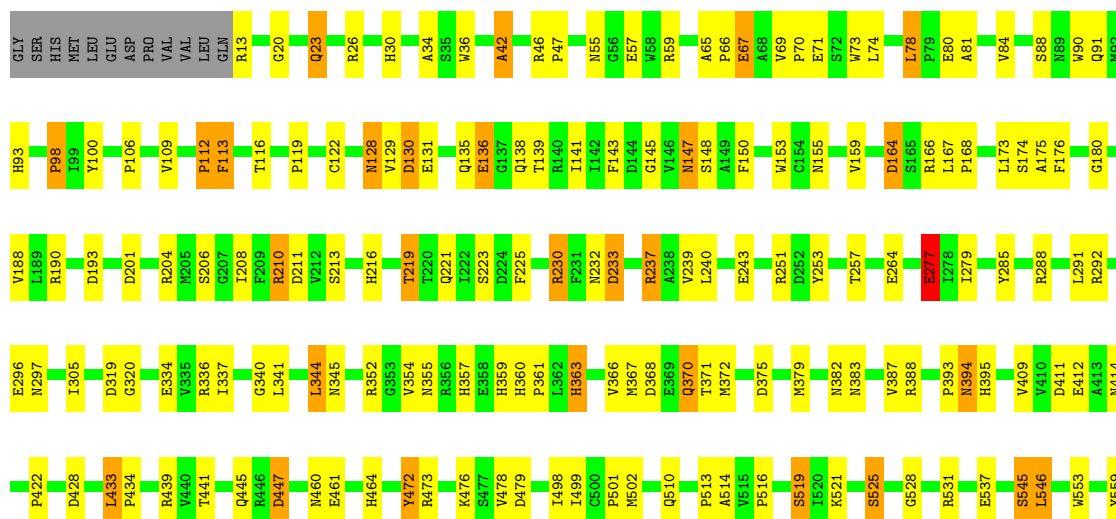


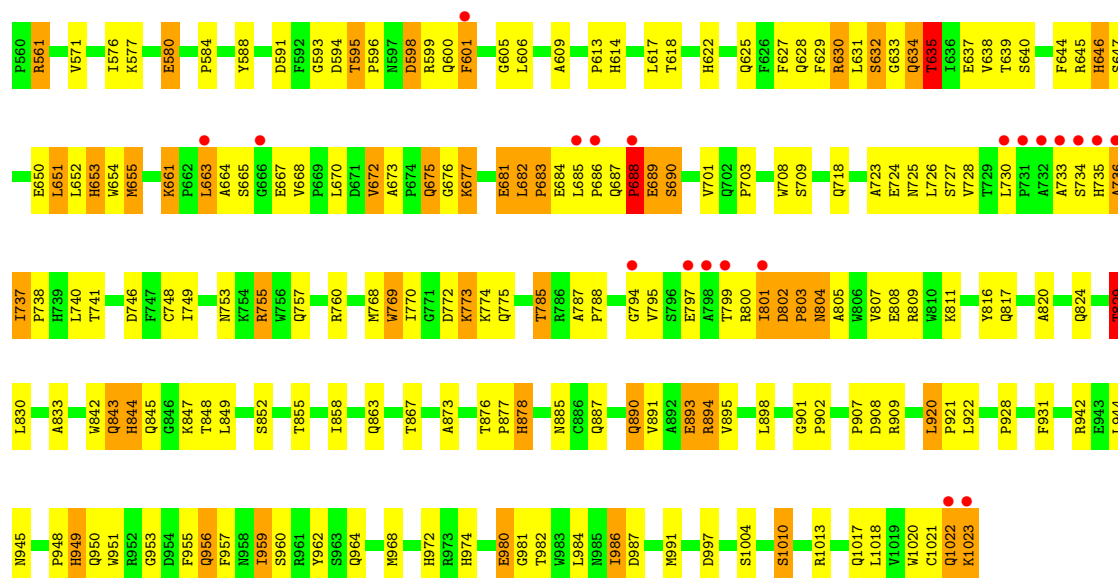
• Molecule 1: Beta-Galactosidase





● 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	149.50Å 169.00Å 200.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 40.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.0 (40.00-2.10) 86.3 (40.00-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.164 , 0.267 0.152 , 0.244	Depositor DCC
R_{free} test set	3827 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 101.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36890	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.06 % 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 5.3009e-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, 2DG, MG, 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	1.31	6/8367 (0.1%)	1.95	176/11415 (1.5%)
1	B	1.32	9/8367 (0.1%)	1.92	191/11415 (1.7%)
1	C	1.31	10/8367 (0.1%)	1.97	223/11415 (2.0%)
1	D	1.34	14/8367 (0.2%)	1.94	190/11415 (1.7%)
All	All	1.32	39/33468 (0.1%)	1.95	780/45660 (1.7%)

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	0	1
1	D	1	0
All	All	1	1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	297	ASN	C-O	-10.80	1.18	1.23
1	D	479	ASP	C-N	-8.38	1.25	1.34
1	C	297	ASN	C-O	-7.07	1.20	1.23
1	D	30	HIS	CE1-NE2	6.56	1.39	1.32
1	D	635	THR	CA-C	-6.34	1.45	1.52
1	D	277	GLU	CD-OE2	6.19	1.37	1.25
1	C	281	GLU	CD-OE2	6.03	1.36	1.25
1	D	71	GLU	CD-OE2	6.03	1.36	1.25
1	B	800	ARG	C-O	5.96	1.30	1.23
1	B	561	ARG	NE-CZ	5.92	1.39	1.33
1	B	120	THR	C-N	5.90	1.36	1.33
1	C	684	GLU	CD-OE2	5.88	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	442	ARG	CZ-NH1	5.88	1.41	1.32
1	C	296	GLU	CD-OE2	5.87	1.36	1.25
1	D	357	HIS	ND1-CE1	5.81	1.38	1.32
1	A	304	GLU	CD-OE2	5.68	1.36	1.25
1	A	896	ASN	N-CA	-5.67	1.39	1.46
1	A	136	GLU	CD-OE2	5.57	1.35	1.25
1	C	1020	TRP	CA-C	-5.54	1.46	1.52
1	B	778	THR	C-O	-5.53	1.18	1.24
1	D	359	HIS	CE1-NE2	5.51	1.38	1.32
1	D	690	SER	CA-C	-5.50	1.45	1.52
1	B	418	HIS	CE1-NE2	5.41	1.38	1.32
1	D	498	ILE	C-O	5.41	1.29	1.24
1	B	920	LEU	CA-CB	5.35	1.60	1.54
1	B	461	GLU	CD-OE2	5.32	1.35	1.25
1	A	93	HIS	ND1-CE1	5.32	1.37	1.32
1	D	243	GLU	CD-OE2	5.21	1.35	1.25
1	C	479	ASP	C-N	-5.21	1.29	1.33
1	D	297	ASN	CA-C	-5.17	1.49	1.53
1	A	18	ASN	C-N	-5.16	1.28	1.34
1	B	403	ASP	CG-OD2	5.14	1.35	1.25
1	C	591	ASP	CG-OD2	5.13	1.35	1.25
1	A	337	ILE	CA-CB	-5.13	1.48	1.54
1	C	856	TYR	CA-C	-5.11	1.46	1.52
1	D	211	ASP	CG-OD2	5.11	1.35	1.25
1	D	136	GLU	CD-OE2	5.08	1.34	1.25
1	C	23	GLN	CA-C	-5.02	1.46	1.52
1	B	997	ASP	CG-OD2	5.00	1.34	1.25

