



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:14 AM UTC

PDB ID : 3DYO / pdb_00003dyo
Title : E. coli (lacZ) beta-galactosidase (H418N) in complex with IPTG
Authors : Juers, D.H.; Huber, R.E.; Matthews, B.W.
Deposited on : 2008-07-28
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

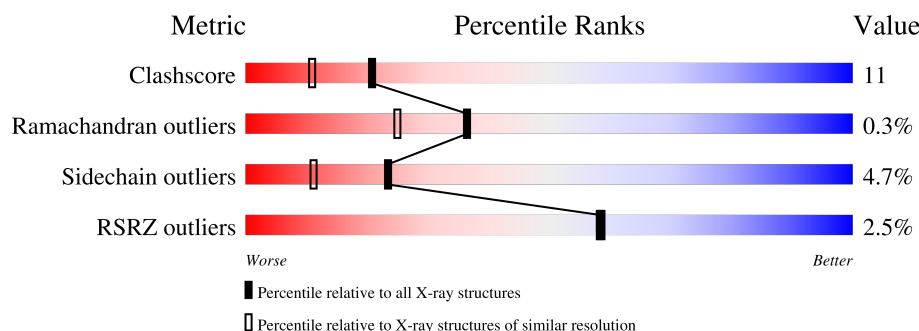
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	3% 66% 27% 5% ..
1	B	1023	2% 72% 22% ..
1	C	1023	2% 76% 19% ..
1	D	1023	2% 71% 22% ..

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	8414	-	-	X	-
5	DMS	B	8412	-	-	X	-
5	DMS	B	8504	-	-	X	-
5	DMS	B	8506	-	-	X	-
5	DMS	C	8411	-	-	X	-
5	DMS	C	8412	-	-	X	-
5	DMS	D	8403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36820 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
			8123	5136	1439	1510	38			
1	B	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	C	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			
1	D	1011	Total	C	N	O	S	0	0	0
			8123	5136	1439	1510	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P00722
A	2	SER	-	expression tag	UNP P00722
A	3	HIS	-	expression tag	UNP P00722
A	4	MET	-	expression tag	UNP P00722
A	5	LEU	-	expression tag	UNP P00722
A	6	GLU	-	expression tag	UNP P00722
A	7	ASP	-	expression tag	UNP P00722
A	8	PRO	-	expression tag	UNP P00722
A	418	ASN	HIS	engineered mutation	UNP P00722
B	1	GLY	-	expression tag	UNP P00722
B	2	SER	-	expression tag	UNP P00722
B	3	HIS	-	expression tag	UNP P00722
B	4	MET	-	expression tag	UNP P00722
B	5	LEU	-	expression tag	UNP P00722
B	6	GLU	-	expression tag	UNP P00722
B	7	ASP	-	expression tag	UNP P00722
B	8	PRO	-	expression tag	UNP P00722
B	418	ASN	HIS	engineered mutation	UNP P00722
C	1	GLY	-	expression tag	UNP P00722
C	2	SER	-	expression tag	UNP P00722
C	3	HIS	-	expression tag	UNP P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP P00722
C	5	LEU	-	expression tag	UNP P00722
C	6	GLU	-	expression tag	UNP P00722
C	7	ASP	-	expression tag	UNP P00722
C	8	PRO	-	expression tag	UNP P00722
C	418	ASN	HIS	engineered mutation	UNP P00722
D	1	GLY	-	expression tag	UNP P00722
D	2	SER	-	expression tag	UNP P00722
D	3	HIS	-	expression tag	UNP P00722
D	4	MET	-	expression tag	UNP P00722
D	5	LEU	-	expression tag	UNP P00722
D	6	GLU	-	expression tag	UNP P00722
D	7	ASP	-	expression tag	UNP P00722
D	8	PRO	-	expression tag	UNP P00722
D	418	ASN	HIS	engineered mutation	UNP P00722