All (780) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	601	PHE	CA-CB-CG	-14.07	99.73	113.80
1	C	297	ASN	CB-CA-C	-12.60	102.25	111.20
1	C	113	PHE	CA-CB-CG	-12.43	101.37	113.80
1	C	294	ASN	CA-CB-CG	-11.94	100.66	112.60
1	A	601	PHE	CA-CB-CG	-10.97	102.83	113.80
1	B	753	ASN	CA-CB-CG	-10.71	101.89	112.60
1	D	829	THR	N-CA-CB	10.07	127.08	110.17
1	D	878	HIS	CA-CB-CG	-9.91	103.89	113.80
1	D	382	ASN	CA-CB-CG	-9.88	102.72	112.60
1	D	320	GLY	CA-C-N	-9.63	108.61	122.19
1	D	320	GLY	C-N-CA	-9.63	108.61	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	844	HIS	CA-CB-CG	-9.62	104.18	113.80
1	A	235	PHE	CA-CB-CG	-9.61	104.19	113.80
1	D	689	GLU	N-CA-CB	9.58	125.21	110.46
1	B	737	ILE	CB-CA-C	9.49	121.05	110.52
1	A	297	ASN	O-C-N	-9.44	117.19	121.53
1	C	878	HIS	CA-CB-CG	-9.39	104.41	113.80
1	A	571	VAL	N-CA-C	9.34	121.19	108.11
1	C	685	LEU	CA-C-N	9.16	128.92	119.76
1	C	685	LEU	C-N-CA	9.16	128.92	119.76
1	C	601	PHE	CA-CB-CG	-9.04	104.75	113.80
1	B	661	LYS	CA-C-N	8.88	129.43	119.93
1	B	661	LYS	C-N-CA	8.88	129.43	119.93
1	B	363	HIS	CA-CB-CG	-8.86	104.94	113.80
1	D	297	ASN	O-C-N	-8.79	117.49	121.53
1	C	809	ARG	NE-CZ-NH1	8.66	130.16	121.50
1	C	778	THR	CA-C-N	8.61	128.67	119.89
1	C	778	THR	C-N-CA	8.61	128.67	119.89
1	D	297	ASN	CB-CA-C	-8.61	105.09	111.20
1	D	844	HIS	CA-CB-CG	-8.57	105.22	113.80
1	C	85	VAL	CA-CB-CG2	-8.54	95.88	110.40
1	D	69	VAL	CA-C-N	8.49	128.82	119.90
1	D	69	VAL	C-N-CA	8.49	128.82	119.90
1	C	553	TRP	CA-CB-CG	-8.47	97.50	113.60
1	C	442	ARG	NE-CZ-NH2	-8.37	111.67	119.20
1	B	832	ASP	N-CA-CB	-8.30	97.71	111.49
1	A	974	HIS	CA-CB-CG	-8.29	105.51	113.80
1	D	997	ASP	N-CA-CB	8.25	124.59	111.56
1	B	297	ASN	CB-CA-C	-8.23	102.97	110.71
1	C	465	GLY	O-C-N	-8.16	116.19	123.29
1	C	855	THR	N-CA-CB	8.14	125.74	111.00
1	A	997	ASP	CA-CB-CG	-8.12	104.48	112.60
1	C	614	HIS	N-CA-C	-8.12	99.48	110.36
1	D	113	PHE	CA-CB-CG	-8.08	105.72	113.80
1	B	777	LEU	N-CA-C	-8.07	103.95	113.88
1	A	777	LEU	N-CA-C	-8.06	103.04	113.12
1	C	297	ASN	O-C-N	-8.04	117.83	121.53
1	B	447	ASP	N-CA-C	8.03	123.26	113.38
1	B	233	ASP	N-CA-C	8.03	120.03	111.28
1	B	360	HIS	CA-CB-CG	-7.98	105.82	113.80
1	B	433	LEU	CA-C-O	7.84	126.41	118.73
1	D	746	ASP	N-CA-C	7.84	121.30	108.99
1	A	746	ASP	CA-CB-CG	-7.74	104.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	410	VAL	N-CA-CB	7.71	121.05	111.41
1	C	306	PRO	N-CA-CB	7.69	107.63	102.25
1	A	770	ILE	N-CA-CB	7.68	121.58	111.90
1	B	759	ASN	CA-CB-CG	-7.68	104.92	112.60
1	C	988	GLY	N-CA-C	-7.67	102.94	112.77
1	A	553	TRP	CA-CB-CG	-7.65	99.07	113.60
1	D	982	THR	N-CA-C	7.64	121.36	108.90
1	A	297	ASN	CB-CA-C	-7.61	105.80	111.20
1	D	433	LEU	CA-C-O	7.58	125.61	118.63
1	A	472	TYR	CA-C-O	7.58	128.77	120.82
1	A	685	LEU	CA-C-N	-7.57	113.03	120.52
1	A	685	LEU	C-N-CA	-7.57	113.03	120.52
1	A	859	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	760	ARG	N-CA-C	7.53	121.73	112.54
1	A	604	ASN	CA-CB-CG	7.51	120.11	112.60
1	A	790	ASP	CA-CB-CG	-7.47	105.13	112.60
1	A	420	MET	CA-C-N	-7.47	116.35	122.85
1	A	420	MET	C-N-CA	-7.47	116.35	122.85
1	B	632	SER	N-CA-CB	7.46	122.12	110.71
1	A	771	GLY	N-CA-C	-7.45	97.14	110.86
1	D	297	ASN	CA-C-N	-7.45	112.65	120.03
1	D	297	ASN	C-N-CA	-7.45	112.65	120.03
1	D	606	LEU	N-CA-C	-7.41	103.71	112.89
1	C	441	THR	CA-CB-OG1	-7.39	98.51	109.60
1	D	646	HIS	CA-CB-CG	-7.30	106.50	113.80
1	D	802	ASP	C-N-CD	-7.28	95.17	125.00
1	C	997	ASP	N-CA-CB	7.27	123.05	111.56
1	A	636	ILE	N-CA-CB	7.26	119.71	111.21
1	A	817	GLN	CB-CG-CD	-7.26	100.25	112.60
1	C	384	PHE	CA-CB-CG	-7.25	106.55	113.80
1	B	931	PHE	CA-CB-CG	-7.23	106.57	113.80
1	A	166	ARG	N-CA-C	7.22	122.19	112.88
1	B	474	TRP	CA-C-O	7.22	128.62	120.90
1	C	989	PHE	CA-CB-CG	-7.22	106.58	113.80
1	D	447	ASP	N-CA-C	7.21	122.08	113.28
1	B	878	HIS	CA-CB-CG	-7.21	106.59	113.80
1	B	82	ASP	CA-CB-CG	-7.16	105.44	112.60
1	D	877	PRO	CB-CA-C	-7.15	102.56	111.64
1	A	949	HIS	CA-CB-CG	-7.14	106.66	113.80
1	D	363	HIS	CA-CB-CG	-7.14	106.66	113.80
1	C	611	ARG	CB-CA-C	7.13	116.89	109.83
1	A	241	GLU	CA-C-N	-7.13	112.95	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	241	GLU	C-N-CA	-7.13	112.95	123.00
1	A	221	GLN	N-CA-CB	-7.09	100.36	111.56
1	C	610	ASP	CA-C-N	-7.08	115.74	126.86
1	C	610	ASP	C-N-CA	-7.08	115.74	126.86
1	C	685	LEU	CB-CA-C	7.08	118.29	110.15
1	D	394	ASN	N-CA-CB	-7.05	99.71	110.42
1	C	294	ASN	CA-C-N	-7.01	113.02	122.98
1	C	294	ASN	C-N-CA	-7.01	113.02	122.98
1	A	598	ASP	CA-CB-CG	-7.01	105.59	112.60
1	D	571	VAL	N-CA-C	6.99	118.88	108.46
1	C	748	CYS	CA-CB-SG	-6.98	98.34	114.40
1	C	854	LYS	N-CA-C	6.98	119.78	109.24
1	B	46	ARG	CD-NE-CZ	-6.98	114.63	124.40
1	D	553	TRP	CA-CB-CG	-6.98	100.34	113.60
1	A	809	ARG	N-CA-CB	-6.96	99.89	110.12
1	A	127	PHE	CA-CB-CG	-6.94	106.86	113.80
1	C	739	HIS	CA-CB-CG	-6.94	106.86	113.80
1	C	893	GLU	N-CA-C	6.91	120.19	111.69
1	B	598	ASP	CA-CB-CG	-6.88	105.72	112.60
1	A	932	PRO	CB-CA-C	-6.84	102.64	111.46
1	B	788	PRO	N-CA-CB	6.82	109.25	103.25
1	C	159	VAL	CB-CA-C	-6.81	105.92	111.71
1	B	611	ARG	N-CA-CB	6.81	120.91	114.10
1	A	395	HIS	N-CA-C	-6.80	101.01	109.64
1	C	279	ILE	N-CA-C	-6.79	106.40	111.90
1	D	164	ASP	CA-CB-CG	-6.78	105.82	112.60
1	B	553	TRP	CA-CB-CG	-6.78	100.73	113.60
1	A	63	PHE	CA-CB-CG	-6.77	107.03	113.80
1	B	211	ASP	N-CA-C	6.77	119.04	110.24
1	C	147	ASN	N-CA-CB	-6.76	99.94	110.55
1	C	690	SER	N-CA-C	6.76	117.19	108.34
1	A	433	LEU	CA-C-O	6.74	125.33	118.73
1	C	890	GLN	N-CA-CB	-6.73	99.44	110.41
1	C	703	PRO	N-CA-CB	6.71	110.64	103.52
1	D	614	HIS	N-CA-C	-6.71	100.27	110.07
1	B	166	ARG	N-CA-C	6.71	122.29	113.30
1	B	221	GLN	N-CA-CB	-6.70	100.98	111.56
1	C	782	ASP	CA-CB-CG	-6.70	105.90	112.60
1	B	113	PHE	N-CA-C	6.70	119.59	110.55
1	B	484	VAL	CA-C-N	-6.70	112.08	122.59
1	B	484	VAL	C-N-CA	-6.70	112.08	122.59
1	B	252	ASP	N-CA-C	6.67	120.52	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	614	HIS	N-CA-CB	6.66	118.21	109.55
1	A	519	SER	N-CA-C	-6.66	100.85	110.24
1	D	297	ASN	CA-CB-CG	-6.65	105.95	112.60
1	D	663	LEU	N-CA-CB	-6.65	100.76	110.40
1	D	733	ALA	N-CA-C	6.64	119.85	110.23
1	C	359	HIS	CA-CB-CG	-6.63	107.17	113.80
1	C	930	VAL	CB-CA-C	6.62	120.45	111.97
1	D	383	ASN	N-CA-C	6.62	120.66	112.58
1	A	155	ASN	CA-CB-CG	-6.60	106.00	112.60
1	A	702	GLN	CA-C-O	6.60	125.05	119.71
1	B	611	ARG	CB-CA-C	6.60	116.36	109.83
1	D	635	THR	CB-CA-C	-6.59	98.87	109.75
1	C	890	GLN	N-CA-C	6.59	120.80	110.32
1	D	672	VAL	CB-CA-C	6.58	119.94	110.33
1	B	570	TRP	N-CA-C	6.58	118.33	111.03
1	A	615	PRO	N-CA-CB	6.58	110.50	103.39
1	C	623	GLN	O-C-N	6.58	129.91	122.22
1	B	964	GLN	CA-C-O	6.56	127.38	120.42
1	A	477	SER	N-CA-CB	6.56	119.58	110.07
1	C	957	PHE	CA-CB-CG	-6.56	107.24	113.80
1	A	448	ARG	N-CA-C	6.55	120.38	112.38
1	C	737	ILE	CB-CA-C	6.55	116.78	110.16
1	B	403	ASP	CB-CA-C	-6.55	99.91	110.79
1	B	362	LEU	CA-C-N	-6.55	111.73	122.54
1	B	362	LEU	C-N-CA	-6.55	111.73	122.54
1	C	209	PHE	N-CA-C	6.54	121.41	113.17
1	A	672	VAL	CB-CA-C	-6.54	100.76	110.82
1	A	997	ASP	N-CA-CB	6.53	121.88	111.56
1	C	405	TYR	CA-C-O	6.53	127.49	119.79
1	A	46	ARG	N-CA-CB	6.52	118.02	109.55
1	B	54	LEU	N-CA-C	-6.51	104.49	112.88
1	D	352	ARG	CA-C-N	-6.49	115.68	122.69
1	D	352	ARG	C-N-CA	-6.49	115.68	122.69
1	C	172	ASP	CA-C-N	-6.48	112.28	122.65
1	C	172	ASP	C-N-CA	-6.48	112.28	122.65
1	A	707	ALA	CA-C-N	-6.47	112.19	122.29
1	A	707	ALA	C-N-CA	-6.47	112.19	122.29
1	B	563	GLN	N-CA-C	6.46	120.08	112.72
1	D	277	GLU	CB-CG-CD	6.44	123.55	112.60
1	A	671	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	745	MET	CB-CA-C	6.43	121.15	110.92
1	D	106	PRO	N-CA-C	-6.43	106.48	114.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	ASN	N-CA-CB	-6.41	100.65	110.65
1	D	193	ASP	N-CA-C	-6.41	105.32	113.01
1	B	384	PHE	CA-CB-CG	-6.41	107.39	113.80
1	A	279	ILE	CA-C-O	6.40	124.66	119.29
1	B	842	TRP	CB-CA-C	-6.39	99.56	110.16
1	B	958	ASN	N-CA-CB	6.38	122.68	111.13
1	C	262	GLN	N-CA-C	-6.38	96.86	108.02
1	B	210	ARG	N-CA-CB	6.37	121.56	111.43
1	B	443	MET	CA-C-O	6.37	127.26	120.70
1	D	129	VAL	N-CA-C	6.37	118.01	108.96
1	D	634	GLN	CB-CG-CD	-6.37	101.77	112.60
1	D	319	ASP	N-CA-C	6.37	120.77	113.19
1	C	249	GLU	N-CA-C	6.36	118.98	109.25
1	C	347	LYS	O-C-N	6.36	127.74	121.57
1	C	745	MET	N-CA-C	6.36	118.78	111.02
1	C	798	ALA	CA-C-N	6.36	129.98	120.31
1	C	798	ALA	C-N-CA	6.36	129.98	120.31
1	A	188	VAL	N-CA-C	6.34	117.94	108.23
1	B	509	ASP	CA-C-N	6.34	129.46	122.74
1	B	509	ASP	C-N-CA	6.34	129.46	122.74
1	D	1018	LEU	CB-CA-C	-6.33	96.45	109.94
1	A	988	GLY	N-CA-C	-6.33	104.37	113.86
1	A	113	PHE	CA-CB-CG	-6.32	107.48	113.80
1	A	513	PRO	CB-CA-C	-6.31	102.71	110.98
1	B	529	GLU	CA-C-N	-6.31	112.15	121.99
1	B	529	GLU	C-N-CA	-6.31	112.15	121.99
1	C	786	ARG	NE-CZ-NH1	6.31	127.81	121.50
1	D	787	ALA	CA-C-N	6.30	127.72	119.84
1	D	787	ALA	C-N-CA	6.30	127.72	119.84
1	C	721	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	A	46	ARG	NE-CZ-NH1	6.30	127.80	121.50
1	B	911	THR	N-CA-C	6.30	118.22	111.36
1	D	632	SER	N-CA-CB	6.29	121.83	110.95
1	A	583	ASN	CA-C-N	6.29	126.20	119.85
1	A	583	ASN	C-N-CA	6.29	126.20	119.85
1	A	519	SER	CA-C-O	-6.28	114.24	121.15
1	D	928	PRO	N-CA-CB	6.27	106.64	102.25
1	D	956	GLN	N-CA-C	-6.27	99.68	109.72
1	D	20	GLY	N-CA-C	-6.27	107.11	115.32
1	C	78	LEU	N-CA-C	-6.26	101.90	109.72
1	A	161	TYR	N-CA-C	6.25	119.69	109.06
1	D	464	HIS	CA-CB-CG	-6.25	107.55	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	860	GLY	CA-C-N	-6.24	111.08	122.38
1	A	860	GLY	C-N-CA	-6.24	111.08	122.38
1	C	345	ASN	CA-CB-CG	-6.24	106.36	112.60
1	C	593	GLY	N-CA-C	-6.24	106.70	115.32
1	C	218	PRO	N-CA-C	-6.24	102.05	111.41
1	A	614	HIS	N-CA-C	-6.23	102.01	110.36
1	A	141	ILE	CA-C-N	-6.23	114.13	122.98
1	A	141	ILE	C-N-CA	-6.23	114.13	122.98
1	C	766	SER	N-CA-C	6.22	120.07	112.23
1	C	501	PRO	CA-C-N	-6.22	114.42	123.00
1	C	501	PRO	C-N-CA	-6.22	114.42	123.00
1	C	429	ASP	CA-C-O	6.21	123.33	119.29
1	D	689	GLU	CA-C-N	6.21	130.18	121.24
1	D	689	GLU	C-N-CA	6.21	130.18	121.24
1	B	52	ARG	CB-CA-C	-6.20	98.22	109.38
1	D	820	ALA	N-CA-C	6.19	119.61	107.98
1	D	188	VAL	N-CA-C	6.17	117.00	107.99
1	A	20	GLY	N-CA-C	-6.17	107.01	114.66
1	C	477	SER	CB-CA-C	-6.16	101.17	110.90
1	A	404	ARG	N-CA-C	6.16	118.07	111.36
1	C	725	ASN	CA-CB-CG	-6.16	106.44	112.60
1	D	931	PHE	CA-CB-CG	-6.16	107.64	113.80
1	B	744	GLU	CA-C-O	6.15	127.48	120.90
1	B	28	ALA	CB-CA-C	-6.14	98.77	109.64
1	C	233	ASP	CA-C-N	-6.14	113.02	122.60
1	C	233	ASP	C-N-CA	-6.14	113.02	122.60
1	C	499	ILE	CA-C-N	-6.14	116.02	122.28
1	C	499	ILE	C-N-CA	-6.14	116.02	122.28
1	B	730	LEU	CB-CA-C	6.13	119.25	109.62
1	B	651	LEU	CA-C-N	-6.13	114.27	122.72
1	B	651	LEU	C-N-CA	-6.13	114.27	122.72
1	C	593	GLY	CA-C-O	6.12	125.91	119.06
1	B	641	GLU	N-CA-CB	6.12	119.49	110.56
1	C	434	PRO	N-CA-CB	6.12	109.77	103.23
1	B	604	ASN	CA-CB-CG	6.11	118.71	112.60
1	C	850	PHE	CA-CB-CG	6.11	119.91	113.80
1	C	81	ALA	N-CA-C	6.11	118.43	110.43
1	B	881	ARG	NE-CZ-NH1	6.10	127.60	121.50
1	C	686	PRO	CA-C-N	-6.10	111.27	120.60
1	C	686	PRO	C-N-CA	-6.10	111.27	120.60
1	A	332	PHE	CA-CB-CG	-6.09	107.71	113.80
1	C	63	PHE	O-C-N	-6.09	117.81	121.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	991	MET	CA-C-N	-6.09	112.36	121.01
1	D	991	MET	C-N-CA	-6.09	112.36	121.01
1	C	454	ILE	CA-C-O	6.09	124.74	118.96
1	D	948	PRO	CB-CA-C	-6.08	101.86	111.04
1	C	404	ARG	N-CA-C	6.08	117.99	111.36
1	C	809	ARG	CD-NE-CZ	6.08	132.91	124.40
1	B	586	SER	O-C-N	6.07	130.11	123.13
1	B	692	GLY	CA-C-O	-6.07	117.41	122.33
1	A	890	GLN	N-CA-C	6.05	119.03	110.50
1	D	661	LYS	CA-C-N	6.05	127.40	119.84
1	D	661	LYS	C-N-CA	6.05	127.40	119.84
1	B	1000	SER	N-CA-C	-6.04	102.78	108.22
1	B	519	SER	N-CA-C	-6.04	101.73	110.24
1	C	802	ASP	CA-CB-CG	-6.04	106.56	112.60
1	B	687	GLN	C-N-CD	-6.03	100.27	125.00
1	C	199	ASP	CA-CB-CG	-6.03	106.57	112.60
1	B	235	PHE	CA-CB-CG	-6.02	107.78	113.80
1	D	605	GLY	N-CA-C	6.02	119.91	112.14
1	C	221	GLN	CB-CG-CD	6.02	122.83	112.60
1	B	337	ILE	N-CA-CB	6.01	118.25	111.21
1	C	576	ILE	N-CA-C	6.01	116.83	108.89
1	C	166	ARG	N-CA-C	6.01	120.22	112.41
1	B	700	VAL	N-CA-CB	6.01	118.24	111.21
1	A	548	GLY	CA-C-O	6.00	125.96	119.06
1	B	208	ILE	N-CA-CB	-6.00	106.24	112.06
1	B	381	GLN	CA-CB-CG	-6.00	102.09	114.10
1	A	788	PRO	N-CA-CB	6.00	108.59	103.19
1	C	688	PRO	CA-C-N	6.00	128.63	120.54
1	C	688	PRO	C-N-CA	6.00	128.63	120.54
1	D	726	LEU	N-CA-CB	5.99	118.88	109.83
1	D	867	THR	CA-C-N	-5.99	114.61	122.94
1	D	867	THR	C-N-CA	-5.99	114.61	122.94
1	C	489	GLY	CA-C-N	-5.98	114.20	122.63
1	C	489	GLY	C-N-CA	-5.98	114.20	122.63
1	C	645	ARG	N-CA-C	5.98	119.37	110.52
1	D	633	GLY	CA-C-N	-5.98	113.22	122.49
1	D	633	GLY	C-N-CA	-5.98	113.22	122.49
1	C	634	GLN	CA-C-O	5.98	127.18	119.95
1	B	737	ILE	N-CA-CB	5.98	120.35	111.86
1	D	931	PHE	CB-CA-C	-5.97	104.26	110.17
1	A	232	ASN	CA-CB-CG	-5.97	106.63	112.60
1	C	63	PHE	CA-C-O	5.96	125.98	120.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	298	PRO	CB-CA-C	-5.95	103.44	111.12
1	A	307	ASN	CB-CA-C	-5.95	100.62	109.90
1	D	890	GLN	N-CA-C	5.95	118.85	110.23
1	D	964	GLN	N-CA-C	-5.94	104.88	111.71
1	D	770	ILE	N-CA-C	-5.94	98.58	107.37
1	A	591	ASP	CA-CB-CG	-5.93	106.67	112.60
1	C	98	PRO	N-CA-C	-5.93	101.95	111.38
1	D	559	TYR	O-C-N	5.93	127.88	121.12
1	B	724	GLU	CA-C-N	-5.93	114.41	123.07
1	B	724	GLU	C-N-CA	-5.93	114.41	123.07
1	A	890	GLN	CA-C-O	5.93	128.02	121.56
1	B	126	THR	CA-CB-OG1	-5.93	100.71	109.60
1	D	233	ASP	CA-CB-CG	-5.92	106.68	112.60
1	A	94	GLY	O-C-N	-5.91	115.02	122.41
1	C	653	HIS	N-CA-CB	5.91	120.06	110.43
1	B	863	GLN	CA-C-N	-5.90	114.74	123.11
1	B	863	GLN	C-N-CA	-5.90	114.74	123.11
1	A	861	SER	CA-C-N	-5.89	112.59	122.25
1	A	861	SER	C-N-CA	-5.89	112.59	122.25
1	A	987	ASP	CA-CB-CG	-5.88	106.72	112.60
1	A	684	GLU	CB-CA-C	-5.88	101.44	110.26
1	B	309	TYR	N-CA-C	-5.88	101.48	109.95
1	B	614	HIS	N-CA-C	-5.88	102.48	110.36
1	D	100	TYR	N-CA-CB	5.87	121.49	110.56
1	C	347	LYS	CB-CA-C	-5.87	99.98	108.84
1	C	667	GLU	CB-CG-CD	-5.87	102.62	112.60
1	C	323	ILE	N-CA-C	-5.87	106.10	111.67
1	C	659	ASP	N-CA-CB	5.86	120.39	110.49
1	D	738	PRO	CB-CA-C	5.86	118.73	111.23
1	B	239	VAL	N-CA-CB	5.86	119.25	111.64
1	B	990	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	604	ASN	CA-CB-CG	5.86	118.45	112.60
1	C	788	PRO	N-CA-CB	5.86	109.40	103.25
1	C	728	VAL	CA-C-N	-5.85	113.13	121.50
1	C	728	VAL	C-N-CA	-5.85	113.13	121.50
1	D	531	ARG	N-CA-C	5.85	118.63	110.20
1	D	949	HIS	CA-CB-CG	-5.85	107.95	113.80
1	B	519	SER	N-CA-CB	-5.84	100.40	109.69
1	D	855	THR	N-CA-CB	5.84	121.70	111.13
1	C	520	ILE	N-CA-C	5.83	116.57	110.62
1	C	760	ARG	N-CA-CB	5.83	119.90	110.40
1	A	297	ASN	CA-CB-CG	-5.83	106.77	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	720	TRP	CA-C-N	-5.82	111.72	121.39
1	C	720	TRP	C-N-CA	-5.82	111.72	121.39
1	D	71	GLU	N-CA-CB	5.82	119.34	110.14
1	D	279	ILE	CB-CA-C	5.82	116.18	111.06
1	A	735	HIS	CA-CB-CG	-5.82	107.98	113.80
1	A	844	HIS	CA-CB-CG	-5.82	107.98	113.80
1	D	319	ASP	N-CA-CB	5.82	120.66	110.42
1	A	171	PHE	CA-CB-CG	-5.81	107.99	113.80
1	D	71	GLU	CB-CA-C	5.81	121.73	110.46
1	C	438	GLU	CB-CA-C	-5.81	99.89	110.63
1	B	735	HIS	N-CA-C	-5.80	105.09	111.82
1	A	225	PHE	N-CA-CB	5.80	121.63	111.13
1	A	540	HIS	CA-CB-CG	-5.80	108.00	113.80
1	C	1001	PRO	N-CA-CB	5.79	108.32	103.17
1	A	614	HIS	N-CA-CB	5.78	116.45	109.74
1	D	686	PRO	N-CA-CB	5.78	109.31	103.25
1	C	330	VAL	O-C-N	5.77	129.49	123.26
1	A	922	LEU	CA-C-O	5.76	126.86	120.63
1	B	640	SER	CA-C-N	-5.76	113.43	122.65
1	B	640	SER	C-N-CA	-5.76	113.43	122.65
1	D	57	GLU	N-CA-C	5.76	118.06	109.25
1	B	530	THR	CA-CB-OG1	-5.75	100.97	109.60
1	B	736	ALA	N-CA-C	5.75	118.16	109.41
1	D	147	ASN	N-CA-CB	-5.75	101.67	110.65
1	A	872	VAL	CA-C-N	-5.75	112.54	120.71
1	A	872	VAL	C-N-CA	-5.75	112.54	120.71
1	B	78	LEU	CA-C-N	5.75	127.03	119.84
1	B	78	LEU	C-N-CA	5.75	127.03	119.84
1	A	779	PRO	CB-CA-C	-5.75	103.42	110.95
1	C	503	TYR	N-CA-C	5.75	119.87	112.86
1	C	757	GLN	N-CA-C	5.75	118.09	108.73
1	D	727	SER	CA-CB-OG	-5.74	99.62	111.10
1	D	136	GLU	N-CA-C	5.74	116.66	108.74
1	B	503	TYR	N-CA-C	5.74	119.86	112.86
1	B	671	ASP	CA-C-N	-5.74	115.63	123.14
1	B	671	ASP	C-N-CA	-5.74	115.63	123.14
1	D	728	VAL	CA-C-N	-5.73	114.11	122.19
1	D	728	VAL	C-N-CA	-5.73	114.11	122.19
1	B	833	ALA	N-CA-CB	-5.72	102.52	111.56
1	D	90	TRP	N-CA-C	5.71	119.06	111.75
1	A	802	ASP	N-CA-CB	5.71	119.32	110.12
1	C	651	LEU	N-CA-CB	5.71	122.15	111.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	TRP	N-CA-C	5.71	118.28	111.71
1	A	632	SER	N-CA-CB	5.71	120.83	110.95
1	A	882	ILE	CA-CB-CG1	-5.71	100.70	110.40
1	C	20	GLY	N-CA-C	-5.71	107.58	114.66
1	C	333	ARG	NE-CZ-NH1	-5.71	115.79	121.50
1	A	877	PRO	CB-CA-C	-5.70	104.10	111.46
1	B	516	PRO	CB-CA-C	-5.70	103.48	110.95
1	B	532	PRO	O-C-N	-5.70	116.05	123.06
1	B	890	GLN	N-CA-C	5.70	119.25	110.42
1	B	21	VAL	O-C-N	5.69	128.23	122.71
1	D	428	ASP	CA-CB-CG	-5.69	106.91	112.60
1	A	415	ILE	CA-C-O	-5.68	114.74	120.31
1	C	76	CYS	N-CA-C	5.68	118.72	109.06
1	B	858	ILE	CA-C-N	-5.68	112.64	123.32
1	B	858	ILE	C-N-CA	-5.68	112.64	123.32
1	C	835	LEU	N-CA-C	5.67	117.94	108.02
1	D	204	ARG	NE-CZ-NH2	5.67	124.30	119.20
1	A	796	SER	N-CA-CB	5.67	118.39	109.83
1	B	889	ALA	CA-C-N	-5.67	112.43	122.74
1	B	889	ALA	C-N-CA	-5.67	112.43	122.74
1	A	663	LEU	CB-CA-C	-5.67	99.15	110.42
1	A	916	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	555	ALA	CB-CA-C	-5.66	99.81	110.67
1	B	128	ASN	CB-CA-C	-5.66	99.84	109.51
1	C	143	PHE	CA-CB-CG	-5.66	108.14	113.80
1	A	958	ASN	N-CA-CB	5.65	121.53	111.69
1	B	185	ALA	N-CA-CB	5.65	119.64	110.77
1	A	25	ASN	N-CA-C	5.65	119.99	113.38
1	B	779	PRO	N-CA-CB	5.65	108.70	103.39
1	B	161	TYR	N-CA-CB	-5.64	101.03	111.13
1	B	113	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	481	SER	N-CA-C	5.64	119.77	113.01
1	C	763	GLY	N-CA-C	-5.63	107.49	115.43
1	A	546	LEU	N-CA-CB	5.63	120.00	110.49
1	C	74	LEU	CA-C-N	-5.62	112.89	122.11
1	C	74	LEU	C-N-CA	-5.62	112.89	122.11
1	C	735	HIS	N-CA-CB	5.62	118.63	110.65
1	C	532	PRO	CB-CA-C	-5.61	102.85	110.60
1	C	659	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	553	TRP	CB-CA-C	5.61	120.21	110.68
1	A	916	ASP	CA-C-N	-5.61	115.31	122.77
1	A	916	ASP	C-N-CA	-5.61	115.31	122.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	216	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	746	ASP	N-CA-C	5.60	117.58	109.07
1	C	363	HIS	CA-CB-CG	-5.60	108.20	113.80
1	B	915	PHE	CA-CB-CG	-5.59	108.21	113.80
1	D	225	PHE	CA-CB-CG	5.59	119.39	113.80
1	C	57	GLU	N-CA-C	5.59	117.85	108.96
1	B	213	SER	O-C-N	5.59	129.62	123.25
1	C	906	TYR	CA-CB-CG	-5.58	103.85	113.90
1	B	794	GLY	CA-C-N	-5.58	113.78	122.09
1	B	794	GLY	C-N-CA	-5.58	113.78	122.09
1	C	447	ASP	N-CA-C	5.58	120.24	113.38
1	C	52	ARG	CB-CA-C	-5.57	99.35	109.38
1	A	357	HIS	CA-CB-CG	-5.57	108.23	113.80
1	C	685	LEU	N-CA-CB	5.57	120.02	110.05
1	A	1003	VAL	N-CA-CB	5.57	117.00	110.82
1	B	111	PRO	CA-C-O	-5.56	116.89	120.90
1	D	802	ASP	CA-C-N	5.56	126.79	119.84
1	D	802	ASP	C-N-CA	5.56	126.79	119.84
1	B	326	GLU	N-CA-C	-5.56	101.30	109.81
1	D	895	VAL	N-CA-CB	5.56	119.38	111.82
1	B	667	GLU	N-CA-C	5.56	117.84	109.23
1	D	264	GLU	CA-C-O	5.56	126.15	119.43
1	A	746	ASP	O-C-N	5.55	129.58	123.25
1	D	472	TYR	CA-C-O	5.55	126.65	120.82
1	C	824	GLN	N-CA-C	5.55	116.96	108.52
1	D	785	THR	CA-CB-OG1	-5.55	101.27	109.60
1	D	949	HIS	N-CA-C	5.55	118.96	110.20
1	B	164	ASP	N-CA-CB	5.54	119.86	110.49
1	D	753	ASN	CA-CB-CG	-5.54	107.06	112.60
1	A	504	ALA	N-CA-C	-5.54	102.08	110.28
1	A	267	VAL	CG1-CB-CG2	-5.53	98.63	110.80
1	C	608	PHE	CA-C-O	-5.53	115.45	121.87
1	B	938	ARG	N-CA-CB	5.53	120.36	110.80
1	C	273	PRO	N-CA-C	-5.53	103.17	111.57
1	C	777	LEU	N-CA-C	-5.53	106.67	113.41
1	B	833	ALA	CA-C-O	5.53	127.36	121.45
1	C	443	MET	CA-C-O	5.53	126.39	120.70
1	D	279	ILE	CB-CG1-CD1	-5.53	102.20	113.80
1	A	573	GLN	N-CA-CB	5.52	118.53	110.25
1	B	568	TRP	CA-CB-CG	-5.52	103.11	113.60
1	C	524	LEU	CA-C-N	-5.52	113.84	122.73
1	C	524	LEU	C-N-CA	-5.52	113.84	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	ARG	N-CA-C	-5.52	101.02	109.41
1	A	337	ILE	O-C-N	-5.51	117.39	123.18
1	D	478	VAL	CA-C-N	-5.51	116.90	122.74
1	D	478	VAL	C-N-CA	-5.51	116.90	122.74
1	C	780	LEU	CA-C-O	-5.51	114.38	120.60
1	B	760	ARG	N-CA-CB	5.50	119.53	110.39
1	B	916	ASP	CA-CB-CG	-5.50	107.09	112.60
1	A	85	VAL	CB-CA-C	-5.50	103.67	111.21
1	A	651	LEU	N-CA-CB	5.50	121.39	111.37
1	C	718	GLN	CB-CA-C	-5.50	101.13	109.99
1	C	90	TRP	N-CA-C	5.49	118.02	111.71
1	C	440	VAL	N-CA-CB	5.49	118.42	110.52
1	A	221	GLN	N-CA-C	5.49	117.14	108.96
1	D	804	ASN	OD1-CG-ND2	5.48	128.08	122.60
1	D	959	ILE	CA-C-N	-5.48	112.70	122.45
1	D	959	ILE	C-N-CA	-5.48	112.70	122.45
1	C	699	ARG	CB-CA-C	-5.48	98.26	109.38
1	A	445	GLN	CA-C-N	-5.48	112.45	121.92
1	A	445	GLN	C-N-CA	-5.48	112.45	121.92
1	B	520	ILE	N-CA-C	5.47	116.20	110.62
1	D	230	ARG	CA-C-O	-5.47	114.94	121.56
1	B	1014	TYR	CA-C-O	5.47	126.61	120.70
1	A	691	ALA	N-CA-C	5.47	117.35	110.24
1	D	843	GLN	N-CA-C	5.47	118.14	109.50
1	D	409	VAL	N-CA-C	5.47	115.82	108.17
1	D	1010	SER	N-CA-C	5.47	119.93	112.88
1	C	856	TYR	N-CA-CB	5.46	119.35	110.77
1	A	593	GLY	CA-C-O	5.46	125.18	119.06
1	A	613	PRO	CB-CA-C	-5.46	103.83	110.98
1	D	155	ASN	CA-CB-CG	-5.46	107.14	112.60
1	B	728	VAL	N-CA-C	-5.45	107.81	113.10
1	C	195	SER	CA-C-O	5.45	126.09	119.49
1	B	726	LEU	N-CA-CB	5.44	117.97	109.97
1	A	684	GLU	N-CA-C	-5.43	101.60	109.59
1	C	776	LEU	N-CA-C	5.43	118.34	109.59
1	C	745	MET	CA-C-N	-5.43	113.79	122.53
1	C	745	MET	C-N-CA	-5.43	113.79	122.53
1	D	119	PRO	O-C-N	5.43	129.47	122.85
1	A	563	GLN	CA-C-N	-5.43	113.40	122.62
1	A	563	GLN	C-N-CA	-5.43	113.40	122.62
1	C	592	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	293	LEU	CA-C-O	5.42	126.22	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	PRO	CA-C-N	-5.42	115.11	122.92
1	D	106	PRO	C-N-CA	-5.42	115.11	122.92
1	A	277	GLU	CB-CG-CD	5.42	121.82	112.60
1	A	279	ILE	CB-CG1-CD1	-5.42	102.42	113.80
1	D	757	GLN	CB-CG-CD	-5.41	103.40	112.60
1	B	99	ILE	CA-C-N	-5.41	115.13	123.14
1	B	99	ILE	C-N-CA	-5.41	115.13	123.14
1	D	561	ARG	N-CA-C	5.41	119.50	113.01
1	A	842	TRP	CE2-CD2-CE3	5.41	124.21	118.80
1	C	33	PHE	CA-CB-CG	5.41	119.21	113.80
1	C	156	GLY	CA-C-N	-5.41	114.60	122.65
1	C	156	GLY	C-N-CA	-5.41	114.60	122.65
1	A	97	ALA	N-CA-C	5.40	118.13	110.24
1	C	648	ASP	N-CA-C	5.39	119.49	113.02
1	C	786	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	C	728	VAL	CA-C-O	5.39	124.07	119.38
1	D	175	ALA	CA-C-N	-5.39	113.27	122.11
1	D	175	ALA	C-N-CA	-5.39	113.27	122.11
1	B	232	ASN	N-CA-CB	5.39	118.21	110.45
1	A	31	PRO	N-CA-CB	5.38	108.30	103.08
1	D	128	ASN	OD1-CG-ND2	5.38	127.98	122.60
1	B	752	GLY	CA-C-N	-5.38	114.06	122.73
1	B	752	GLY	C-N-CA	-5.38	114.06	122.73
1	B	961	ARG	CA-C-N	-5.38	115.41	122.99
1	B	961	ARG	C-N-CA	-5.38	115.41	122.99
1	C	623	GLN	CA-CB-CG	-5.37	103.35	114.10
1	C	377	LEU	CA-C-N	-5.37	112.66	120.29
1	C	377	LEU	C-N-CA	-5.37	112.66	120.29
1	B	782	ASP	CA-CB-CG	5.37	117.97	112.60
1	C	482	ARG	CB-CA-C	-5.37	101.15	109.20
1	C	685	LEU	O-C-N	5.37	127.95	121.29
1	D	644	PHE	CA-C-N	-5.37	112.89	122.07
1	D	644	PHE	C-N-CA	-5.37	112.89	122.07
1	C	535	LEU	CA-C-O	-5.36	114.64	120.81
1	B	375	ASP	CA-CB-CG	-5.36	107.24	112.60
1	C	770	ILE	N-CA-CB	5.36	118.65	111.90
1	D	479	ASP	CA-C-O	5.36	127.44	121.22
1	D	760	ARG	N-CA-CB	5.36	119.41	110.41
1	D	908	ASP	N-CA-C	-5.36	106.33	112.92
1	B	996	ASP	CA-CB-CG	-5.35	107.25	112.60
1	D	987	ASP	N-CA-C	5.35	118.54	109.76
1	B	52	ARG	CA-C-O	-5.35	115.04	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ASN	CA-CB-CG	-5.35	107.25	112.60
1	A	734	SER	CA-C-O	5.35	127.14	121.05
1	A	14	ARG	N-CA-CB	-5.34	104.37	110.35
1	C	944	LEU	CA-C-N	-5.34	114.93	122.94
1	C	944	LEU	C-N-CA	-5.34	114.93	122.94
1	A	446	ARG	CA-C-N	-5.34	114.21	122.49
1	A	446	ARG	C-N-CA	-5.34	114.21	122.49
1	B	907	PRO	N-CA-CB	5.33	108.96	103.15
1	B	949	HIS	N-CA-C	5.33	118.75	110.17
1	C	103	VAL	N-CA-C	5.33	116.41	111.45
1	B	287	ASP	N-CA-C	5.33	118.79	112.72
1	D	997	ASP	CA-C-O	-5.32	115.76	121.45
1	C	382	ASN	N-CA-CB	5.32	118.63	110.70
1	B	928	PRO	N-CA-CB	5.32	105.97	102.25
1	C	279	ILE	CB-CA-C	-5.32	106.19	111.30
1	D	150	PHE	O-C-N	5.32	129.11	123.42
1	D	628	GLN	CA-C-N	-5.32	113.60	122.21
1	D	628	GLN	C-N-CA	-5.32	113.60	122.21
1	B	384	PHE	N-CA-C	-5.32	101.87	110.32
1	A	613	PRO	N-CA-CB	5.31	108.27	103.33
1	A	662	PRO	N-CA-CB	5.31	108.05	103.27
1	B	877	PRO	N-CA-CB	5.31	107.97	103.35
1	A	890	GLN	N-CA-CB	-5.31	102.52	110.17
1	B	583	ASN	N-CA-CB	5.31	116.46	110.03
1	C	735	HIS	CA-CB-CG	5.31	119.11	113.80
1	B	39	SER	N-CA-C	5.31	117.06	111.28
1	D	760	ARG	CA-C-N	-5.31	111.75	121.52
1	D	760	ARG	C-N-CA	-5.31	111.75	121.52
1	D	510	GLN	N-CA-C	-5.30	96.98	108.81
1	C	499	ILE	N-CA-C	-5.30	101.84	108.84
1	B	320	GLY	CA-C-N	-5.30	114.04	121.72
1	B	320	GLY	C-N-CA	-5.30	114.04	121.72
1	B	183	ARG	N-CA-C	5.29	117.03	108.41
1	B	846	GLY	CA-C-N	-5.29	115.26	122.93
1	B	846	GLY	C-N-CA	-5.29	115.26	122.93
1	A	93	HIS	ND1-CE1-NE2	5.29	113.69	108.40
1	B	71	GLU	CB-CG-CD	5.29	121.59	112.60
1	D	519	SER	N-CA-C	-5.29	102.78	110.24
1	C	99	ILE	CA-C-N	-5.28	115.51	122.85
1	C	99	ILE	C-N-CA	-5.28	115.51	122.85
1	D	675	GLN	CA-C-O	-5.28	114.13	119.78
1	A	618	THR	CA-C-O	5.28	126.14	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	868	VAL	N-CA-C	5.28	115.50	108.11
1	C	717	TRP	N-CA-C	5.27	116.30	108.60
1	C	33	PHE	CB-CA-C	-5.27	99.86	110.30
1	C	642	TYR	CA-CB-CG	-5.27	104.41	113.90
1	D	736	ALA	N-CA-C	5.27	117.67	109.60
1	B	771	GLY	CA-C-N	-5.27	114.22	122.65
1	B	771	GLY	C-N-CA	-5.27	114.22	122.65
1	A	257	THR	CA-C-N	-5.26	116.66	123.19
1	A	257	THR	C-N-CA	-5.26	116.66	123.19
1	B	303	ALA	N-CA-C	-5.26	105.66	111.71
1	C	297	ASN	CA-CB-CG	-5.26	107.34	112.60
1	D	627	PHE	N-CA-CB	5.26	119.53	110.68
1	B	98	PRO	N-CA-C	-5.26	103.02	111.38
1	A	833	ALA	CA-C-N	-5.26	115.81	123.06
1	A	833	ALA	C-N-CA	-5.26	115.81	123.06
1	C	507	ASP	CA-CB-CG	-5.25	107.35	112.60
1	C	1019	VAL	CA-CB-CG1	-5.25	101.47	110.40
1	B	651	LEU	CB-CA-C	5.25	119.74	109.35
1	D	139	THR	CA-C-N	-5.24	114.00	122.81
1	D	139	THR	C-N-CA	-5.24	114.00	122.81
1	D	561	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	A	685	LEU	CB-CA-C	5.24	120.50	110.17
1	A	699	ARG	NE-CZ-NH2	-5.24	114.48	119.20
1	B	692	GLY	N-CA-C	-5.24	106.30	111.85
1	C	360	HIS	CA-CB-CG	-5.24	108.56	113.80
1	D	211	ASP	N-CA-C	5.24	117.48	110.35
1	C	274	PHE	CA-CB-CG	-5.24	108.56	113.80
1	D	894	ARG	CB-CA-C	-5.23	101.04	110.36
1	D	922	LEU	N-CA-C	5.23	117.39	111.11
1	C	977	HIS	CA-CB-CG	-5.23	108.57	113.80
1	A	653	HIS	CA-CB-CG	-5.23	108.57	113.80
1	D	907	PRO	N-CA-CB	5.23	109.22	103.26
1	D	609	ALA	CA-C-N	-5.22	113.57	122.56
1	D	609	ALA	C-N-CA	-5.22	113.57	122.56
1	A	226	HIS	CA-C-N	-5.22	116.16	123.10
1	A	226	HIS	C-N-CA	-5.22	116.16	123.10
1	B	264	GLU	CA-C-O	5.22	125.39	119.18
1	B	823	LEU	N-CA-C	-5.22	107.46	113.88
1	C	790	ASP	CA-CB-CG	-5.22	107.38	112.60
1	D	598	ASP	CA-CB-CG	-5.22	107.38	112.60
1	A	164	ASP	N-CA-CB	5.21	119.30	110.49
1	A	928	PRO	N-CA-CB	5.21	105.90	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	969	GLU	N-CA-C	-5.21	106.60	113.17
1	A	583	ASN	CA-CB-CG	-5.21	107.39	112.60
1	A	231	PHE	N-CA-C	5.21	117.59	109.52
1	D	34	ALA	N-CA-CB	5.21	117.85	110.98
1	A	945	ASN	CA-CB-CG	-5.20	107.40	112.60
1	D	955	PHE	CA-CB-CG	-5.20	108.60	113.80
1	A	863	GLN	CA-CB-CG	-5.20	103.71	114.10
1	B	78	LEU	CB-CA-C	-5.19	104.11	110.08
1	B	386	ALA	CA-C-N	-5.19	115.23	122.71
1	B	386	ALA	C-N-CA	-5.19	115.23	122.71
1	C	320	GLY	CA-C-N	-5.19	115.56	122.72
1	C	320	GLY	C-N-CA	-5.19	115.56	122.72
1	B	209	PHE	N-CA-C	5.19	119.71	113.17
1	D	683	PRO	CB-CA-C	-5.19	104.43	111.12
1	D	546	LEU	N-CA-CB	5.19	119.26	110.49
1	D	653	HIS	N-CA-CB	5.19	119.04	110.69
1	A	1004	SER	CB-CA-C	5.18	118.33	109.72
1	B	721	ARG	CB-CA-C	-5.18	100.77	109.53
1	C	600	GLN	N-CA-C	5.18	119.36	113.19
1	C	358	GLU	CA-CB-CG	-5.18	103.74	114.10
1	A	784	PHE	CA-CB-CG	-5.18	108.62	113.80
1	C	748	CYS	N-CA-CB	5.18	119.03	110.69
1	C	428	ASP	CA-C-N	5.17	128.57	121.74
1	C	428	ASP	C-N-CA	5.17	128.57	121.74
1	A	809	ARG	O-C-N	-5.17	116.64	122.12
1	A	1013	ARG	NE-CZ-NH2	5.17	123.85	119.20
1	B	501	PRO	O-C-N	5.17	129.27	122.86
1	B	323	ILE	N-CA-C	-5.17	106.76	111.67
1	B	610	ASP	CA-C-N	-5.17	118.75	126.86
1	B	610	ASP	C-N-CA	-5.17	118.75	126.86
1	B	806	TRP	CA-C-O	5.17	126.21	120.63
1	B	1005	ALA	O-C-N	5.17	127.60	122.12
1	C	230	ARG	CB-CA-C	5.16	119.50	109.33
1	C	809	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	D	638	VAL	CA-C-N	-5.16	115.72	122.99
1	D	638	VAL	C-N-CA	-5.16	115.72	122.99
1	C	910	LEU	CA-C-N	-5.16	112.85	120.28
1	C	910	LEU	C-N-CA	-5.16	112.85	120.28
1	D	221	GLN	N-CA-CB	-5.16	103.41	111.56
1	D	109	VAL	CB-CA-C	-5.15	106.34	111.80
1	A	1011	ALA	N-CA-C	5.15	118.66	112.38
1	D	688	PRO	CA-C-N	-5.15	112.01	122.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	688	PRO	C-N-CA	-5.15	112.01	122.31
1	C	793	ILE	N-CA-C	5.15	115.81	110.82
1	B	447	ASP	N-CA-CB	-5.14	102.87	110.53
1	C	40	GLU	CG-CD-OE1	5.14	130.22	118.40
1	C	440	VAL	CB-CA-C	-5.14	105.31	112.04
1	A	634	GLN	CG-CD-NE2	-5.14	108.69	116.40
1	C	498	ILE	CA-CB-CG2	5.14	119.23	110.50
1	B	762	SER	N-CA-CB	5.14	117.86	110.20
1	A	183	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	D	1018	LEU	O-C-N	5.13	129.13	123.33
1	A	412	GLU	N-CA-C	5.13	117.25	108.90
1	B	764	PHE	CA-C-O	5.13	127.11	121.11
1	D	78	LEU	N-CA-CB	5.12	118.36	110.01
1	A	737	ILE	N-CA-CB	5.12	118.38	111.21
1	B	39	SER	CA-CB-OG	-5.12	100.86	111.10
1	B	974	HIS	CA-C-N	-5.12	113.76	122.56
1	B	974	HIS	C-N-CA	-5.12	113.76	122.56
1	C	277	GLU	CA-CB-CG	-5.12	103.87	114.10
1	C	570	TRP	N-CA-C	5.11	116.70	111.03
1	D	129	VAL	N-CA-CB	-5.11	106.00	112.60
1	A	741	THR	CA-CB-CG2	-5.11	101.81	110.50
1	D	42	ALA	CA-C-O	5.11	125.97	120.55
1	A	556	PHE	CA-CB-CG	5.11	118.91	113.80
1	C	556	PHE	O-C-N	-5.11	116.71	122.12
1	B	868	VAL	N-CA-C	5.11	115.33	107.77
1	B	664	ALA	N-CA-CB	-5.10	103.06	111.69
1	A	675	GLN	CB-CA-C	-5.10	100.70	110.65
1	A	159	VAL	CA-C-N	-5.09	114.30	120.51
1	A	159	VAL	C-N-CA	-5.09	114.30	120.51
1	C	76	CYS	N-CA-CB	-5.09	102.01	111.13
1	D	755	ARG	O-C-N	-5.09	117.17	123.33
1	A	427	THR	CA-C-N	-5.09	114.14	122.54
1	A	427	THR	C-N-CA	-5.09	114.14	122.54
1	B	383	ASN	N-CA-C	5.09	119.44	113.23
1	D	559	TYR	CB-CA-C	-5.09	104.52	110.17
1	A	627	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	513	PRO	N-CA-CB	5.09	107.84	103.31
1	B	756	TRP	CA-C-N	-5.09	115.81	122.99
1	B	756	TRP	C-N-CA	-5.09	115.81	122.99
1	A	838	THR	N-CA-C	5.09	117.41	109.52
1	D	525	SER	N-CA-C	5.09	118.52	112.72
1	C	69	VAL	N-CA-C	5.08	113.93	108.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	352	ARG	CA-C-N	-5.08	117.20	122.69
1	C	352	ARG	C-N-CA	-5.08	117.20	122.69
1	D	23	GLN	CA-CB-CG	-5.08	103.93	114.10
1	B	930	VAL	CB-CA-C	5.08	118.39	111.88
1	B	181	GLU	CA-C-O	-5.08	114.97	120.81
1	D	528	GLY	CA-C-N	-5.08	114.16	121.42
1	D	528	GLY	C-N-CA	-5.08	114.16	121.42
1	C	687	GLN	CB-CA-C	5.07	117.78	109.46
1	D	70	PRO	CB-CA-C	-5.07	105.32	111.46
1	D	223	SER	N-CA-C	-5.07	107.26	113.50
1	D	769	TRP	N-CA-CB	5.06	120.19	111.13
1	A	942	ARG	CD-NE-CZ	-5.06	117.31	124.40
1	C	52	ARG	CA-CB-CG	5.06	124.22	114.10
1	D	219	THR	CA-CB-OG1	-5.06	102.01	109.60
1	B	151	HIS	CA-CB-CG	-5.06	108.74	113.80
1	B	1007	PHE	CA-CB-CG	-5.05	108.75	113.80
1	C	611	ARG	CA-C-O	5.05	123.32	119.18
1	C	176	PHE	N-CA-CB	-5.05	103.91	110.88
1	C	441	THR	N-CA-C	5.05	117.68	111.82
1	C	662	PRO	N-CA-CB	5.05	107.67	103.17
1	A	673	ALA	N-CA-CB	-5.05	103.78	109.49
1	C	383	ASN	N-CA-C	5.05	119.39	113.23
1	C	578	TYR	CA-CB-CG	-5.05	104.81	113.90
1	C	43	ARG	NE-CZ-NH1	5.05	126.55	121.50
1	D	166	ARG	N-CA-C	5.05	119.39	112.88
1	D	689	GLU	O-C-N	5.05	130.54	122.42
1	D	723	ALA	N-CA-CB	5.05	117.45	109.83
1	A	625	GLN	CA-CB-CG	-5.04	104.01	114.10
1	D	630	ARG	NE-CZ-NH1	5.04	126.54	121.50
1	B	741	THR	CA-CB-OG1	-5.04	102.04	109.60
1	C	249	GLU	CA-C-O	5.04	126.33	120.49
1	C	996	ASP	N-CA-CB	5.04	118.10	110.14
1	A	802	ASP	CB-CA-C	5.03	115.46	110.33
1	B	449	ASN	CA-CB-CG	5.03	117.63	112.60
1	C	221	GLN	O-C-N	5.03	128.88	123.10
1	B	871	GLU	CB-CG-CD	-5.03	104.05	112.60
1	D	580	GLU	N-CA-CB	5.03	118.08	110.14
1	B	777	LEU	N-CA-CB	5.03	117.27	110.59
1	D	130	ASP	CA-C-O	5.03	126.72	121.19
1	A	65	ALA	CA-C-O	5.02	124.63	119.76
1	A	177	LEU	N-CA-C	5.02	117.89	110.46
1	D	920	LEU	CA-C-O	5.02	126.01	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ASN	CA-CB-CG	5.02	117.62	112.60
1	D	69	VAL	O-C-N	5.02	126.82	121.10
1	C	917	ARG	CD-NE-CZ	-5.02	117.37	124.40
1	C	52	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	640	SER	CB-CA-C	-5.01	101.58	109.80
1	B	392	TYR	CB-CA-C	-5.01	103.17	110.03
1	D	67	GLU	CB-CA-C	-5.01	100.45	110.42
1	D	150	PHE	CA-C-N	5.01	130.19	122.93
1	D	150	PHE	C-N-CA	5.01	130.19	122.93
1	D	516	PRO	CB-CA-C	-5.01	104.42	110.98
1	C	98	PRO	CB-CA-C	-5.00	104.42	110.98
1	D	98	PRO	N-CA-CB	5.00	107.98	103.33
1	C	740	LEU	CA-C-O	5.00	126.67	120.92