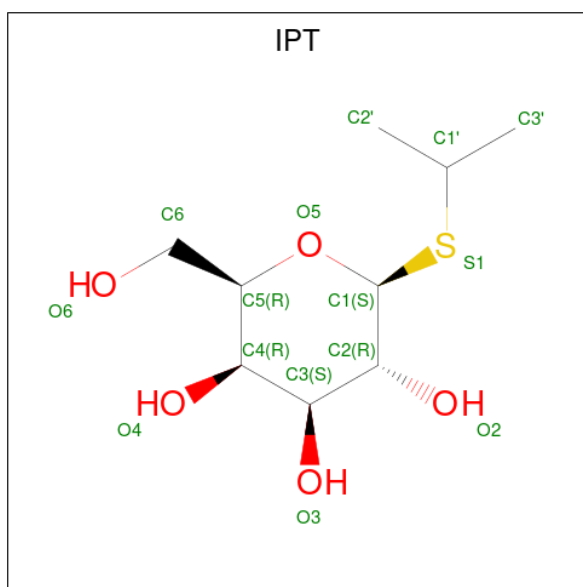
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

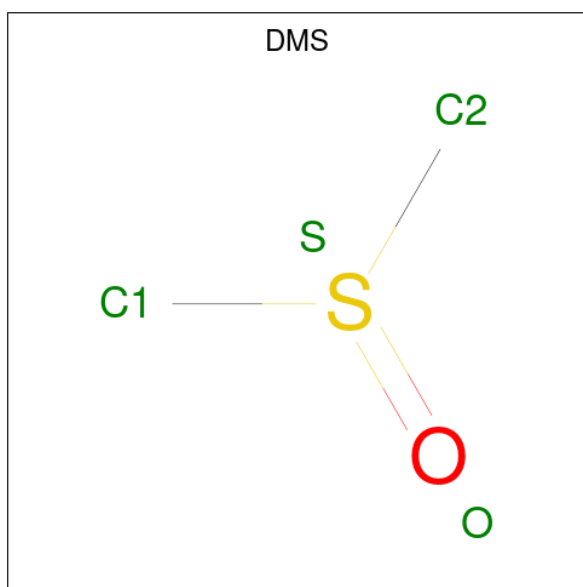
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Na 4 4	0	0
3	B	5	Total Na 5 5	0	0
3	C	5	Total Na 5 5	0	0
3	D	4	Total Na 4 4	0	0

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



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

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



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

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

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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	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

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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	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

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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
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

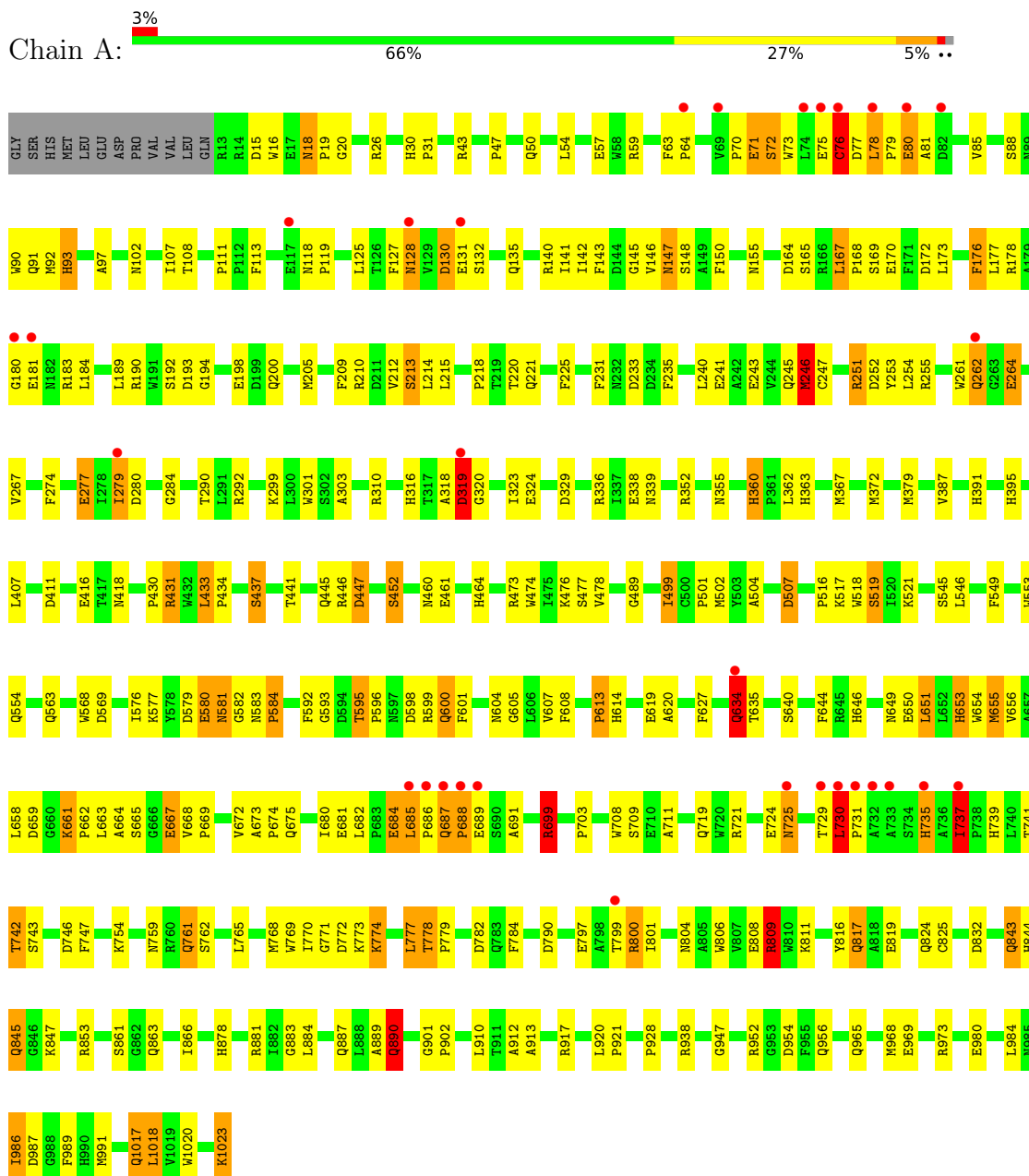
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	862	Total 862	O 862	0	0
6	B	995	Total 995	O 995	0	0