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	689	GLU	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	329	ASP	Sidechain

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	206	1
1	B	8125	0	7716	223	0
1	C	8125	0	7716	247	0
1	D	8125	0	7716	230	0
2	A	10	0	9	0	0
2	B	10	0	9	1	0
2	C	10	0	9	0	0
2	D	10	0	9	2	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	A	100	0	150	24	0
5	B	108	0	162	29	0
5	C	112	0	168	30	0
5	D	92	0	138	21	0
6	A	992	0	0	27	0
6	B	995	0	0	16	0
6	C	946	0	0	22	1
6	D	980	0	0	22	0
All	All	36890	0	31518	920	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (920) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:GLN:H	1:C:634:GLN:NE2	1.47	1.13
1:C:102:ASN:HD22	5:C:8506:DMS:H11	1.12	1.13
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.33	1.10
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.54	1.05
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.37	1.02
1:B:797:GLU:HG2	1:B:799:THR:HG23	1.35	1.02
1:B:600:GLN:H	1:B:600:GLN:HE21	1.09	0.98
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.45	0.96
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.30	0.94
1:B:699:ARG:NH2	5:B:8415:DMS:H11	1.82	0.94
1:D:653:HIS:CD2	1:D:667:GLU:HB3	2.03	0.93
1:C:755:ARG:HG2	1:C:769:TRP:CE3	2.02	0.93
1:D:804:ASN:HA	1:D:809:ARG:HE	1.30	0.93
1:B:744:GLU:CB	1:B:745:MET:HE3	1.98	0.92
1:D:653:HIS:HD2	1:D:667:GLU:HB3	1.36	0.91
1:A:600:GLN:H	1:A:600:GLN:HE21	1.17	0.91
1:B:367:MET:HE2	1:B:372:MET:HG3	1.51	0.91
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.34	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:CD2	1:D:701:VAL:HB	2.01	0.91
1:D:804:ASN:HD22	1:D:809:ARG:CZ	1.85	0.90
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.88	0.89
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.38	0.88
1:B:655:MET:HE2	1:B:665:SER:HB3	1.55	0.86
1:D:804:ASN:HA	1:D:809:ARG:NE	1.89	0.85
1:A:735:HIS:ND1	1:A:735:HIS:N	2.24	0.85
1:B:102:ASN:ND2	5:B:8506:DMS:H11	1.92	0.84
1:B:668:VAL:HG12	1:B:669:PRO:HD2	1.57	0.83
1:C:634:GLN:NE2	1:C:634:GLN:N	2.26	0.83
1:B:744:GLU:HB3	1:B:745:MET:HE3	1.61	0.83
1:A:797:GLU:O	1:A:801:ILE:HD13	1.79	0.82
1:B:102:ASN:HD22	5:B:8506:DMS:H11	1.42	0.82
1:D:843:GLN:HG2	1:D:848:THR:HA	1.61	0.82
1:B:730:LEU:HD12	1:B:730:LEU:H	1.44	0.82
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.29	0.81
1:B:634:GLN:HG2	1:B:682:LEU:O	1.80	0.81
1:C:824:GLN:HG2	1:C:825:CYS:N	1.96	0.81
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.62	0.80
1:A:267:VAL:O	5:A:8602:DMS:H23	1.82	0.80
1:D:804:ASN:CB	1:D:809:ARG:HH21	1.93	0.80
1:C:367:MET:HE3	1:C:367:MET:HA	1.61	0.79
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.17	0.79
1:D:807:VAL:O	1:D:811:LYS:HG3	1.83	0.79
1:D:802:ASP:OD1	1:D:803:PRO:HD2	1.83	0.79
1:C:634:GLN:H	1:C:634:GLN:HE21	1.30	0.79
1:A:655:MET:HE2	1:A:656:VAL:O	1.82	0.78
1:D:651:LEU:HD23	1:D:701:VAL:HB	1.63	0.78
1:A:797:GLU:HB3	1:A:799:THR:HG23	1.63	0.78
1:B:508:GLU:OE2	5:B:8407:DMS:H11	1.82	0.78
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.17	0.78
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.64	0.77
1:C:72:SER:HB3	6:C:9337:HOH:O	1.84	0.77
1:C:765:LEU:HD21	1:C:768:MET:HE3	1.66	0.77
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.67	0.77
1:D:230:ARG:HD3	6:D:9630:HOH:O	1.84	0.76
1:A:646:HIS:ND1	6:A:9408:HOH:O	2.17	0.76
1:C:777:LEU:HG	1:C:889:ALA:HA	1.68	0.76
1:D:797:GLU:O	1:D:801:ILE:HD13	1.85	0.76
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.50	0.76
6:B:9363:HOH:O	5:C:8420:DMS:H22	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:ASN:ND2	5:C:8506:DMS:H11	1.96	0.76
1:B:655:MET:HG3	6:B:8989:HOH:O	1.85	0.75
1:C:292:ARG:HH12	5:C:8412:DMS:H23	1.51	0.75
1:B:142:ILE:CG1	1:B:170:GLU:HG2	2.14	0.75
1:A:65:ALA:HB1	1:A:66:PRO:HD2	1.67	0.75
5:C:8417:DMS:H22	6:C:9210:HOH:O	1.87	0.75
1:C:785:THR:O	1:C:881:ARG:HD2	1.88	0.74
1:B:797:GLU:HG2	1:B:799:THR:CG2	2.17	0.74
1:C:748:CYS:C	1:C:749:ILE:HD12	2.12	0.74
1:A:668:VAL:HG13	1:A:669:PRO:HD2	1.69	0.74
1:A:887:GLN:NE2	1:A:980:GLU:O	2.20	0.74
1:D:237:ARG:NH1	6:D:9257:HOH:O	2.20	0.74
1:B:142:ILE:HG12	1:B:170:GLU:CG	2.18	0.74
1:B:531:ARG:HB3	1:B:532:PRO:HD2	1.70	0.73
1:C:749:ILE:HD12	1:C:749:ILE:N	2.03	0.73
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.04	0.73
1:C:878:HIS:HD2	6:C:8694:HOH:O	1.71	0.73
1:C:687:GLN:HE21	1:C:687:GLN:N	1.86	0.73
1:D:634:GLN:NE2	1:D:682:LEU:O	2.22	0.73
1:C:768:MET:HE2	1:C:864:MET:HE1	1.71	0.73
1:A:233:ASP:HA	5:A:8417:DMS:H13	1.71	0.72
1:D:651:LEU:HD21	1:D:653:HIS:CE1	2.23	0.72
1:A:46:ARG:HB3	1:A:47:PRO:HD2	1.69	0.72
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.01	0.72
1:D:292:ARG:HH12	5:D:8412:DMS:C2	2.03	0.72
1:B:651:LEU:C	1:B:651:LEU:HD23	2.15	0.72
5:B:8410:DMS:H22	6:B:8878:HOH:O	1.88	0.72
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.69	0.72
1:A:277:GLU:H	1:A:277:GLU:CD	1.98	0.72
1:B:360:HIS:HE1	1:B:362:LEU:HB2	1.55	0.71
1:D:749:ILE:HD12	1:D:749:ILE:N	2.04	0.71
1:C:797:GLU:O	1:C:801:ILE:HD13	1.90	0.71
1:B:651:LEU:HD23	1:B:651:LEU:O	1.91	0.71
1:A:595:THR:HA	1:A:596:PRO:C	2.16	0.71
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.72	0.70
1:C:356:ARG:HD2	1:C:379:MET:CE	2.22	0.70
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.92	0.70
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.74	0.70
1:D:112:PRO:HD2	1:D:113:PHE:CE1	2.26	0.69
1:A:84:VAL:HA	5:A:8414:DMS:O	1.92	0.69
1:A:473:ARG:NH1	6:A:9273:HOH:O	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:730:LEU:H	1:B:730:LEU:CD1	2.00	0.69
1:B:878:HIS:HD2	6:B:8690:HOH:O	1.74	0.69
1:C:768:MET:CE	1:C:864:MET:HE1	2.22	0.69
1:D:135:GLN:C	1:D:136:GLU:HG2	2.18	0.68
1:D:622:HIS:O	1:D:625:GLN:HG3	1.92	0.68
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.29	0.68
1:A:800:ARG:O	1:A:800:ARG:HG2	1.92	0.68
1:A:749:ILE:HD12	1:A:749:ILE:N	2.08	0.68
1:B:634:GLN:HE22	1:B:684:GLU:HA	1.57	0.68
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.22	0.68
1:C:745:MET:HE3	1:C:745:MET:HA	1.76	0.68
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.23	0.68
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.27	0.68
1:C:651:LEU:HD21	1:C:653:HIS:HE1	1.57	0.68
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.76	0.68
1:C:765:LEU:HD21	1:C:768:MET:CE	2.24	0.68
1:B:236:SER:C	1:B:237:ARG:HG2	2.17	0.67
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.27	0.67
1:D:595:THR:O	5:D:8413:DMS:H12	1.94	0.67
1:D:804:ASN:HD22	1:D:809:ARG:HH21	1.39	0.67
1:A:829:THR:HG23	1:A:834:VAL:HG22	1.77	0.67
1:D:748:CYS:C	1:D:749:ILE:HD12	2.19	0.67
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.24	0.67
1:C:651:LEU:CD1	1:C:701:VAL:HB	2.24	0.67
1:B:1022:GLN:HG2	1:B:1023:LYS:N	2.09	0.67
1:D:725:ASN:HB2	6:D:9521:HOH:O	1.94	0.67
1:D:88:SER:HA	1:D:366:VAL:HG21	1.76	0.67
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:A:599:ARG:HG3	1:A:600:GLN:NE2	2.10	0.66
1:D:367:MET:HB3	1:D:372:MET:HE3	1.77	0.66
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.11	0.66
1:B:637:GLU:OE2	1:B:677:LYS:HD3	1.95	0.66
1:B:699:ARG:HH22	5:B:8415:DMS:H11	1.56	0.66
1:C:858:ILE:CD1	1:C:864:MET:HB2	2.26	0.66
5:C:8415:DMS:H11	6:C:9520:HOH:O	1.96	0.66
1:C:718:GLN:HG2	5:C:8503:DMS:C1	2.26	0.65
1:D:635:THR:HG23	1:D:681:GLU:OE1	1.95	0.65
1:A:316:HIS:CB	5:A:8406:DMS:H23	2.26	0.65
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.78	0.65
1:C:133:TRP:CD1	5:C:8504:DMS:H21	2.31	0.65
1:C:655:MET:HE2	1:C:665:SER:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ASN:HD22	5:B:8506:DMS:C1	2.10	0.65
1:B:246:MET:HE3	1:B:250:LEU:HD23	1.78	0.65
1:B:684:GLU:O	1:B:686:PRO:HD3	1.97	0.65
1:B:634:GLN:NE2	1:B:684:GLU:HA	2.12	0.65
1:C:232:ASN:ND2	1:C:237:ARG:HG3	2.12	0.65
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.26	0.65
1:A:857:ARG:HG2	6:A:9068:HOH:O	1.97	0.64
1:A:46:ARG:HB3	1:A:47:PRO:CD	2.28	0.64
1:C:367:MET:HE3	1:C:367:MET:CA	2.26	0.64
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.08	0.64
1:D:804:ASN:CA	1:D:809:ARG:HH21	2.09	0.64
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.10	0.64
1:C:658:LEU:O	1:C:661:LYS:HB2	1.98	0.64
1:C:743:SER:O	1:C:760:ARG:NH1	2.28	0.64
1:B:699:ARG:HH21	5:B:8415:DMS:H11	1.61	0.64
1:D:804:ASN:HA	1:D:809:ARG:NH2	2.13	0.64
1:C:749:ILE:HG13	1:C:834:VAL:HG11	1.81	0.63
1:D:595:THR:HA	1:D:596:PRO:C	2.23	0.63
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.79	0.63
1:B:668:VAL:CG1	1:B:669:PRO:HD2	2.29	0.63
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.79	0.63
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.78	0.63
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.04	0.63
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.95	0.63
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.30	0.63
5:A:8415:DMS:H11	6:A:9499:HOH:O	1.99	0.62
1:B:241:GLU:HG3	1:B:292:ARG:HG3	1.79	0.62
1:C:596:PRO:HB3	6:C:9379:HOH:O	1.98	0.62
1:B:615:PRO:O	1:B:618:THR:HG22	1.99	0.62
1:C:822:LEU:HD13	1:C:840:HIS:NE2	2.14	0.62
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.81	0.62
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.64	0.62
1:C:292:ARG:HH12	5:C:8412:DMS:C2	2.12	0.62
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.62
5:B:8601:DMS:H11	6:B:9437:HOH:O	2.00	0.62
1:A:878:HIS:HD2	6:A:8674:HOH:O	1.83	0.62
1:B:962:TYR:OH	5:B:8423:DMS:H21	2.00	0.61
1:D:805:ALA:O	1:D:809:ARG:HG3	2.00	0.61
1:C:858:ILE:HD11	1:C:864:MET:HB2	1.81	0.61
1:A:599:ARG:HG3	1:A:600:GLN:HE21	1.65	0.61
1:A:892:ALA:HB3	1:A:946:TYR:CE1	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.82	0.61
1:D:804:ASN:HA	1:D:809:ARG:HH21	1.65	0.61
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.35	0.61
1:A:844:HIS:HD2	6:A:9406:HOH:O	1.83	0.61
1:A:431:ARG:HG3	6:A:9338:HOH:O	1.99	0.61
1:C:887:GLN:NE2	1:C:980:GLU:O	2.32	0.61
5:B:8421:DMS:H23	6:B:9132:HOH:O	1.99	0.61
1:C:454:ILE:HG13	1:C:455:ILE:HG13	1.83	0.61
1:D:795:VAL:HG23	6:D:9473:HOH:O	1.99	0.61
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.36	0.60
1:C:734:SER:HB3	1:C:860:GLY:C	2.26	0.60
1:D:55:ASN:O	5:D:8408:DMS:H21	2.01	0.60
1:D:230:ARG:HH12	1:D:239:VAL:HG11	1.65	0.60
1:D:240:LEU:HD23	1:D:240:LEU:C	2.25	0.60
1:D:634:GLN:HB3	1:D:682:LEU:HB2	1.82	0.60
1:C:133:TRP:NE1	5:C:8504:DMS:H21	2.16	0.60
1:D:804:ASN:CA	1:D:809:ARG:HE	2.07	0.60
1:C:1020:TRP:HD1	1:C:1021:CYS:N	1.99	0.60
1:B:367:MET:CE	1:B:372:MET:HG3	2.29	0.60
1:D:804:ASN:HB2	1:D:809:ARG:HH21	1.66	0.60
1:D:472:TYR:O	1:D:476:LYS:HG2	2.02	0.60
1:A:110:ASN:OD1	6:A:9307:HOH:O	2.15	0.60
1:A:1017:GLN:HG3	1:A:1017:GLN:O	1.99	0.59
1:C:88:SER:HA	1:C:366:VAL:HG21	1.83	0.59
1:C:278:ILE:HD13	1:C:278:ILE:N	2.16	0.59
1:D:794:GLY:HA3	6:D:8986:HOH:O	2.01	0.59
1:D:91:GLN:HB3	1:D:98:PRO:HD3	1.84	0.59
1:A:640:SER:O	1:A:675:GLN:HA	2.03	0.59
1:D:128:ASN:HB3	1:D:180:GLY:O	2.03	0.59
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.68	0.59
1:A:890:GLN:HG3	1:A:891:VAL:N	2.17	0.59
1:B:37:ARG:NH1	5:B:8504:DMS:H21	2.18	0.59
1:D:473:ARG:NH1	1:D:476:LYS:HB2	2.17	0.58
1:C:237:ARG:HH11	1:C:237:ARG:HB2	1.68	0.58
1:C:719:GLN:O	5:C:8427:DMS:H13	2.03	0.58
1:D:795:VAL:HG12	6:D:9678:HOH:O	2.03	0.58
1:B:200:GLN:HG2	1:B:391:HIS:HB2	1.84	0.58
1:A:587:ALA:HB1	1:A:591:ASP:HB2	1.85	0.58
1:C:690:SER:HB2	6:C:9334:HOH:O	2.03	0.58
1:C:744:GLU:O	1:C:760:ARG:HD3	2.03	0.58
1:A:832:ASP:OD1	1:A:832:ASP:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:630:ARG:NE	1:B:637:GLU:OE1	2.36	0.58
1:D:804:ASN:C	1:D:809:ARG:HE	2.12	0.58
1:B:685:LEU:O	1:B:686:PRO:C	2.47	0.58
1:C:796:SER:OG	1:C:802:ASP:N	2.28	0.58
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.39	0.58
1:B:600:GLN:HE21	1:B:600:GLN:N	1.91	0.58
1:B:1022:GLN:HG2	1:B:1023:LYS:O	2.04	0.58
1:D:593:GLY:O	1:D:595:THR:HG22	2.03	0.58
1:D:393:PRO:HD3	1:D:412:GLU:O	2.03	0.58
1:B:631:LEU:HD12	1:B:635:THR:O	2.04	0.58
1:A:336:ARG:HB2	5:A:8409:DMS:H21	1.85	0.57
1:A:687:GLN:HG3	6:A:9416:HOH:O	2.02	0.57
1:C:768:MET:O	1:C:775:GLN:N	2.37	0.57
1:C:778:THR:HG23	1:C:887:GLN:CB	2.34	0.57
1:A:599:ARG:HG3	1:A:600:GLN:H	1.68	0.57
1:D:375:ASP:O	1:D:379:MET:HG3	2.05	0.57
1:C:249:GLU:OE2	1:C:251:ARG:HD3	2.04	0.57
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.85	0.57
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.69	0.57
1:D:873:ALA:O	1:D:876:THR:HG22	2.05	0.57
1:A:132:SER:HB2	5:A:8504:DMS:H21	1.87	0.57
1:D:878:HIS:HD2	6:D:8814:HOH:O	1.88	0.57
1:A:279:ILE:HD11	1:D:422:PRO:HG2	1.86	0.56
1:A:683:PRO:O	1:A:685:LEU:HG	2.04	0.56
1:C:508:GLU:OE2	5:C:8407:DMS:H11	2.05	0.56
1:C:906:TYR:HB3	1:C:907:PRO:HD2	1.87	0.56
1:D:130:ASP:OD2	5:D:8703:DMS:H23	2.05	0.56
1:C:781:ARG:NH1	6:C:9326:HOH:O	2.38	0.56
1:C:802:ASP:O	1:C:808:GLU:HG3	2.05	0.56
1:A:745:MET:HE1	1:A:761:GLN:HB2	1.87	0.56
1:B:577:LYS:O	1:B:584:PRO:HA	2.04	0.56
1:A:290:THR:O	5:A:8412:DMS:H23	2.04	0.56
1:B:429:ASP:OD1	1:B:430:PRO:HD2	2.04	0.56
1:D:682:LEU:HD22	1:D:683:PRO:HD2	1.85	0.56
1:C:651:LEU:HD11	1:C:701:VAL:HB	1.88	0.56
1:C:843:GLN:NE2	1:C:848:THR:OG1	2.37	0.56
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.38	0.56
1:A:668:VAL:CG1	1:A:669:PRO:HD2	2.36	0.55
1:B:646:HIS:CE1	1:B:673:ALA:HB2	2.42	0.55
1:D:277:GLU:OE1	5:D:8412:DMS:O	2.25	0.55
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:GLY:HA3	5:B:8408:DMS:H11	1.89	0.55
1:A:625:GLN:NE2	6:A:8804:HOH:O	2.39	0.55
1:C:651:LEU:CD2	1:C:653:HIS:HE1	2.19	0.55
1:A:649:ASN:HA	5:A:8425:DMS:H12	1.88	0.55
1:A:655:MET:HE3	1:A:664:ALA:O	2.07	0.55
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.42	0.55
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.89	0.55
1:A:653:HIS:CD2	1:A:667:GLU:HG2	2.42	0.55
1:B:233:ASP:HA	5:B:8417:DMS:H13	1.88	0.55
1:D:629:PHE:O	1:D:630:ARG:NH1	2.35	0.55
1:D:891:VAL:HG23	1:D:981:GLY:HA2	1.89	0.55
1:C:786:ARG:HG2	1:C:880:ALA:HB1	1.89	0.55
1:B:595:THR:HA	1:B:596:PRO:C	2.32	0.55
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.89	0.55
1:B:634:GLN:HG2	1:B:682:LEU:HB2	1.89	0.55
1:B:37:ARG:HH12	5:B:8504:DMS:H21	1.71	0.54
1:B:655:MET:SD	1:B:656:VAL:N	2.80	0.54
1:D:688:PRO:C	1:D:690:SER:H	2.14	0.54
5:B:8420:DMS:H23	6:C:9115:HOH:O	2.06	0.54
1:C:654:TRP:O	1:C:665:SER:HB2	2.07	0.54
1:D:128:ASN:HB2	6:D:9631:HOH:O	2.06	0.54
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.14	0.54
1:A:316:HIS:HB2	5:A:8406:DMS:H23	1.88	0.54
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.36	0.54
1:B:878:HIS:CD2	6:B:8690:HOH:O	2.54	0.54
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.89	0.54
1:A:843:GLN:HG2	1:A:848:THR:HA	1.89	0.54
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.42	0.54
1:B:863:GLN:HG3	1:B:1021:CYS:CB	2.37	0.54
1:C:765:LEU:CD2	1:C:768:MET:HE3	2.36	0.54
1:A:416:GLU:OE2	1:A:418:HIS:HB2	2.07	0.54
1:D:521:LYS:HE2	6:D:9163:HOH:O	2.08	0.54
1:A:759:ASN:OD1	1:A:761:GLN:N	2.38	0.54
1:A:830:LEU:HD12	1:A:833:ALA:HB3	1.90	0.54
5:A:8420:DMS:H22	6:D:9470:HOH:O	2.07	0.54
1:B:30:HIS:HB2	1:B:31:PRO:HD2	1.89	0.54
1:D:340:GLY:O	1:D:561:ARG:HG2	2.08	0.54
1:D:847:LYS:HG3	1:D:848:THR:N	2.18	0.54
5:C:8503:DMS:H21	6:C:9425:HOH:O	2.08	0.54
1:D:843:GLN:CG	1:D:848:THR:HA	2.35	0.54
1:B:499:ILE:HD11	1:B:529:GLU:CD	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:824:GLN:OE1	1:C:837:THR:HG22	2.08	0.54
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.76	0.54
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.38	0.53
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.76	0.53
1:D:801:ILE:CG2	1:D:802:ASP:H	2.21	0.53
1:A:518:TRP:O	1:A:519:SER:C	2.51	0.53
1:C:652:LEU:HD23	1:C:680:ILE:HD13	1.90	0.53
1:C:832:ASP:OD1	1:C:832:ASP:N	2.41	0.53
1:C:843:GLN:HA	1:C:847:LYS:O	2.07	0.53
1:D:577:LYS:O	1:D:584:PRO:HA	2.08	0.53
5:D:8409:DMS:H23	6:D:9076:HOH:O	2.06	0.53
1:A:240:LEU:C	1:A:240:LEU:HD23	2.32	0.53
1:C:595:THR:HA	1:C:596:PRO:C	2.32	0.53
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.43	0.53
5:A:8406:DMS:H12	6:A:9397:HOH:O	2.07	0.53
1:C:948:PRO:O	1:C:1023:LYS:N	2.34	0.53
1:B:599:ARG:HH11	1:B:600:GLN:NE2	2.05	0.53
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.43	0.53
1:D:36:TRP:CD2	1:D:42:ALA:HA	2.43	0.53
1:C:333:ARG:O	1:C:333:ARG:HD3	2.08	0.53
1:D:736:ALA:C	1:D:737:ILE:HG22	2.34	0.53
1:C:46:ARG:HG2	6:C:9473:HOH:O	2.07	0.53
1:D:802:ASP:O	1:D:804:ASN:N	2.42	0.53
1:D:843:GLN:HG2	1:D:848:THR:CA	2.36	0.53
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.39	0.53
1:A:577:LYS:O	1:A:584:PRO:HA	2.09	0.53
1:C:809:ARG:NH2	1:C:1001:PRO:CG	2.72	0.53
1:A:77:ASP:O	1:A:79:PRO:HD3	2.10	0.52
1:B:272:ALA:HB1	1:B:273:PRO:HD2	1.90	0.52
1:C:600:GLN:HB2	1:C:603:MET:HE2	1.91	0.52
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.17	0.52
1:B:231:PHE:O	5:B:8417:DMS:H23	2.10	0.52
1:C:796:SER:HB2	1:C:802:ASP:HB3	1.92	0.52
1:B:797:GLU:HB3	1:B:800:ARG:H	1.73	0.52
1:C:755:ARG:HG2	1:C:769:TRP:HE3	1.70	0.52
1:D:292:ARG:HH12	5:D:8412:DMS:H23	1.73	0.52
1:A:93:HIS:CD2	5:A:8414:DMS:H11	2.45	0.52
1:C:572:ASP:HB3	1:C:603:MET:HG2	1.91	0.52
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.39	0.52
1:A:527:PRO:HB3	1:B:339:ASN:O	2.09	0.52
1:C:367:MET:HB3	1:C:372:MET:HE3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:687:GLN:HE21	1:C:687:GLN:H	1.56	0.52
1:D:84:VAL:HA	5:D:8414:DMS:H11	1.90	0.52
1:B:890:GLN:HB3	6:B:9524:HOH:O	2.09	0.52
1:D:801:ILE:HG22	1:D:802:ASP:N	2.25	0.52
1:A:446:ARG:HG2	1:A:447:ASP:OD1	2.09	0.52
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.22	0.52
1:C:78:LEU:HB3	1:C:80:GLU:HG3	1.92	0.52
1:C:622:HIS:CE1	5:C:8402:DMS:H12	2.45	0.52
1:D:718:GLN:NE2	5:D:8503:DMS:H11	2.24	0.52
1:C:861:SER:OG	1:C:863:GLN:HG3	2.10	0.52
1:C:890:GLN:HG3	1:C:891:VAL:N	2.22	0.52
1:C:750:GLU:OE2	1:C:755:ARG:HB2	2.10	0.52
1:B:863:GLN:CG	1:B:1021:CYS:HB3	2.38	0.51
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.92	0.51
1:D:167:LEU:HB3	1:D:168:PRO:HD2	1.92	0.51
1:A:433:LEU:N	1:A:434:PRO:CD	2.73	0.51
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.45	0.51
1:C:824:GLN:HG2	1:C:825:CYS:H	1.74	0.51
1:D:800:ARG:O	1:D:801:ILE:O	2.29	0.51
1:C:746:ASP:CA	1:C:760:ARG:HG3	2.24	0.51
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.93	0.51
1:D:972:HIS:HB3	1:D:974:HIS:ND1	2.25	0.51
1:B:847:LYS:HG2	1:B:849:LEU:HD23	1.93	0.51
1:C:367:MET:HE3	1:C:368:ASP:H	1.76	0.51
1:C:749:ILE:CG1	1:C:834:VAL:HG11	2.40	0.51
1:A:949:HIS:HB2	1:A:951:TRP:CH2	2.46	0.51
1:B:105:TYR:CE1	1:B:419:GLY:HA3	2.46	0.51
1:B:873:ALA:O	1:B:876:THR:HG22	2.11	0.51
1:D:640:SER:O	1:D:675:GLN:HA	2.10	0.51
1:A:250:LEU:HD11	1:A:286:ALA:O	2.11	0.51
1:C:615:PRO:O	1:C:618:THR:HG22	2.11	0.51
1:A:433:LEU:N	1:A:434:PRO:HD2	2.26	0.51
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.93	0.51
1:A:316:HIS:CG	5:A:8406:DMS:H23	2.46	0.51
1:A:735:HIS:O	1:A:736:ALA:HB2	2.09	0.51
1:C:796:SER:CB	1:C:802:ASP:H	2.24	0.51
1:C:114:VAL:HB	1:C:115:PRO:HD2	1.92	0.50
1:C:745:MET:HA	1:C:745:MET:CE	2.32	0.50
1:A:106:PRO:O	5:A:8410:DMS:H23	2.11	0.50
1:B:730:LEU:HD12	1:B:730:LEU:N	2.21	0.50
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:LEU:O	1:D:345:ASN:C	2.52	0.50
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.47	0.50
1:B:173:LEU:O	1:B:174:SER:C	2.52	0.50
1:C:784:PHE:CD1	1:C:850:PHE:CD1	2.99	0.50
1:C:906:TYR:HB3	1:C:907:PRO:CD	2.42	0.50
1:A:352:ARG:HD3	1:A:624:GLN:HB3	1.93	0.50
1:A:844:HIS:CE1	1:A:845:GLN:HG3	2.47	0.50
1:B:230:ARG:NH1	1:B:241:GLU:OE1	2.44	0.50
1:B:531:ARG:HB3	1:B:532:PRO:CD	2.41	0.50
1:B:753:ASN:N	1:B:753:ASN:OD1	2.45	0.50
1:C:680:ILE:O	1:C:680:ILE:HG22	2.07	0.50
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.10	0.50
1:D:891:VAL:CG2	1:D:981:GLY:HA2	2.42	0.50
1:A:237:ARG:HH11	1:A:237:ARG:CB	2.23	0.50
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.93	0.50
1:C:833:ALA:HB1	1:C:858:ILE:O	2.11	0.50
1:D:599:ARG:HG3	1:D:600:GLN:H	1.76	0.50
1:A:473:ARG:NH1	1:A:476:LYS:CB	2.74	0.50
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.93	0.50
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.46	0.50
1:C:847:LYS:NZ	1:D:724:GLU:O	2.45	0.50
5:D:8406:DMS:H22	6:D:9612:HOH:O	2.12	0.50
1:A:127:PHE:N	1:A:127:PHE:CD2	2.79	0.50
1:A:167:LEU:HD21	1:A:393:PRO:HG2	1.94	0.50
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.12	0.50
1:D:78:LEU:HD23	6:D:9218:HOH:O	2.11	0.50
1:D:801:ILE:CG2	1:D:802:ASP:N	2.75	0.50
1:A:921:PRO:O	1:A:922:LEU:C	2.55	0.50
1:B:1017:GLN:HB2	6:B:9517:HOH:O	2.12	0.50
1:C:266:GLN:NE2	5:C:8602:DMS:S	2.85	0.50
1:B:320:GLY:O	5:B:8406:DMS:O	2.29	0.49
1:C:37:ARG:HG3	1:C:37:ARG:HH11	1.77	0.49
1:A:717:TRP:CH2	5:A:8415:DMS:H12	2.47	0.49
1:B:684:GLU:HG2	1:B:685:LEU:N	2.27	0.49
1:D:513:PRO:O	1:D:514:ALA:HB3	2.12	0.49
1:B:872:VAL:O	1:B:873:ALA:C	2.55	0.49
1:C:724:GLU:O	1:D:847:LYS:NZ	2.44	0.49
1:D:667:GLU:C	1:D:668:VAL:HG23	2.36	0.49
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.09	0.49
1:A:809:ARG:HH11	1:A:809:ARG:CG	2.20	0.49
1:B:450:HIS:HE1	6:B:9574:HOH:O	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:797:GLU:CG	1:B:799:THR:HG23	2.25	0.49
1:D:219:THR:HG21	6:D:9649:HOH:O	2.12	0.49
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.95	0.49
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.94	0.49
1:B:869:ASP:OD1	1:B:1015:HIS:ND1	2.45	0.49
1:C:249:GLU:CD	1:C:251:ARG:HD3	2.38	0.49
1:B:291:LEU:HD12	5:B:8405:DMS:H12	1.94	0.49
5:C:8427:DMS:H22	6:C:9051:HOH:O	2.12	0.49
1:B:142:ILE:HG22	6:B:8857:HOH:O	2.12	0.49
1:B:262:GLN:HE21	1:B:262:GLN:C	2.21	0.49
1:C:608:PHE:CE1	1:C:614:HIS:CD2	3.00	0.49
1:C:824:GLN:O	1:C:838:THR:HA	2.13	0.49
1:D:441:THR:O	1:D:445:GLN:HG3	2.12	0.49
1:D:829:THR:HG22	1:D:830:LEU:N	2.28	0.49
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.12	0.49
1:A:624:GLN:NE2	6:A:8624:HOH:O	2.45	0.49
1:C:92:MET:HE3	1:C:205:MET:SD	2.53	0.49
1:D:251:ARG:HD2	5:D:8416:DMS:C1	2.42	0.49
1:D:654:TRP:CZ3	1:D:665:SER:HA	2.48	0.49
5:A:8502:DMS:H13	6:A:9319:HOH:O	2.12	0.49
1:B:729:THR:HG23	6:B:9217:HOH:O	2.12	0.49
1:B:843:GLN:HA	1:B:847:LYS:O	2.13	0.49
1:C:240:LEU:C	1:C:240:LEU:HD23	2.37	0.49
1:C:696:LEU:O	1:C:719:GLN:HA	2.12	0.49
1:D:847:LYS:HG2	1:D:849:LEU:HD23	1.95	0.49
1:B:601:PHE:HB3	6:B:9551:HOH:O	2.13	0.48
1:B:694:LEU:HD12	1:B:723:ALA:HB3	1.94	0.48
1:C:796:SER:OG	1:C:801:ILE:HA	2.13	0.48
1:D:502:MET:HA	1:D:537:GLU:O	2.13	0.48
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.95	0.48
1:A:702:GLN:O	1:A:712:GLY:N	2.43	0.48
1:B:133:TRP:CD1	5:B:8504:DMS:H12	2.47	0.48
1:C:237:ARG:NH1	1:C:237:ARG:CB	2.76	0.48
1:C:285:TYR:HB3	1:C:288:ARG:HG3	1.95	0.48
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.95	0.48
1:A:59:ARG:HG2	5:A:8502:DMS:H12	1.95	0.48
1:A:237:ARG:HH11	1:A:237:ARG:CG	2.26	0.48
1:A:768:MET:CE	1:A:1020:TRP:CZ2	2.94	0.48
5:A:8503:DMS:H13	6:A:9015:HOH:O	2.13	0.48
1:B:843:GLN:HG2	1:B:848:THR:HA	1.95	0.48
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:844:HIS:HD2	6:C:9418:HOH:O	1.95	0.48
1:D:143:PHE:O	1:D:168:PRO:HA	2.13	0.48
1:D:305:ILE:HD11	1:D:645:ARG:HB3	1.95	0.48
1:A:344:LEU:O	1:A:345:ASN:C	2.56	0.48
1:C:546:LEU:HA	6:C:8749:HOH:O	2.13	0.48
5:C:8427:DMS:H11	6:C:8829:HOH:O	2.13	0.48
1:D:893:GLU:HG3	1:D:894:ARG:CD	2.44	0.48
1:A:587:ALA:HB1	1:A:591:ASP:CB	2.42	0.48
1:A:651:LEU:C	1:A:651:LEU:HD12	2.39	0.48
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.81	0.48
1:B:262:GLN:NE2	1:B:263:GLY:N	2.61	0.48
1:C:102:ASN:HD22	5:C:8506:DMS:C1	2.03	0.48
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.49	0.48
1:D:598:ASP:O	1:D:601:PHE:HB2	2.14	0.48
1:A:806:TRP:CE2	1:A:991:MET:HE1	2.49	0.48
1:B:102:ASN:OD1	1:B:201:ASP:HB2	2.12	0.48
1:C:703:PRO:O	1:C:711:ALA:HB1	2.13	0.48
1:C:740:LEU:HA	1:C:748:CYS:O	2.14	0.48
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.95	0.48
1:C:242:ALA:O	1:C:290:THR:HA	2.14	0.48
1:D:159:VAL:HG22	1:D:176:PHE:CE2	2.48	0.48
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.13	0.48
1:C:746:ASP:HA	1:C:760:ARG:CG	2.23	0.48
1:D:201:ASP:OD2	2:D:2001:2DG:O4	2.25	0.48
1:D:808:GLU:OE1	1:D:811:LYS:HE3	2.13	0.48
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.14	0.48
1:B:568:TRP:CH2	2:B:2001:2DG:H3	2.49	0.48
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.96	0.48
1:A:279:ILE:HG23	1:A:279:ILE:HD13	1.62	0.47
1:A:974:HIS:HB3	6:A:9019:HOH:O	2.14	0.47
1:B:14:ARG:HA	1:B:16:TRP:CZ3	2.48	0.47
1:B:36:TRP:CD1	1:B:48:SER:HB2	2.48	0.47
1:D:145:GLY:N	1:D:210:ARG:HB2	2.28	0.47
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.28	0.47
1:D:1020:TRP:HD1	1:D:1021:CYS:N	2.11	0.47
1:D:354:VAL:O	1:D:387:VAL:HA	2.14	0.47
1:A:249:GLU:HG2	1:A:251:ARG:NE	2.29	0.47
1:B:537:GLU:HA	1:B:566:PHE:O	2.14	0.47
1:C:220:THR:HG23	1:C:246:MET:HE2	1.97	0.47
1:D:718:GLN:HG2	5:D:8503:DMS:C1	2.44	0.47
1:A:646:HIS:NE2	1:A:671:ASP:OD1	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:542:MET:HA	1:C:604:ASN:HA	1.95	0.47
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.49	0.47
1:B:646:HIS:CE1	1:B:673:ALA:CB	2.97	0.47
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.96	0.47
1:C:533:LEU:C	1:C:533:LEU:HD23	2.39	0.47
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.97	0.47
1:B:126:THR:HA	1:B:182:ASN:O	2.14	0.47
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.45	0.47
1:D:654:TRP:CZ2	1:D:683:PRO:HG2	2.50	0.47
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.31	0.47
1:B:71:GLU:H	1:B:71:GLU:CD	2.22	0.47
1:B:377:LEU:O	1:B:381:GLN:HG3	2.15	0.47
1:B:807:VAL:CG1	1:B:808:GLU:N	2.76	0.47
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.68	0.47
1:C:780:LEU:HA	1:C:886:CYS:HB3	1.97	0.47
1:D:230:ARG:HH12	1:D:239:VAL:CG1	2.25	0.47
1:D:292:ARG:NH1	5:D:8412:DMS:C2	2.76	0.47
1:D:545:SER:O	1:D:909:ARG:HD3	2.15	0.47
1:D:893:GLU:HG3	1:D:894:ARG:HD2	1.96	0.47
1:D:986:ILE:O	1:D:986:ILE:HG22	2.10	0.47
1:B:655:MET:SD	1:B:656:VAL:O	2.72	0.47
1:C:91:GLN:HG2	1:C:98:PRO:HA	1.96	0.47
1:A:871:GLU:OE1	1:B:726:LEU:HD22	2.15	0.47
1:A:50:GLN:N	1:A:50:GLN:CD	2.73	0.47
1:A:628:GLN:HG3	6:A:9028:HOH:O	2.15	0.47
1:A:959:ILE:HG23	1:A:959:ILE:O	2.14	0.47
1:A:1013:ARG:HH11	1:A:1013:ARG:HD3	1.58	0.47
1:B:628:GLN:HE22	5:B:8402:DMS:C2	2.28	0.47
1:C:525:SER:HB3	1:D:525:SER:HB3	1.97	0.47
1:B:13:ARG:O	1:B:14:ARG:C	2.58	0.46
1:B:807:VAL:HG13	1:B:808:GLU:N	2.31	0.46
1:D:785:THR:HB	1:D:816:TYR:CE2	2.50	0.46
1:A:260:LEU:O	1:A:267:VAL:HG22	2.15	0.46
1:C:749:ILE:O	1:C:755:ARG:HA	2.15	0.46
1:D:277:GLU:CD	1:D:277:GLU:H	2.19	0.46
1:D:473:ARG:HH11	1:D:476:LYS:HB2	1.79	0.46
1:A:125:LEU:O	1:A:183:ARG:HA	2.15	0.46
1:B:578:TYR:HA	1:B:583:ASN:O	2.15	0.46
1:B:661:LYS:O	1:B:663:LEU:HD23	2.15	0.46
1:C:651:LEU:HD22	1:C:667:GLU:HG2	1.97	0.46
1:D:363:HIS:HD2	6:D:9298:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:TYR:CD1	1:B:419:GLY:HA3	2.51	0.46
1:D:112:PRO:HD2	1:D:113:PHE:CD1	2.51	0.46
1:D:291:LEU:HD22	1:D:291:LEU:N	2.30	0.46
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.98	0.46
1:D:654:TRP:CZ2	1:D:683:PRO:CG	2.98	0.46
1:A:117:GLU:HG3	6:A:9004:HOH:O	2.16	0.46
1:A:599:ARG:CG	1:A:600:GLN:NE2	2.79	0.46
1:A:863:GLN:HG2	1:A:1021:CYS:CB	2.39	0.46
1:B:282:ARG:HB2	1:C:423:MET:N	2.31	0.46
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.34	0.46
1:B:519:SER:HB3	1:B:522:LYS:HB3	1.96	0.46
1:C:13:ARG:O	1:C:14:ARG:C	2.58	0.46
1:C:720:TRP:HA	5:C:8427:DMS:H11	1.97	0.46
1:C:749:ILE:N	1:C:749:ILE:CD1	2.75	0.46
1:C:995:GLY:O	1:C:996:ASP:C	2.57	0.46
1:A:65:ALA:CB	1:A:66:PRO:HD2	2.39	0.46
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.80	0.46
1:C:1020:TRP:CD1	1:C:1021:CYS:N	2.82	0.46
1:B:433:LEU:N	1:B:434:PRO:CD	2.79	0.46
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.49	0.46
1:D:65:ALA:HB1	1:D:67:GLU:OE1	2.15	0.46
1:D:972:HIS:HB3	1:D:974:HIS:HD1	1.79	0.46
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.98	0.46
5:C:8423:DMS:H21	6:C:9152:HOH:O	2.15	0.46
1:D:618:THR:HG21	6:D:9054:HOH:O	2.15	0.46
5:D:8419:DMS:H21	6:D:9465:HOH:O	2.14	0.46
1:B:88:SER:HA	1:B:366:VAL:HG21	1.98	0.46
1:B:183:ARG:NH1	6:B:8921:HOH:O	2.39	0.46
1:C:629:PHE:HA	1:C:637:GLU:O	2.16	0.46
1:C:658:LEU:O	1:C:659:ASP:C	2.57	0.46
1:C:858:ILE:HD13	1:C:864:MET:HB2	1.97	0.46
1:C:96:ASP:HB2	6:C:8977:HOH:O	2.15	0.46
1:C:743:SER:O	1:C:744:GLU:C	2.56	0.46
1:A:59:ARG:HG2	5:A:8502:DMS:C1	2.47	0.45
1:A:158:TRP:CZ2	1:A:160:GLY:HA2	2.50	0.45
1:C:178:ARG:HE	1:C:178:ARG:HB3	1.28	0.45
5:C:8427:DMS:H13	6:C:9051:HOH:O	2.15	0.45
1:B:658:LEU:O	1:B:661:LYS:HG3	2.16	0.45
1:B:661:LYS:HA	1:B:662:PRO:HD3	1.48	0.45
1:C:367:MET:HA	1:C:367:MET:CE	2.39	0.45
1:C:475:ILE:HD13	1:C:475:ILE:HG21	1.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:664:ALA:O	1:D:665:SER:HB3	2.15	0.45
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.98	0.45
5:A:8420:DMS:C2	6:D:9470:HOH:O	2.64	0.45
1:B:91:GLN:HG2	1:B:98:PRO:HA	1.98	0.45
1:C:230:ARG:O	1:C:238:ALA:HA	2.17	0.45
1:C:651:LEU:CD2	1:C:653:HIS:CE1	2.99	0.45
1:A:88:SER:HA	1:A:366:VAL:HG21	1.98	0.45
1:A:593:GLY:O	1:A:595:THR:HG22	2.15	0.45
1:B:925:MET:HB3	6:B:8644:HOH:O	2.16	0.45
1:C:581:ASN:HB2	1:C:583:ASN:ND2	2.32	0.45
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.51	0.45
1:D:804:ASN:HD22	1:D:809:ARG:NE	2.12	0.45
1:A:802:ASP:O	1:A:808:GLU:HG3	2.17	0.45
1:D:749:ILE:N	1:D:749:ILE:CD1	2.72	0.45
1:A:685:LEU:CB	1:A:686:PRO:CD	2.95	0.45
1:B:252:ASP:OD2	5:B:8416:DMS:H12	2.16	0.45
1:B:474:TRP:O	1:B:478:VAL:HG13	2.16	0.45
1:B:601:PHE:CE2	5:B:8506:DMS:H23	2.52	0.45
1:B:734:SER:CB	1:B:860:GLY:HA3	2.47	0.45
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.51	0.45
1:D:942:ARG:HA	1:D:953:GLY:O	2.17	0.45
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.44	0.45
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.52	0.45
1:B:663:LEU:O	1:B:664:ALA:HB2	2.16	0.45
1:C:838:THR:OG1	1:C:854:LYS:HB2	2.17	0.45
1:C:933:SER:O	1:C:934:GLU:C	2.58	0.45
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.77	0.45
1:D:473:ARG:HD2	1:D:473:ARG:HA	1.80	0.45
1:D:654:TRP:CE3	1:D:655:MET:HA	2.51	0.45
1:B:73:TRP:CZ2	1:B:122:CYS:HB3	2.52	0.45
1:B:822:LEU:HD11	1:B:824:GLN:O	2.17	0.45
1:B:937:LEU:HA	1:B:957:PHE:O	2.16	0.45
1:C:737:ILE:HA	1:C:738:PRO:HD3	1.90	0.45
1:B:262:GLN:C	1:B:262:GLN:NE2	2.75	0.45
1:B:734:SER:HB2	1:B:860:GLY:HA3	1.99	0.45
1:C:809:ARG:HH21	1:C:1001:PRO:HG3	1.81	0.45
1:D:842:TRP:C	1:D:843:GLN:HG3	2.42	0.45
1:A:701:VAL:O	1:A:703:PRO:HD3	2.17	0.45
1:A:990:HIS:HD2	1:A:991:MET:O	2.00	0.45
1:B:646:HIS:CE1	1:B:673:ALA:CA	3.00	0.45
1:D:370:GLN:HB2	6:D:9235:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:639:THR:OG1	1:D:677:LYS:HG3	2.16	0.45
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.52	0.45
1:A:1004:SER:O	1:A:1005:ALA:C	2.59	0.44
1:B:945:ASN:HB3	1:B:1023:LYS:CE	2.46	0.44
1:C:375:ASP:HB3	1:C:379:MET:HE3	1.99	0.44
1:C:756:TRP:CE2	1:C:858:ILE:HD12	2.52	0.44
1:C:777:LEU:HD23	1:C:777:LEU:HA	1.69	0.44
1:C:881:ARG:C	1:C:882:ILE:HG13	2.42	0.44
1:D:251:ARG:HD2	5:D:8416:DMS:H12	1.99	0.44
1:A:80:GLU:O	1:A:80:GLU:HG2	2.15	0.44
1:A:262:GLN:HG3	6:A:9568:HOH:O	2.17	0.44
1:A:429:ASP:HA	1:A:430:PRO:HD2	1.86	0.44
1:A:460:ASN:O	1:A:461:GLU:C	2.60	0.44
1:A:472:TYR:O	1:A:476:LYS:HG2	2.18	0.44
1:A:712:GLY:O	1:A:713:HIS:C	2.59	0.44
1:C:557:ARG:HD2	6:C:8638:HOH:O	2.17	0.44
1:D:147:ASN:HA	1:D:148:SER:HA	1.60	0.44
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.52	0.44
1:B:923:SER:HA	5:B:8508:DMS:H12	1.99	0.44
1:C:746:ASP:C	1:C:760:ARG:HD2	2.42	0.44
1:D:650:GLU:HB3	1:D:670:LEU:HD12	1.99	0.44
1:A:126:THR:HA	1:A:182:ASN:O	2.18	0.44
1:A:577:LYS:HD3	1:A:587:ALA:HB2	1.98	0.44
1:B:347:LYS:HB2	1:B:643:LEU:HD13	1.99	0.44
1:B:367:MET:HE2	1:B:372:MET:CG	2.34	0.44
1:B:674:PRO:O	1:B:675:GLN:HB2	2.18	0.44
1:B:817:GLN:NE2	1:B:817:GLN:HA	2.32	0.44
1:D:844:HIS:O	1:D:845:GLN:C	2.57	0.44
1:B:670:LEU:HD23	1:B:670:LEU:HA	1.68	0.44
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.69	0.44
1:D:130:ASP:O	1:D:131:GLU:C	2.61	0.44
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.52	0.44
1:A:90:TRP:CZ3	1:A:121:GLY:HA3	2.53	0.44
1:A:339:ASN:O	1:B:527:PRO:HB3	2.17	0.44
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.52	0.44
1:A:668:VAL:HA	1:A:669:PRO:HD3	1.81	0.44
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.18	0.44
1:C:50:GLN:CD	1:C:50:GLN:N	2.75	0.44
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.99	0.44
5:A:8420:DMS:H22	6:A:9586:HOH:O	2.18	0.44
1:C:152:LEU:HD11	1:C:184:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:326:GLU:O	1:C:327:ALA:HB2	2.17	0.44
1:C:781:ARG:NH1	1:C:781:ARG:HG2	2.33	0.44
1:C:872:VAL:O	1:C:873:ALA:C	2.58	0.44
1:D:688:PRO:C	1:D:690:SER:N	2.76	0.44
1:B:416:GLU:HA	1:B:460:ASN:O	2.17	0.44
1:C:100:TYR:OH	1:C:201:ASP:OD1	2.26	0.44
1:C:1020:TRP:CD1	1:C:1020:TRP:C	2.95	0.44
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.36	0.44
1:D:588:TYR:O	1:D:591:ASP:HB2	2.17	0.44
1:D:599:ARG:HG3	1:D:600:GLN:N	2.33	0.44
1:A:600:GLN:HE21	1:A:600:GLN:N	1.99	0.44
1:C:561:ARG:HD3	1:D:525:SER:O	2.18	0.44
1:D:190:ARG:HG3	1:D:206:SER:HB3	2.00	0.44
1:D:368:ASP:O	1:D:372:MET:HG3	2.18	0.44
1:A:178:ARG:HD2	6:A:9436:HOH:O	2.16	0.43
1:A:561:ARG:HD3	1:B:525:SER:O	2.18	0.43
1:A:696:LEU:O	1:A:719:GLN:HA	2.18	0.43
1:B:824:GLN:O	1:B:838:THR:HA	2.18	0.43
1:C:255:ARG:HB2	1:C:316:HIS:CE1	2.53	0.43
1:C:472:TYR:O	1:C:476:LYS:HG2	2.18	0.43
1:D:138:GLN:O	1:D:216:HIS:HA	2.17	0.43
1:D:630:ARG:NH1	6:D:9277:HOH:O	2.50	0.43
1:B:255:ARG:HB2	1:B:316:HIS:CE1	2.53	0.43
1:B:367:MET:HE3	1:B:368:ASP:H	1.82	0.43
1:B:847:LYS:HG3	1:B:848:THR:N	2.33	0.43
1:C:75:GLU:CD	1:C:156:GLY:HA3	2.44	0.43
1:C:505:ARG:HG2	1:C:996:ASP:OD2	2.18	0.43
1:C:638:VAL:O	1:C:677:LYS:HA	2.18	0.43
1:C:842:TRP:O	1:C:849:LEU:N	2.44	0.43
1:C:990:HIS:HD2	1:C:991:MET:O	2.01	0.43
1:D:367:MET:HE1	1:D:371:THR:CG2	2.47	0.43
1:A:654:TRP:CE3	1:A:654:TRP:C	2.96	0.43
1:B:262:GLN:HE21	1:B:263:GLY:N	2.14	0.43
1:B:613:PRO:HG2	6:B:9240:HOH:O	2.17	0.43
1:B:693:GLN:HG2	1:B:695:TRP:NE1	2.34	0.43
1:C:111:PRO:HA	1:C:112:PRO:HA	1.67	0.43
1:C:651:LEU:CD1	1:C:651:LEU:C	2.91	0.43
1:D:93:HIS:CD2	5:D:8414:DMS:H23	2.53	0.43
1:A:742:THR:HG22	1:A:743:SER:N	2.32	0.43
1:B:110:ASN:N	1:B:111:PRO:CD	2.82	0.43
1:B:473:ARG:O	1:B:474:TRP:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ILE:HG22	5:C:8410:DMS:H23	2.01	0.43
1:C:262:GLN:HB2	1:C:309:TYR:CE2	2.53	0.43
1:D:701:VAL:O	1:D:703:PRO:HD3	2.19	0.43
1:A:367:MET:HA	1:A:367:MET:HE2	2.00	0.43
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.36	0.43
1:C:46:ARG:O	1:C:47:PRO:C	2.59	0.43
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.85	0.43
1:C:799:THR:O	1:C:800:ARG:HG2	2.18	0.43
1:D:23:GLN:HB2	1:D:26:ARG:HB2	2.00	0.43
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.48	0.43
1:A:142:ILE:HG23	1:A:170:GLU:HG2	2.00	0.43
1:A:774:LYS:NZ	6:A:9275:HOH:O	2.51	0.43
1:B:369:GLU:HB2	1:B:397:LEU:CD2	2.49	0.43
1:B:427:THR:HG22	1:B:436:MET:SD	2.59	0.43
1:B:599:ARG:HH11	1:B:599:ARG:HG3	1.84	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.18	0.43
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.77	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.54	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:C:344:LEU:CB	1:C:349:LEU:HD21	2.49	0.43
1:C:608:PHE:CZ	1:C:614:HIS:CD2	3.06	0.43
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.82	0.43
1:D:598:ASP:C	1:D:599:ARG:HG2	2.44	0.43
1:D:833:ALA:HB1	1:D:858:ILE:O	2.18	0.43
1:D:986:ILE:HD13	1:D:986:ILE:HG21	1.51	0.43
1:A:583:ASN:HB3	1:A:584:PRO:HD2	2.00	0.43
1:A:1017:GLN:HE21	1:A:1017:GLN:HB2	1.74	0.43
1:B:626:PHE:O	1:B:641:GLU:N	2.36	0.43
1:B:864:MET:HE3	1:B:866:ILE:HD11	2.00	0.43
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.54	0.43
1:C:610:ASP:O	1:C:611:ARG:HB2	2.18	0.43
5:C:8410:DMS:H11	6:C:8964:HOH:O	2.19	0.43
1:D:433:LEU:N	1:D:434:PRO:CD	2.81	0.43
1:D:842:TRP:HZ3	1:D:852:SER:HB3	1.84	0.43
1:A:749:ILE:HD12	1:A:749:ILE:H	1.83	0.43
1:B:377:LEU:HD22	1:B:708:TRP:HA	2.01	0.43
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.49	0.43
1:B:899:GLY:HA2	1:B:915:PHE:CE1	2.54	0.43
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.01	0.43
1:B:143:PHE:O	1:B:168:PRO:HA	2.19	0.43
1:B:316:HIS:CD2	5:B:8406:DMS:H23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:HIS:CE1	1:B:362:LEU:H	2.36	0.43
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.80	0.43
1:C:431:ARG:NH2	6:C:9033:HOH:O	2.29	0.43
1:C:526:LEU:HD23	1:C:526:LEU:HA	1.78	0.43
1:D:968:MET:HE3	1:D:968:MET:HB2	1.88	0.43
1:A:835:LEU:HD11	1:A:855:THR:HB	2.02	0.42
1:B:291:LEU:CD1	5:B:8405:DMS:H12	2.49	0.42
1:B:654:TRP:O	1:B:665:SER:HB2	2.19	0.42
1:D:629:PHE:HA	1:D:637:GLU:O	2.19	0.42
5:C:8410:DMS:H22	6:C:8882:HOH:O	2.17	0.42
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.54	0.42
1:B:598:ASP:C	1:B:599:ARG:HG2	2.44	0.42
1:B:797:GLU:O	1:B:800:ARG:N	2.51	0.42
1:B:869:ASP:HA	1:B:1014:TYR:O	2.18	0.42
1:C:73:TRP:CE2	1:C:122:CYS:HB3	2.55	0.42
1:C:655:MET:CE	1:C:662:PRO:HB3	2.49	0.42
1:D:1022:GLN:O	1:D:1023:LYS:HB2	2.20	0.42
1:A:75:GLU:OE1	1:A:75:GLU:HA	2.18	0.42
1:A:100:TYR:HB3	1:A:589:GLY:HA2	2.01	0.42
1:B:36:TRP:CD2	1:B:42:ALA:HA	2.54	0.42
1:C:237:ARG:NH2	1:C:296:GLU:OE2	2.52	0.42
1:C:653:HIS:ND1	1:C:667:GLU:HG2	2.34	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CG	2.55	0.42
1:C:930:VAL:HA	1:C:973:ARG:HD3	2.01	0.42
1:D:36:TRP:NE1	1:D:46:ARG:O	2.43	0.42
1:D:59:ARG:NH2	1:D:81:ALA:HB3	2.34	0.42
1:D:673:ALA:O	1:D:676:GLY:N	2.40	0.42
1:D:804:ASN:CG	1:D:809:ARG:HH21	2.25	0.42
1:A:360:HIS:HE1	1:A:362:LEU:HB2	1.84	0.42
1:A:1020:TRP:C	1:A:1020:TRP:CD1	2.97	0.42
1:C:127:PHE:N	1:C:127:PHE:CD2	2.87	0.42
1:C:335:VAL:HG22	1:C:344:LEU:HD12	2.01	0.42
1:C:649:ASN:O	1:C:702:GLN:HG2	2.20	0.42
1:D:959:ILE:O	1:D:960:SER:HB3	2.19	0.42
1:D:984:LEU:HD11	1:D:986:ILE:HG13	2.01	0.42
5:A:8409:DMS:H23	6:A:8937:HOH:O	2.18	0.42
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.54	0.42
1:B:975:LEU:HD23	1:B:975:LEU:HA	1.82	0.42
1:D:208:ILE:HG21	1:D:208:ILE:HD13	1.75	0.42
1:D:253:TYR:CD1	1:D:253:TYR:C	2.97	0.42
1:D:962:TYR:CE1	5:D:8508:DMS:H22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HG3	1:A:600:GLN:N	2.32	0.42
1:C:178:ARG:O	1:C:179:ALA:C	2.63	0.42
1:C:720:TRP:HA	5:C:8427:DMS:C1	2.50	0.42
1:C:930:VAL:O	1:C:932:PRO:HD3	2.20	0.42
1:C:974:HIS:HA	5:C:8423:DMS:H12	2.02	0.42
1:D:830:LEU:N	1:D:833:ALA:O	2.45	0.42
1:A:521:LYS:HE2	6:A:9023:HOH:O	2.19	0.42
1:B:367:MET:HE3	1:B:368:ASP:N	2.35	0.42
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.31	0.42
1:C:416:GLU:HA	1:C:460:ASN:O	2.19	0.42
1:D:141:ILE:HD13	1:D:143:PHE:CE1	2.54	0.42
1:D:360:HIS:ND1	1:D:361:PRO:HD2	2.35	0.42
1:A:655:MET:HG3	1:A:656:VAL:N	2.25	0.42
1:A:726:LEU:HD12	1:B:848:THR:HG22	2.01	0.42
1:B:658:LEU:HD11	1:B:692:GLY:HA3	2.02	0.42
1:B:777:LEU:HG	1:B:889:ALA:HA	2.01	0.42
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.19	0.42
1:D:173:LEU:O	1:D:174:SER:C	2.62	0.42
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.02	0.42
1:D:898:LEU:HA	1:D:898:LEU:HD12	1.81	0.42
1:A:660:GLY:O	1:A:662:PRO:HD3	2.20	0.42
1:B:56:GLY:CA	5:B:8408:DMS:H11	2.50	0.42
1:B:86:VAL:HG13	1:B:87:PRO:HA	2.02	0.42
1:C:376:ILE:HG13	1:C:398:TRP:CH2	2.55	0.42
1:D:588:TYR:N	1:D:591:ASP:OD2	2.37	0.42
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.02	0.42
1:A:646:HIS:ND1	1:A:673:ALA:HA	2.34	0.41
1:C:415:ILE:HD13	1:C:415:ILE:HG21	1.87	0.41
1:C:430:PRO:C	1:C:432:TRP:N	2.75	0.41
1:C:608:PHE:CE1	1:C:614:HIS:HD2	2.37	0.41
1:D:292:ARG:NH1	5:D:8412:DMS:H23	2.33	0.41
1:D:718:GLN:CD	5:D:8503:DMS:C1	2.93	0.41
1:A:542:MET:HE1	1:A:601:PHE:CE1	2.55	0.41
1:B:472:TYR:O	1:B:476:LYS:HG2	2.19	0.41
1:C:667:GLU:C	1:C:668:VAL:HG23	2.44	0.41
1:C:745:MET:HE3	1:C:745:MET:O	2.19	0.41
1:C:787:ALA:HA	1:C:788:PRO:HD3	1.95	0.41
1:A:253:TYR:CD1	1:A:253:TYR:C	2.98	0.41
1:B:37:ARG:NH1	5:B:8504:DMS:C2	2.82	0.41
1:C:147:ASN:HA	1:C:148:SER:HA	1.59	0.41
1:C:661:LYS:HB2	1:C:661:LYS:HE3	1.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.55	0.41
1:A:475:ILE:HG21	1:A:475:ILE:HD13	1.80	0.41
1:A:933:SER:O	1:A:934:GLU:C	2.60	0.41
1:B:569:ASP:O	1:B:605:GLY:HA2	2.20	0.41
1:C:347:LYS:HB3	1:C:348:PRO:HD2	2.01	0.41
1:C:708:TRP:H	1:C:708:TRP:CD1	2.37	0.41
1:D:460:ASN:O	1:D:461:GLU:C	2.63	0.41
1:A:279:ILE:CD1	1:D:422:PRO:CG	2.98	0.41
1:A:542:MET:HA	1:A:604:ASN:HA	2.02	0.41
1:B:250:LEU:C	1:B:251:ARG:HG2	2.45	0.41
1:B:314:GLU:OE2	5:B:8406:DMS:H21	2.20	0.41
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.34	0.41
1:C:851:ILE:O	1:C:870:VAL:HA	2.20	0.41
1:D:232:ASN:O	1:D:233:ASP:C	2.63	0.41
1:A:390:SER:HA	1:A:391:HIS:HA	1.88	0.41
1:A:615:PRO:O	1:A:618:THR:HG22	2.20	0.41
1:A:845:GLN:HE21	1:A:845:GLN:HB3	1.62	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.61	0.41
1:C:733:ALA:O	1:C:734:SER:C	2.64	0.41
5:C:8503:DMS:H13	6:C:9034:HOH:O	2.19	0.41
1:D:646:HIS:CD2	1:D:647:SER:N	2.88	0.41
1:D:801:ILE:HG22	1:D:802:ASP:H	1.85	0.41
1:A:854:LYS:HA	1:A:867:THR:O	2.21	0.41
1:B:542:MET:HA	1:B:604:ASN:HA	2.02	0.41
1:C:769:TRP:HA	1:C:773:LYS:O	2.21	0.41
1:D:74:LEU:HD22	1:D:153:TRP:CG	2.55	0.41
1:D:91:GLN:CD	1:D:91:GLN:H	2.29	0.41
1:D:461:GLU:OE1	2:D:2001:2DG:H21	2.21	0.41
1:A:781:ARG:NH1	6:A:9309:HOH:O	2.53	0.41
1:B:19:PRO:HD3	1:B:112:PRO:HB3	2.02	0.41
1:C:143:PHE:HB3	1:C:146:VAL:HG23	2.00	0.41
1:C:292:ARG:NH1	5:C:8412:DMS:H23	2.27	0.41
1:C:795:VAL:HG12	5:C:8506:DMS:H23	2.03	0.41
1:D:414:ASN:ND2	1:D:439:ARG:NH1	2.69	0.41
1:A:128:ASN:CG	1:A:129:VAL:N	2.79	0.41
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.41
1:A:571:VAL:CG2	1:A:609:ALA:HA	2.51	0.41
1:A:577:LYS:HB3	1:A:577:LYS:HE3	1.91	0.41
1:A:694:LEU:HD23	1:A:694:LEU:HA	1.89	0.41
1:B:231:PHE:CD1	1:B:231:PHE:N	2.89	0.41
1:B:412:GLU:CG	1:B:459:GLY:HA2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ALA:HB3	1:C:445:GLN:OE1	2.21	0.41
1:C:344:LEU:HB3	1:C:349:LEU:HD21	2.03	0.41
1:C:498:ILE:HD13	1:C:498:ILE:HG21	1.89	0.41
1:C:526:LEU:O	1:C:527:PRO:C	2.60	0.41
1:C:718:GLN:CG	5:C:8503:DMS:C1	2.97	0.41
1:C:789:LEU:O	1:C:790:ASP:C	2.62	0.41
1:D:67:GLU:CD	1:D:67:GLU:H	2.28	0.41
1:D:337:ILE:HA	1:D:341:LEU:O	2.21	0.41
1:B:78:LEU:HA	1:B:79:PRO:HD3	1.75	0.41
1:B:658:LEU:O	1:B:659:ASP:C	2.61	0.41
1:D:367:MET:HE1	1:D:371:THR:HG22	2.03	0.41
1:D:654:TRP:CE3	1:D:665:SER:HA	2.56	0.41
1:D:890:GLN:HG3	1:D:891:VAL:N	2.36	0.41
1:D:949:HIS:HB3	1:D:951:TRP:CH2	2.56	0.41
1:A:370:GLN:HB2	6:A:9098:HOH:O	2.21	0.40
1:A:502:MET:HB2	1:A:537:GLU:HB2	2.02	0.40
1:B:510:GLN:O	1:B:512:PHE:N	2.49	0.40
1:B:689:GLU:O	1:B:690:SER:CB	2.69	0.40
1:A:352:ARG:HH11	1:A:352:ARG:HG3	1.86	0.40
1:A:908:ASP:HB3	1:A:1007:PHE:CD1	2.56	0.40
5:A:8503:DMS:H22	6:A:9015:HOH:O	2.21	0.40
1:B:766:SER:HA	1:B:779:PRO:HB3	2.04	0.40
1:B:876:THR:O	1:B:877:PRO:C	2.63	0.40
1:C:221:GLN:O	1:C:246:MET:HA	2.22	0.40
1:C:496:THR:O	1:C:496:THR:HG23	2.21	0.40
5:D:8413:DMS:H22	6:D:9300:HOH:O	2.20	0.40
1:A:663:LEU:CD1	1:A:686:PRO:HG2	2.51	0.40
1:A:826:THR:OG1	1:A:837:THR:HB	2.21	0.40
1:D:740:LEU:HD12	1:D:741:THR:N	2.36	0.40
1:A:240:LEU:HD13	1:A:260:LEU:HD13	2.04	0.40
1:A:388:ARG:HH11	1:A:388:ARG:HD3	1.63	0.40
1:A:579:ASP:OD1	1:A:581:ASN:HB2	2.22	0.40
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.04	0.40
1:C:573:GLN:HB2	1:C:602:CYS:O	2.22	0.40
1:D:576:ILE:HA	1:D:576:ILE:HD13	1.82	0.40
5:D:8410:DMS:H12	6:D:9625:HOH:O	2.20	0.40
1:A:18:ASN:N	1:A:193:ASP:OD2	2.53	0.40
1:A:546:LEU:HA	6:A:8730:HOH:O	2.20	0.40
1:A:576:ILE:HD13	1:A:576:ILE:HA	1.84	0.40
1:A:756:TRP:CD1	1:A:768:MET:HG2	2.57	0.40
1:D:957:PHE:CD1	1:D:957:PHE:C	2.98	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:773:LYS:NZ	6:C:9410:HOH:O[3_544]	2.18	0.02