6	C	974	Total 974	O 974	0	0
6	D	897	Total 897	O 897	0	0

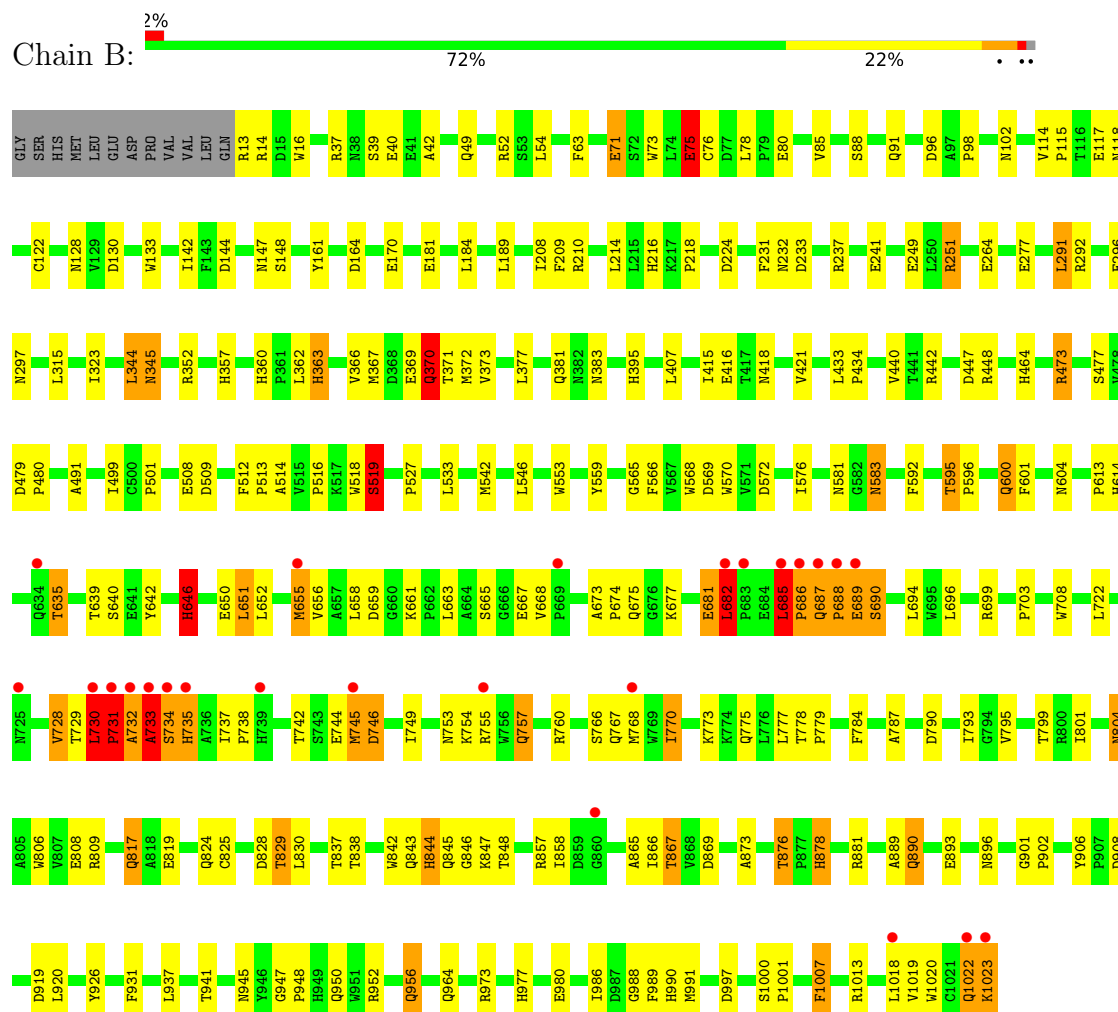
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