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%)	964 (96%)	44 (4%)	1 (0%)	48	50
1	B	1009/1023 (99%)	956 (95%)	48 (5%)	5 (0%)	24	22
1	C	1009/1023 (99%)	963 (95%)	46 (5%)	0	100	100
1	D	1009/1023 (99%)	962 (95%)	43 (4%)	4 (0%)	30	28
All	All	4036/4092 (99%)	3845 (95%)	181 (4%)	10 (0%)	43	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	D	688	PRO
1	D	801	ILE
1	B	688	PRO
1	D	803	PRO
1	B	732	ALA
1	D	164	ASP
1	B	164	ASP
1	A	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	18
1	B	864/875 (99%)	815 (94%)	49 (6%)	18	17
1	C	864/875 (99%)	809 (94%)	55 (6%)	16	14
1	D	864/875 (99%)	807 (93%)	57 (7%)	15	13
All	All	3456/3500 (99%)	3248 (94%)	208 (6%)	17	15

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	75	GLU
1	A	116	THR
1	A	214	LEU
1	A	230	ARG
1	A	237	ARG
1	A	250	LEU
1	A	277	GLU
1	A	279	ILE
1	A	336	ARG
1	A	344	LEU
1	A	362	LEU
1	A	377	LEU
1	A	446	ARG
1	A	477	SER
1	A	478	VAL
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

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Mol	Chain	Res	Type
1	A	663	LEU
1	A	672	VAL
1	A	682	LEU
1	A	684	GLU
1	A	685	LEU
1	A	735	HIS
1	A	737	ILE
1	A	741	THR
1	A	796	SER
1	A	799	THR
1	A	800	ARG
1	A	801	ILE
1	A	809	ARG
1	A	817	GLN
1	A	829	THR
1	A	885	ASN
1	A	890	GLN
1	A	956	GLN
1	A	986	ILE
1	A	1013	ARG
1	A	1017	GLN
1	A	1018	LEU
1	A	1023	LYS
1	B	49	GLN
1	B	71	GLU
1	B	80	GLU
1	B	165	SER
1	B	230	ARG
1	B	237	ARG
1	B	262	GLN
1	B	264	GLU
1	B	344	LEU
1	B	362	LEU
1	B	370	GLN
1	B	395	HIS
1	B	439	ARG
1	B	477	SER
1	B	478	VAL
1	B	515	VAL
1	B	546	LEU
1	B	594	ASP
1	B	595	THR

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Mol	Chain	Res	Type
1	B	600	GLN
1	B	634	GLN
1	B	651	LEU
1	B	661	LYS
1	B	663	LEU
1	B	667	GLU
1	B	668	VAL
1	B	672	VAL
1	B	681	GLU
1	B	685	LEU
1	B	687	GLN
1	B	730	LEU
1	B	737	ILE
1	B	744	GLU
1	B	745	MET
1	B	754	LYS
1	B	797	GLU
1	B	799	THR
1	B	809	ARG
1	B	819	GLU
1	B	824	GLN
1	B	829	THR
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	868	VAL
1	B	885	ASN
1	B	890	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	72	SER
1	C	75	GLU
1	C	117	GLU
1	C	135	GLN
1	C	178	ARG
1	C	189	LEU
1	C	213	SER
1	C	214	LEU
1	C	230	ARG
1	C	237	ARG
1	C	262	GLN

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Mol	Chain	Res	Type
1	C	278	ILE
1	C	333	ARG
1	C	344	LEU
1	C	400	THR
1	C	477	SER
1	C	546	LEU
1	C	580	GLU
1	C	595	THR
1	C	634	GLN
1	C	635	THR
1	C	646	HIS
1	C	651	LEU
1	C	655	MET
1	C	661	LYS
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	687	GLN
1	C	699	ARG
1	C	729	THR
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	746	ASP
1	C	749	ILE
1	C	750	GLU
1	C	755	ARG
1	C	773	LYS
1	C	778	THR
1	C	797	GLU
1	C	799	THR
1	C	819	GLU
1	C	824	GLN
1	C	830	LEU
1	C	832	ASP
1	C	843	GLN
1	C	888	LEU
1	C	890	GLN
1	C	934	GLU
1	C	956	GLN
1	C	986	ILE

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Mol	Chain	Res	Type
1	C	1023	LYS
1	D	13	ARG
1	D	80	GLU
1	D	112	PRO
1	D	116	THR
1	D	213	SER
1	D	237	ARG
1	D	257	THR
1	D	277	GLU
1	D	344	LEU
1	D	370	GLN
1	D	394	ASN
1	D	519	SER
1	D	545	SER
1	D	546	LEU
1	D	580	GLU
1	D	594	ASP
1	D	595	THR
1	D	631	LEU
1	D	632	SER
1	D	635	THR
1	D	651	LEU
1	D	652	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	672	VAL
1	D	677	LYS
1	D	681	GLU
1	D	682	LEU
1	D	684	GLU
1	D	685	LEU
1	D	687	GLN
1	D	689	GLU
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	755	ARG
1	D	769	TRP
1	D	772	ASP
1	D	773	LYS

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Mol	Chain	Res	Type
1	D	774	LYS
1	D	799	THR
1	D	817	GLN
1	D	824	GLN
1	D	829	THR
1	D	885	ASN
1	D	893	GLU
1	D	944	LEU
1	D	956	GLN
1	D	980	GLU
1	D	986	ILE
1	D	1004	SER
1	D	1013	ARG
1	D	1017	GLN
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	50	GLN
1	A	445	GLN
1	A	558	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	653	HIS
1	A	757	GLN
1	A	761	GLN
1	A	817	GLN
1	A	824	GLN
1	A	844	HIS
1	A	845	GLN
1	A	903	GLN
1	A	977	HIS
1	A	1017	GLN
1	B	25	ASN
1	B	262	GLN
1	B	363	HIS
1	B	485	GLN
1	B	600	GLN

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Mol	Chain	Res	Type
1	B	624	GLN
1	B	628	GLN
1	B	646	HIS
1	B	653	HIS
1	B	687	GLN
1	B	757	GLN
1	B	817	GLN
1	B	824	GLN
1	B	843	GLN
1	B	844	HIS
1	B	878	HIS
1	C	102	ASN
1	C	262	GLN
1	C	266	GLN
1	C	363	HIS
1	C	394	ASN
1	C	634	GLN
1	C	653	HIS
1	C	687	GLN
1	C	843	GLN
1	C	844	HIS
1	C	878	HIS
1	C	977	HIS
1	D	163	GLN
1	D	363	HIS
1	D	365	GLN
1	D	624	GLN
1	D	653	HIS
1	D	702	GLN
1	D	757	GLN
1	D	804	ASN
1	D	878	HIS
1	D	903	GLN
1	D	977	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 132 ligands modelled in this entry, 25 are monoatomic - leaving 107 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	D	8501	-	3,3,3	0.87	0	3,3,3	0.90	0
5	DMS	B	8504	-	3,3,3	0.11	0	3,3,3	0.08	0
2	2DG	A	2001	1,4	10,10,11	1.02	1 (10%)	13,13,15	1.87	3 (23%)
5	DMS	A	8411	-	3,3,3	1.61	1 (33%)	3,3,3	0.15	0
5	DMS	A	8407	-	3,3,3	1.78	2 (66%)	3,3,3	0.54	0
5	DMS	D	8705	-	3,3,3	1.27	0	3,3,3	0.21	0
5	DMS	D	8703	-	3,3,3	0.87	0	3,3,3	0.32	0
5	DMS	C	8413	-	3,3,3	3.02	2 (66%)	3,3,3	0.45	0
5	DMS	C	8427	-	3,3,3	0.92	0	3,3,3	0.10	0
5	DMS	A	8504	-	3,3,3	0.36	0	3,3,3	0.43	0
5	DMS	C	8404	-	3,3,3	1.32	1 (33%)	3,3,3	0.68	0
5	DMS	C	8601	-	3,3,3	1.12	0	3,3,3	0.62	0
5	DMS	A	8425	4	3,3,3	1.46	1 (33%)	3,3,3	0.56	0
5	DMS	A	8503	-	3,3,3	0.67	0	3,3,3	0.18	0
5	DMS	D	8503	-	3,3,3	1.38	1 (33%)	3,3,3	0.79	0
5	DMS	A	8420	-	3,3,3	1.62	1 (33%)	3,3,3	1.03	0
5	DMS	D	8402	-	3,3,3	1.17	0	3,3,3	0.64	0
5	DMS	D	8421	-	3,3,3	1.06	0	3,3,3	0.08	0
5	DMS	C	8602	-	3,3,3	1.11	0	3,3,3	0.16	0
5	DMS	D	8405	-	3,3,3	0.85	0	3,3,3	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8415	-	3,3,3	1.62	1 (33%)	3,3,3	0.97	0
5	DMS	B	8402	-	3,3,3	1.94	2 (66%)	3,3,3	0.18	0
5	DMS	C	8504	-	3,3,3	1.14	0	3,3,3	0.23	0
5	DMS	C	8401	-	3,3,3	0.90	0	3,3,3	0.77	0
5	DMS	B	8405	-	3,3,3	0.90	0	3,3,3	0.39	0
5	DMS	B	8601	-	3,3,3	0.43	0	3,3,3	0.29	0
5	DMS	C	8403	-	3,3,3	0.86	0	3,3,3	0.44	0
5	DMS	A	8413	-	3,3,3	2.09	2 (66%)	3,3,3	0.16	0
5	DMS	D	8701	-	3,3,3	2.97	2 (66%)	3,3,3	0.77	0
5	DMS	A	8404	-	3,3,3	1.88	1 (33%)	3,3,3	0.31	0
5	DMS	B	8423	-	3,3,3	0.58	0	3,3,3	0.15	0
5	DMS	D	8404	-	3,3,3	1.62	1 (33%)	3,3,3	0.52	0
5	DMS	C	8506	-	3,3,3	1.64	1 (33%)	3,3,3	1.26	1 (33%)
5	DMS	D	8409	-	3,3,3	2.27	1 (33%)	3,3,3	0.59	0
5	DMS	B	8420	-	3,3,3	1.34	1 (33%)	3,3,3	0.39	0
5	DMS	A	8602	-	3,3,3	0.88	0	3,3,3	0.83	0
5	DMS	A	8405	-	3,3,3	1.55	1 (33%)	3,3,3	0.24	0
5	DMS	A	8401	-	3,3,3	1.99	1 (33%)	3,3,3	0.12	0
5	DMS	D	8401	-	3,3,3	1.83	1 (33%)	3,3,3	0.33	0
5	DMS	B	8417	-	3,3,3	1.21	0	3,3,3	0.48	0
5	DMS	C	8402	-	3,3,3	2.13	1 (33%)	3,3,3	0.73	0
5	DMS	C	8416	-	3,3,3	1.14	0	3,3,3	0.72	0
5	DMS	B	8401	-	3,3,3	0.69	0	3,3,3	0.44	0
5	DMS	C	8405	-	3,3,3	1.87	1 (33%)	3,3,3	0.26	0
5	DMS	D	8417	-	3,3,3	1.31	0	3,3,3	0.73	0
2	2DG	B	2001	1,4	10,10,11	1.39	1 (10%)	13,13,15	1.26	1 (7%)
5	DMS	B	8416	-	3,3,3	1.33	0	3,3,3	0.06	0
5	DMS	B	8502	-	3,3,3	0.77	0	3,3,3	1.27	1 (33%)
5	DMS	A	8402	-	3,3,3	1.61	1 (33%)	3,3,3	0.14	0
2	2DG	C	2001	1,4	10,10,11	1.28	1 (10%)	13,13,15	1.85	1 (7%)
5	DMS	A	8417	-	3,3,3	1.14	0	3,3,3	0.51	0
5	DMS	C	8408	-	3,3,3	0.70	0	3,3,3	0.25	0
5	DMS	C	8411	-	3,3,3	1.72	1 (33%)	3,3,3	0.34	0
5	DMS	B	8409	-	3,3,3	0.72	0	3,3,3	1.29	1 (33%)
5	DMS	C	8423	-	3,3,3	1.33	0	3,3,3	0.32	0
5	DMS	A	8502	-	3,3,3	1.19	0	3,3,3	1.37	1 (33%)
5	DMS	B	8425	4	3,3,3	1.96	1 (33%)	3,3,3	0.37	0
5	DMS	C	8414	-	3,3,3	1.66	1 (33%)	3,3,3	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	8419	-	3,3,3	1.43	0	3,3,3	0.19	0
5	DMS	D	8408	-	3,3,3	1.18	0	3,3,3	0.31	0
5	DMS	A	8408	-	3,3,3	1.11	0	3,3,3	0.23	0
5	DMS	B	8413	-	3,3,3	2.28	2 (66%)	3,3,3	0.83	0
5	DMS	D	8403	-	3,3,3	0.53	0	3,3,3	0.31	0
5	DMS	D	8410	-	3,3,3	1.33	0	3,3,3	0.50	0
5	DMS	B	8404	-	3,3,3	0.83	0	3,3,3	0.36	0
5	DMS	B	8410	-	3,3,3	1.33	0	3,3,3	0.49	0
5	DMS	A	8415	-	3,3,3	1.99	1 (33%)	3,3,3	0.16	0
5	DMS	D	8419	-	3,3,3	0.91	0	3,3,3	0.36	0
5	DMS	A	8414	-	3,3,3	0.78	0	3,3,3	0.44	0
5	DMS	D	8414	-	3,3,3	1.26	0	3,3,3	0.09	0
5	DMS	C	8501	-	3,3,3	1.58	0	3,3,3	1.19	1 (33%)
5	DMS	C	8412	-	3,3,3	0.88	0	3,3,3	0.56	0
5	DMS	D	8416	-	3,3,3	0.80	0	3,3,3	0.23	0
5	DMS	A	8406	-	3,3,3	1.96	1 (33%)	3,3,3	0.45	0
5	DMS	A	8403	-	3,3,3	0.99	0	3,3,3	0.74	0
5	DMS	B	8407	-	3,3,3	1.55	0	3,3,3	0.26	0
5	DMS	B	8406	-	3,3,3	1.29	1 (33%)	3,3,3	0.25	0
5	DMS	B	8427	-	3,3,3	0.91	0	3,3,3	0.61	0
5	DMS	C	8410	-	3,3,3	1.13	0	3,3,3	0.37	0
5	DMS	D	8406	-	3,3,3	1.05	0	3,3,3	0.38	0
5	DMS	C	8421	-	3,3,3	0.62	0	3,3,3	0.23	0
5	DMS	D	8412	-	3,3,3	1.52	1 (33%)	3,3,3	0.60	0
5	DMS	D	8411	-	3,3,3	0.95	0	3,3,3	0.50	0
5	DMS	B	8412	-	3,3,3	1.97	1 (33%)	3,3,3	0.17	0
5	DMS	B	8403	-	3,3,3	1.50	0	3,3,3	1.26	1 (33%)
5	DMS	C	8417	-	3,3,3	0.88	0	3,3,3	0.52	0
5	DMS	B	8408	-	3,3,3	1.45	0	3,3,3	0.41	0
5	DMS	B	8421	-	3,3,3	0.87	0	3,3,3	0.14	0
5	DMS	A	8410	-	3,3,3	0.73	0	3,3,3	0.10	0
5	DMS	B	8414	-	3,3,3	0.56	0	3,3,3	0.77	0
5	DMS	B	8415	-	3,3,3	1.13	0	3,3,3	1.34	1 (33%)
5	DMS	A	8409	-	3,3,3	2.40	2 (66%)	3,3,3	0.37	0
5	DMS	B	8411	-	3,3,3	0.37	0	3,3,3	0.76	0
5	DMS	A	8412	-	3,3,3	0.77	0	3,3,3	0.20	0
5	DMS	B	8506	-	3,3,3	1.42	0	3,3,3	0.79	0
5	DMS	A	8419	-	3,3,3	0.69	0	3,3,3	0.40	0
5	DMS	C	8420	-	3,3,3	1.31	0	3,3,3	0.67	0
5	DMS	D	8413	-	3,3,3	0.91	0	3,3,3	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	2DG	D	2001	1,4	10,10,11	1.39	2 (20%)	13,13,15	2.35	4 (30%)
5	DMS	D	8508	-	3,3,3	0.57	0	3,3,3	0.60	0
5	DMS	C	8407	-	3,3,3	1.18	0	3,3,3	0.10	0
5	DMS	A	8501	-	3,3,3	1.48	1 (33%)	3,3,3	0.32	0
5	DMS	C	8409	-	3,3,3	1.61	1 (33%)	3,3,3	0.39	0
5	DMS	A	8421	-	3,3,3	0.91	0	3,3,3	0.98	0
5	DMS	B	8508	-	3,3,3	2.57	3 (100%)	3,3,3	0.39	0
5	DMS	C	8425	4	3,3,3	1.52	1 (33%)	3,3,3	1.66	1 (33%)
5	DMS	C	8503	-	3,3,3	0.80	0	3,3,3	0.42	0