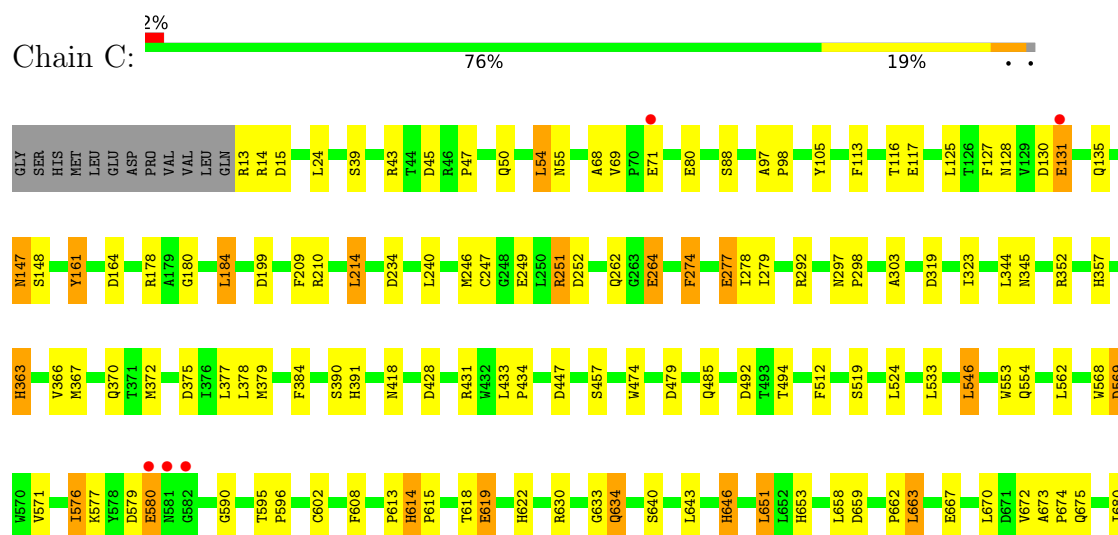
• Molecule 1: Beta-galactosidase

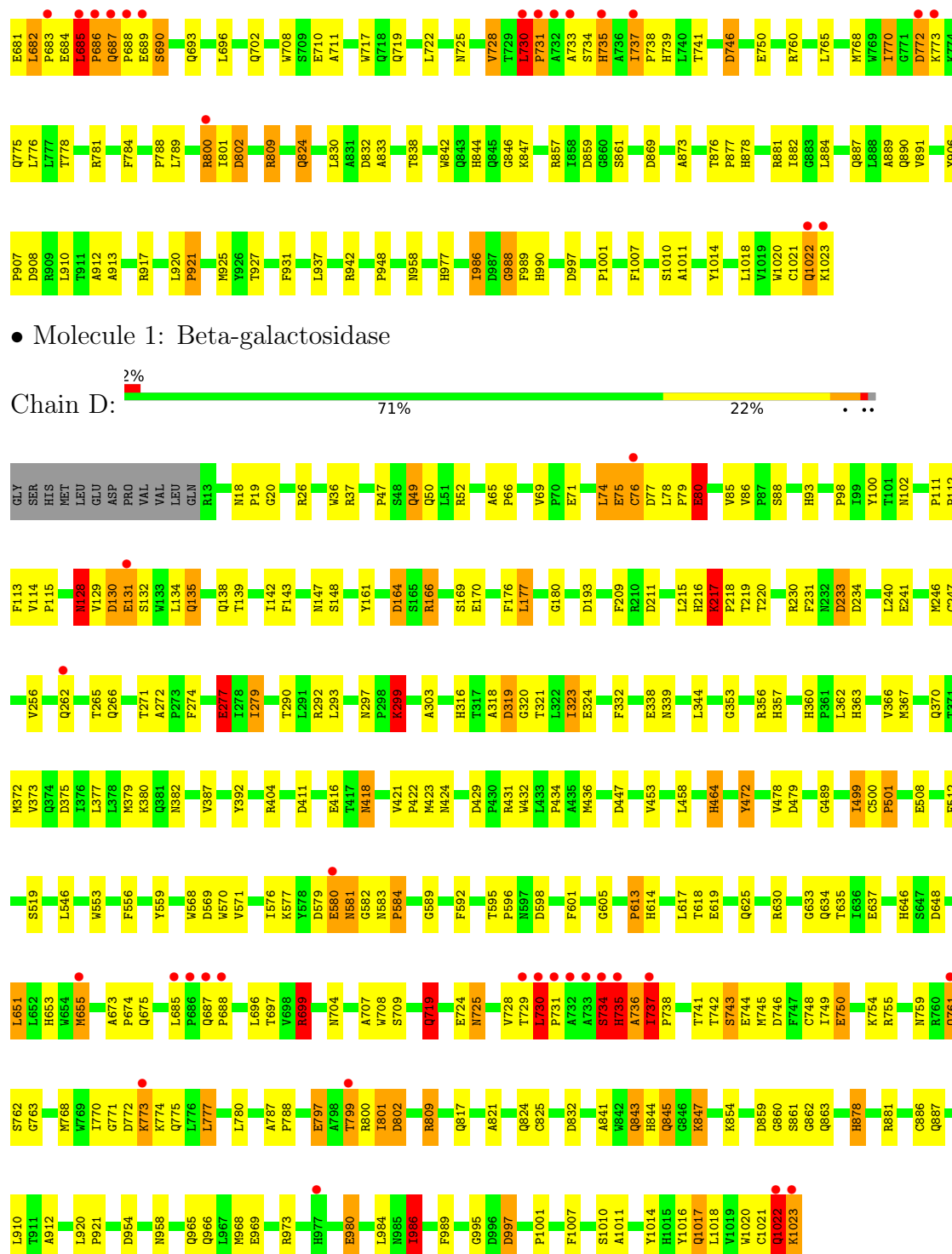


- Molecule 1: Beta-galactosidase



- Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	152.01Å 162.52Å 204.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (30.00-1.80) 97.7 (30.00-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.173 , 0.241 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 87.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36820	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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 40.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.5942e-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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, IPT, DMS, MG