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

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

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	8413	DMS	O-S	4.61	1.80	1.50
5	D	8701	DMS	O-S	3.84	1.75	1.50
5	D	8409	DMS	O-S	3.82	1.75	1.50
5	A	8406	DMS	C2-S	-3.39	1.51	1.76
5	A	8409	DMS	O-S	3.37	1.72	1.50
2	D	2001	2DG	C2-C3	3.27	1.57	1.52
5	C	8402	DMS	C2-S	3.22	1.99	1.76
5	A	8401	DMS	O-S	3.21	1.71	1.50
5	B	8508	DMS	C1-S	3.17	1.98	1.76
5	A	8415	DMS	C2-S	3.09	1.98	1.76
5	B	8412	DMS	C2-S	3.03	1.97	1.76
2	B	2001	2DG	C4-C5	2.99	1.59	1.53
5	A	8404	DMS	C2-S	2.97	1.97	1.76
5	B	8425	DMS	O-S	2.89	1.69	1.50
5	D	8701	DMS	C2-S	2.88	1.96	1.76
5	B	8413	DMS	C1-S	2.83	1.96	1.76
5	A	8420	DMS	C2-S	2.76	1.95	1.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	8413	DMS	C2-S	2.70	1.95	1.76
5	C	8414	DMS	C1-S	-2.69	1.56	1.76
5	C	8405	DMS	O-S	2.69	1.68	1.50
5	C	8415	DMS	C2-S	2.68	1.95	1.76
5	C	8409	DMS	O-S	2.67	1.67	1.50
5	A	8411	DMS	C1-S	2.63	1.94	1.76
5	B	8402	DMS	C2-S	2.61	1.94	1.76
5	D	8401	DMS	C2-S	2.54	1.94	1.76
5	D	8404	DMS	C2-S	2.50	1.93	1.76
2	C	2001	2DG	C4-C5	2.48	1.58	1.53
5	A	8409	DMS	C1-S	2.43	1.93	1.76
5	A	8402	DMS	C2-S	2.42	1.93	1.76
5	B	8413	DMS	O-S	2.41	1.66	1.50
5	A	8405	DMS	O-S	2.35	1.65	1.50
5	C	8425	DMS	C2-S	2.33	1.92	1.76
5	A	8413	DMS	O-S	2.33	1.65	1.50
5	A	8501	DMS	C2-S	2.25	1.92	1.76
5	B	8420	DMS	C2-S	2.23	1.92	1.76
5	C	8506	DMS	C2-S	2.22	1.91	1.76
5	B	8508	DMS	C2-S	2.21	1.91	1.76
5	B	8406	DMS	C1-S	2.21	1.91	1.76
5	C	8413	DMS	C2-S	2.20	1.91	1.76
2	A	2001	2DG	C2-C3	2.19	1.55	1.52
5	B	8508	DMS	O-S	2.19	1.64	1.50
5	A	8425	DMS	C2-S	2.17	1.91	1.76
5	A	8407	DMS	C2-S	2.15	1.91	1.76
5	D	8503	DMS	C1-S	2.14	1.91	1.76
5	C	8411	DMS	C1-S	2.10	1.91	1.76
2	D	2001	2DG	C4-C5	2.10	1.57	1.53
5	B	8402	DMS	O-S	2.09	1.64	1.50
5	D	8412	DMS	O-S	2.08	1.64	1.50
5	A	8407	DMS	O-S	2.05	1.63	1.50
5	C	8404	DMS	O-S	2.01	1.63	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	2001	2DG	C3-C4-C5	-5.76	104.22	109.99
2	A	2001	2DG	C3-C4-C5	-4.73	105.25	109.99
2	D	2001	2DG	C2-C3-C4	4.27	116.04	111.16
2	D	2001	2DG	C1-O5-C5	4.22	119.43	112.01
2	D	2001	2DG	C3-C4-C5	-4.21	105.77	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2001	2DG	C1-C2-C3	-2.97	105.79	110.61
5	C	8425	DMS	C2-S-C1	2.86	113.06	98.42
2	D	2001	2DG	C1-C2-C3	-2.58	106.42	110.61
5	A	8502	DMS	C2-S-C1	2.37	110.59	98.42
5	B	8415	DMS	C2-S-C1	2.29	110.17	98.42
5	B	8409	DMS	C2-S-C1	2.21	109.74	98.42
5	B	8502	DMS	C2-S-C1	2.19	109.65	98.42
5	C	8506	DMS	C2-S-C1	2.17	109.54	98.42
2	A	2001	2DG	O4-C4-C3	-2.16	105.64	110.05
5	B	8403	DMS	C2-S-C1	2.09	109.16	98.42
2	B	2001	2DG	O3-C3-C2	-2.07	104.93	109.99
5	C	8501	DMS	C2-S-C1	-2.03	88.00	98.42

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	2DG	O5-C5-C6-O6
2	A	2001	2DG	O5-C5-C6-O6
2	D	2001	2DG	O5-C5-C6-O6
2	B	2001	2DG	O5-C5-C6-O6

There are no ring outliers.

56 monomers are involved in 107 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8504	DMS	4	0
5	D	8703	DMS	1	0
5	C	8427	DMS	6	0
5	A	8504	DMS	1	0
5	A	8425	DMS	1	0
5	A	8503	DMS	2	0
5	D	8503	DMS	3	0
5	A	8420	DMS	3	0
5	C	8602	DMS	1	0
5	C	8415	DMS	1	0
5	B	8402	DMS	1	0
5	C	8504	DMS	2	0
5	B	8405	DMS	2	0
5	B	8601	DMS	1	0
5	B	8423	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8506	DMS	4	0
5	D	8409	DMS	1	0
5	B	8420	DMS	1	0
5	A	8602	DMS	1	0
5	B	8417	DMS	2	0
5	C	8402	DMS	1	0
2	B	2001	2DG	1	0
5	B	8416	DMS	1	0
5	A	8417	DMS	1	0
5	C	8423	DMS	2	0
5	A	8502	DMS	3	0
5	D	8408	DMS	1	0
5	D	8410	DMS	1	0
5	B	8410	DMS	1	0
5	A	8415	DMS	2	0
5	D	8419	DMS	1	0
5	A	8414	DMS	2	0
5	D	8414	DMS	2	0
5	C	8412	DMS	3	0
5	D	8416	DMS	2	0
5	A	8406	DMS	4	0
5	B	8407	DMS	1	0
5	B	8406	DMS	3	0
5	C	8410	DMS	3	0
5	D	8406	DMS	1	0
5	D	8412	DMS	5	0
5	C	8417	DMS	1	0
5	B	8408	DMS	2	0
5	B	8421	DMS	1	0
5	A	8410	DMS	1	0
5	B	8415	DMS	3	0
5	A	8409	DMS	2	0
5	A	8412	DMS	1	0
5	B	8506	DMS	4	0
5	C	8420	DMS	1	0
5	D	8413	DMS	2	0
2	D	2001	2DG	2	0
5	D	8508	DMS	1	0
5	C	8407	DMS	1	0
5	B	8508	DMS	1	0
5	C	8503	DMS	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.69	11 (1%) 78 80	5, 15, 44, 98	0
1	B	1011/1023 (98%)	-0.68	14 (1%) 73 75	5, 15, 45, 100	0
1	C	1011/1023 (98%)	-0.64	12 (1%) 76 78	6, 15, 46, 100	0
1	D	1011/1023 (98%)	-0.62	20 (1%) 65 67	4, 16, 46, 99	0
All	All	4044/4092 (98%)	-0.66	57 (1%) 73 75	4, 15, 45, 100	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	686	PRO	6.3
1	D	601	PHE	4.9
1	D	798	ALA	4.5
1	B	732	ALA	4.2
1	B	731	PRO	4.1
1	B	686	PRO	3.6
1	B	730	LEU	3.6
1	A	688	PRO	3.5
1	C	799	THR	3.5
1	B	733	ALA	3.5
1	B	685	LEU	3.5
1	D	799	THR	3.3
1	D	733	ALA	3.2
1	D	801	ILE	3.2
1	A	730	LEU	3.2
1	C	732	ALA	3.2
1	C	733	ALA	3.1
1	D	732	ALA	3.1
1	D	797	GLU	3.1
1	A	1023	LYS	3.1
1	C	730	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	732	ALA	3.0
1	A	731	PRO	3.0
1	C	735	HIS	3.0
1	D	686	PRO	2.9
1	C	685	LEU	2.8
1	A	687	GLN	2.8
1	A	735	HIS	2.7
1	D	685	LEU	2.7
1	D	730	LEU	2.7
1	C	686	PRO	2.7
1	B	798	ALA	2.7
1	D	736	ALA	2.6
1	D	735	HIS	2.6
1	A	685	LEU	2.6
1	C	731	PRO	2.6
1	C	734	SER	2.5
1	D	734	SER	2.5
1	B	799	THR	2.4
1	B	735	HIS	2.4
1	C	736	ALA	2.4
1	D	1023	LYS	2.4
1	A	689	GLU	2.4
1	C	798	ALA	2.4
1	D	688	PRO	2.3
1	D	663	LEU	2.3
1	B	1023	LYS	2.2
1	B	729	THR	2.2
1	B	845	GLN	2.2
1	C	1023	LYS	2.2
1	B	689	GLU	2.2
1	D	666	GLY	2.1
1	D	1022	GLN	2.1
1	D	794	GLY	2.1
1	B	797	GLU	2.0
1	A	798	ALA	2.0
1	D	731	PRO	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($\text{\AA}^2$)	Q<0.9
5	DMS	A	8502	4/4	0.87	0.15	14,21,75,84	0
5	DMS	C	8417	4/4	0.88	0.13	24,51,57,58	0
5	DMS	A	8417	4/4	0.89	0.17	25,26,61,100	0
5	DMS	B	8406	4/4	0.90	0.16	34,40,61,78	0
5	DMS	D	8703	4/4	0.90	0.15	24,53,80,80	0
5	DMS	B	8508	4/4	0.91	0.10	27,31,46,64	0
5	DMS	A	8421	4/4	0.91	0.17	42,43,67,100	0
5	DMS	C	8602	4/4	0.91	0.11	27,32,53,77	0
5	DMS	D	8417	4/4	0.91	0.11	18,26,39,73	0
5	DMS	D	8503	4/4	0.91	0.16	33,53,64,100	0
5	DMS	B	8427	4/4	0.91	0.09	28,31,42,65	0
5	DMS	B	8502	4/4	0.92	0.10	13,30,45,50	0
5	DMS	D	8409	4/4	0.92	0.11	25,30,39,53	0
5	DMS	B	8421	4/4	0.92	0.12	14,46,60,85	0
5	DMS	B	8420	4/4	0.92	0.19	36,45,63,100	0
5	DMS	C	8425	4/4	0.92	0.11	33,37,39,48	0
5	DMS	C	8503	4/4	0.93	0.16	20,31,54,100	0
5	DMS	B	8413	4/4	0.93	0.10	22,32,35,42	0
5	DMS	B	8414	4/4	0.93	0.15	24,43,49,100	0
5	DMS	B	8416	4/4	0.93	0.12	35,42,52,88	0
5	DMS	D	8421	4/4	0.93	0.09	36,45,48,52	0
5	DMS	A	8415	4/4	0.93	0.10	24,27,28,70	0
5	DMS	B	8408	4/4	0.93	0.12	15,25,43,60	0
5	DMS	D	8705	4/4	0.93	0.10	24,32,51,51	0
5	DMS	C	8415	4/4	0.94	0.09	20,26,33,52	0
5	DMS	C	8416	4/4	0.94	0.07	31,33,49,64	0
4	NA	D	3103	1/1	0.94	0.09	38,38,38,38	0
5	DMS	C	8419	4/4	0.94	0.10	33,44,54,61	0
5	DMS	C	8423	4/4	0.94	0.09	26,27,32,61	0
5	DMS	B	8417	4/4	0.94	0.09	26,31,34,63	0
5	DMS	B	8407	4/4	0.94	0.12	34,34,63,66	0
5	DMS	C	8601	4/4	0.94	0.14	31,53,55,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8407	4/4	0.94	0.11	28,40,42,43	0
5	DMS	B	8425	4/4	0.94	0.08	22,30,32,54	0
5	DMS	A	8425	4/4	0.94	0.12	34,40,45,45	0
4	NA	B	3104	1/1	0.94	0.07	37,37,37,37	0
5	DMS	B	8415	4/4	0.94	0.10	22,26,33,67	0
5	DMS	B	8601	4/4	0.94	0.16	36,60,100,100	0
5	DMS	C	8413	4/4	0.94	0.11	31,32,34,38	0
5	DMS	A	8409	4/4	0.95	0.09	24,27,39,42	0
5	DMS	A	8413	4/4	0.95	0.15	34,34,53,100	0
5	DMS	C	8506	4/4	0.95	0.10	15,24,47,89	0
5	DMS	C	8407	4/4	0.95	0.11	35,39,51,52	0
5	DMS	C	8409	4/4	0.95	0.10	23,35,41,41	0
5	DMS	A	8406	4/4	0.95	0.14	7,53,55,100	0
5	DMS	D	8416	4/4	0.95	0.12	16,34,42,89	0
5	DMS	B	8423	4/4	0.95	0.12	28,44,71,87	0
5	DMS	A	8503	4/4	0.95	0.13	42,47,48,100	0
5	DMS	A	8602	4/4	0.95	0.15	42,45,100,100	0
3	MG	B	3001	1/1	0.95	0.05	11,11,11,11	0
5	DMS	B	8506	4/4	0.95	0.16	31,39,63,100	0
5	DMS	C	8420	4/4	0.96	0.14	34,36,53,100	0
5	DMS	B	8504	4/4	0.96	0.10	31,37,51,52	0
2	2DG	A	2001	10/11	0.96	0.06	10,15,18,25	0
5	DMS	C	8427	4/4	0.96	0.13	37,43,81,82	0
2	2DG	C	2001	10/11	0.96	0.07	7,15,26,27	0
5	DMS	C	8504	4/4	0.96	0.08	32,34,42,64	0
5	DMS	A	8414	4/4	0.96	0.10	16,37,47,100	0
4	NA	C	3104	1/1	0.96	0.07	26,26,26,26	0
2	2DG	D	2001	10/11	0.96	0.06	9,15,24,24	0
5	DMS	D	8406	4/4	0.96	0.07	18,19,20,34	0
5	DMS	C	8412	4/4	0.96	0.13	18,31,67,100	0
5	DMS	D	8410	4/4	0.96	0.13	22,35,39,100	0
5	DMS	D	8413	4/4	0.96	0.07	21,24,34,35	0
5	DMS	D	8414	4/4	0.96	0.12	17,32,44,92	0
3	MG	A	3001	1/1	0.96	0.04	13,13,13,13	0
5	DMS	C	8414	4/4	0.96	0.07	17,18,23,39	0
5	DMS	B	8409	4/4	0.96	0.07	18,32,33,38	0
5	DMS	B	8410	4/4	0.96	0.09	18,27,41,54	0
5	DMS	D	8508	4/4	0.96	0.10	19,46,50,80	0
5	DMS	B	8412	4/4	0.96	0.08	21,33,34,38	0
3	MG	A	3005	1/1	0.96	0.04	36,36,36,36	0
5	DMS	A	8420	4/4	0.97	0.11	33,35,39,46	0
3	MG	D	3005	1/1	0.97	0.06	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	8408	4/4	0.97	0.10	13,35,46,83	0
4	NA	A	3101	1/1	0.97	0.06	13,13,13,13	0
5	DMS	A	8501	4/4	0.97	0.07	12,13,29,33	0
5	DMS	A	8408	4/4	0.97	0.10	14,23,31,82	0
4	NA	A	3102	1/1	0.97	0.03	15,15,15,15	0
5	DMS	A	8504	4/4	0.97	0.09	23,35,38,100	0
5	DMS	A	8411	4/4	0.97	0.12	24,26,28,100	0
5	DMS	A	8412	4/4	0.97	0.08	24,33,37,37	0
4	NA	A	3104	1/1	0.97	0.06	21,21,21,21	0
2	2DG	B	2001	10/11	0.97	0.06	13,15,19,24	0
5	DMS	D	8419	4/4	0.97	0.06	18,32,40,44	0
5	DMS	C	8421	4/4	0.97	0.08	26,26,41,64	0
5	DMS	D	8501	4/4	0.97	0.08	16,34,36,46	0
3	MG	C	3001	1/1	0.97	0.03	12,12,12,12	0
3	MG	D	3001	1/1	0.97	0.03	15,15,15,15	0
5	DMS	D	8701	4/4	0.97	0.09	15,17,22,37	0
5	DMS	A	8419	4/4	0.97	0.11	24,26,55,100	0
5	DMS	C	8501	4/4	0.97	0.08	23,23,34,38	0
4	NA	B	3103	1/1	0.98	0.03	19,19,19,19	0
5	DMS	A	8410	4/4	0.98	0.09	28,39,55,58	0
3	MG	A	3002	1/1	0.98	0.07	14,14,14,14	0
5	DMS	C	8410	4/4	0.98	0.08	21,35,37,43	0
5	DMS	D	8403	4/4	0.98	0.07	21,26,27,45	0
5	DMS	D	8405	4/4	0.98	0.09	18,23,42,100	0
5	DMS	C	8411	4/4	0.98	0.07	18,20,34,50	0
5	DMS	D	8408	4/4	0.98	0.06	14,27,28,36	0
4	NA	C	3101	1/1	0.98	0.02	11,11,11,11	0
4	NA	C	3102	1/1	0.98	0.04	16,16,16,16	0
5	DMS	D	8411	4/4	0.98	0.11	11,27,27,100	0
5	DMS	D	8412	4/4	0.98	0.09	15,25,32,33	0
3	MG	C	3002	1/1	0.98	0.03	12,12,12,12	0
5	DMS	B	8402	4/4	0.98	0.06	8,21,25,29	0
5	DMS	B	8403	4/4	0.98	0.05	12,12,18,21	0
5	DMS	B	8404	4/4	0.98	0.06	16,20,30,40	0
5	DMS	B	8405	4/4	0.98	0.11	23,28,62,71	0
3	MG	B	3002	1/1	0.98	0.04	14,14,14,14	0
5	DMS	A	8402	4/4	0.98	0.08	11,26,30,47	0
4	NA	A	3103	1/1	0.98	0.06	25,25,25,25	0
3	MG	D	3002	1/1	0.98	0.09	19,19,19,19	0
4	NA	B	3102	1/1	0.98	0.04	13,13,13,13	0
5	DMS	B	8411	4/4	0.98	0.07	15,17,32,100	0
5	DMS	C	8402	4/4	0.98	0.06	6,31,38,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8403	4/4	0.99	0.05	15,20,21,23	0
5	DMS	A	8404	4/4	0.99	0.05	9,22,22,30	0
5	DMS	A	8405	4/4	0.99	0.04	11,22,25,27	0
4	NA	D	3101	1/1	0.99	0.05	16,16,16,16	0
4	NA	D	3102	1/1	0.99	0.02	18,18,18,18	0
4	NA	C	3103	1/1	0.99	0.05	22,22,22,22	0
5	DMS	A	8401	4/4	0.99	0.05	6,13,16,19	0
5	DMS	C	8401	4/4	0.99	0.05	10,11,21,30	0
5	DMS	B	8401	4/4	0.99	0.05	13,13,21,22	0
5	DMS	D	8401	4/4	0.99	0.06	10,11,20,27	0
5	DMS	D	8402	4/4	0.99	0.06	9,23,27,32	0
5	DMS	C	8403	4/4	0.99	0.04	10,12,16,19	0
5	DMS	D	8404	4/4	0.99	0.07	14,19,26,80	0
5	DMS	C	8404	4/4	0.99	0.05	11,13,21,21	0
5	DMS	C	8405	4/4	0.99	0.05	16,23,25,38	0
4	NA	B	3101	1/1	0.99	0.03	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.