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	1.28	4/8364 (0.0%)	1.82	146/11411 (1.3%)
1	B	1.31	10/8364 (0.1%)	1.81	148/11411 (1.3%)
1	C	1.30	8/8364 (0.1%)	1.78	118/11411 (1.0%)
1	D	1.25	10/8364 (0.1%)	1.79	136/11411 (1.2%)
All	All	1.28	32/33456 (0.1%)	1.80	548/45644 (1.2%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	297	ASN	C-O	-6.42	1.20	1.23
1	A	233	ASP	CA-C	-5.99	1.45	1.52
1	B	990	HIS	CE1-NE2	5.99	1.38	1.32
1	D	353	GLY	N-CA	5.94	1.50	1.44
1	D	802	ASP	C-N	-5.85	1.26	1.33
1	B	297	ASN	CA-C	-5.82	1.48	1.53
1	D	319	ASP	CG-OD2	5.76	1.36	1.25
1	C	619	GLU	CD-OE2	5.72	1.36	1.25
1	B	668	VAL	C-N	-5.65	1.26	1.33
1	C	474	TRP	NE1-CE2	5.58	1.43	1.37
1	C	1022	GLN	CD-NE2	-5.56	1.21	1.33
1	B	735	HIS	N-CA	-5.50	1.39	1.46
1	C	492	ASP	CG-OD2	5.49	1.35	1.25
1	B	742	THR	CA-C	-5.45	1.46	1.52
1	D	375	ASP	CG-OD2	5.45	1.35	1.25
1	D	472	TYR	CA-CB	5.35	1.61	1.53
1	D	954	ASP	CA-C	-5.24	1.47	1.53
1	B	646	HIS	CE1-NE2	5.24	1.37	1.32
1	C	1022	GLN	CA-C	-5.19	1.45	1.52
1	A	395	HIS	CE1-NE2	5.19	1.37	1.32
1	C	942	ARG	NE-CZ	5.18	1.38	1.33
1	A	452	SER	N-CA	5.17	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	357	HIS	CE1-NE2	5.16	1.37	1.32
1	C	569	ASP	CG-OD2	5.12	1.35	1.25
1	D	881	ARG	NE-CZ	5.09	1.38	1.33
1	D	233	ASP	CG-OD2	5.08	1.35	1.25
1	B	447	ASP	CG-OD2	5.07	1.34	1.25
1	B	926	TYR	CA-C	5.06	1.58	1.52
1	A	18	ASN	C-O	-5.03	1.19	1.24
1	D	500	CYS	CA-CB	5.03	1.58	1.53
1	B	241	GLU	CD-OE2	5.01	1.34	1.25
1	C	479	ASP	C-N	-5.00	1.29	1.34

All (548) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1022	GLN	OE1-CD-NE2	-15.95	106.65	122.60
1	B	735	HIS	CA-CB-CG	-14.00	99.80	113.80
1	A	319	ASP	CA-CB-CG	12.04	124.64	112.60
1	C	735	HIS	CA-CB-CG	-11.95	101.86	113.80
1	B	734	SER	N-CA-C	11.83	128.73	108.02
1	B	733	ALA	CA-C-N	-11.29	106.59	123.07
1	B	733	ALA	C-N-CA	-11.29	106.59	123.07
1	C	948	PRO	CB-CA-C	-10.49	96.73	110.27
1	A	598	ASP	CA-CB-CG	-9.98	102.62	112.60
1	D	802	ASP	CA-C-O	9.82	128.53	119.99
1	A	667	GLU	CB-CG-CD	-9.51	96.44	112.60
1	D	209	PHE	CA-CB-CG	-9.41	104.39	113.80
1	B	297	ASN	CB-CA-C	-9.39	104.53	111.20
1	D	297	ASN	CA-CB-CG	-9.27	103.33	112.60
1	D	274	PHE	CA-CB-CG	-9.07	104.73	113.80
1	C	809	ARG	NE-CZ-NH1	8.98	130.49	121.50
1	B	210	ARG	N-CA-CB	8.85	124.32	111.05
1	B	889	ALA	CA-C-N	-8.85	107.36	122.67
1	B	889	ALA	C-N-CA	-8.85	107.36	122.67
1	B	869	ASP	CA-CB-CG	-8.82	103.78	112.60
1	A	737	ILE	N-CA-CB	8.79	121.69	112.37
1	C	68	ALA	CA-C-N	-8.79	116.26	122.59
1	C	68	ALA	C-N-CA	-8.79	116.26	122.59
1	D	989	PHE	CA-CB-CG	-8.64	105.16	113.80
1	C	634	GLN	N-CA-CB	8.56	123.99	110.73
1	B	988	GLY	N-CA-C	-8.46	101.94	112.77
1	D	421	VAL	CA-C-O	-8.41	115.57	119.94
1	C	1022	GLN	CG-CD-OE1	8.25	137.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	464	HIS	CA-CB-CG	-8.24	105.56	113.80
1	C	682	LEU	CA-C-N	8.16	128.22	119.90
1	C	682	LEU	C-N-CA	8.16	128.22	119.90
1	C	1022	GLN	N-CA-CB	8.02	124.04	110.49
1	D	279	ILE	CA-CB-CG2	7.97	124.05	110.50
1	D	318	ALA	N-CA-CB	-7.93	98.16	110.06
1	B	614	HIS	N-CA-C	-7.79	99.93	110.36
1	A	687	GLN	N-CA-C	7.76	121.01	110.31
1	A	433	LEU	CA-C-O	7.75	125.86	118.34
1	B	233	ASP	CA-C-N	-7.58	110.62	122.67
1	B	233	ASP	C-N-CA	-7.58	110.62	122.67
1	D	279	ILE	CB-CA-C	7.56	117.71	111.06
1	D	209	PHE	N-CA-C	7.55	122.49	113.28
1	D	382	ASN	CA-CB-CG	-7.49	105.11	112.60
1	D	570	TRP	N-CA-C	7.45	119.30	111.03
1	D	633	GLY	CA-C-N	-7.45	110.98	122.60
1	D	633	GLY	C-N-CA	-7.45	110.98	122.60
1	B	685	LEU	C-N-CD	-7.39	94.69	125.00
1	D	272	ALA	CA-C-O	7.37	126.47	120.13
1	C	735	HIS	CB-CA-C	7.36	123.26	110.01
1	D	646	HIS	ND1-CE1-NE2	7.35	115.75	108.40
1	C	770	ILE	N-CA-CB	7.35	121.04	112.15
1	D	729	THR	N-CA-C	7.34	121.14	110.28
1	C	363	HIS	CA-CB-CG	-7.33	106.47	113.80
1	B	997	ASP	N-CA-CB	7.31	123.11	111.56
1	D	265	THR	CA-CB-OG1	-7.31	98.63	109.60
1	A	554	GLN	OE1-CD-NE2	7.25	129.85	122.60
1	B	76	CYS	N-CA-CB	-7.24	98.05	111.52
1	B	682	LEU	CA-C-N	7.20	127.24	119.89
1	B	682	LEU	C-N-CA	7.20	127.24	119.89
1	A	634	GLN	CB-CA-C	7.11	122.53	111.02
1	D	614	HIS	N-CA-C	-7.08	100.88	110.36
1	D	113	PHE	CA-CB-CG	-7.04	106.76	113.80
1	A	93	HIS	CA-CB-CG	-7.03	106.77	113.80
1	A	604	ASN	CA-CB-CG	7.02	119.62	112.60
1	D	323	ILE	N-CA-C	-7.01	105.78	111.81
1	A	209	PHE	N-CA-C	7.01	122.00	113.38
1	B	78	LEU	CA-C-O	7.00	125.99	119.76
1	B	828	ASP	CA-C-N	-6.98	113.08	122.72
1	B	828	ASP	C-N-CA	-6.98	113.08	122.72
1	A	221	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	C	357	HIS	CA-CB-CG	-6.94	106.86	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	319	ASP	N-CA-CB	6.94	120.53	110.47
1	B	685	LEU	CA-C-N	6.93	128.51	119.84
1	B	685	LEU	C-N-CA	6.93	128.51	119.84
1	D	598	ASP	CA-CB-CG	-6.92	105.67	112.60
1	A	190	ARG	N-CA-CB	6.91	120.03	110.01
1	B	184	LEU	CB-CA-C	-6.91	97.87	109.48
1	B	790	ASP	CA-CB-CG	-6.91	105.69	112.60
1	A	76	CYS	N-CA-C	6.90	119.56	109.07
1	A	989	PHE	CA-CB-CG	-6.90	106.90	113.80
1	B	646	HIS	CA-CB-CG	-6.89	106.91	113.80
1	B	738	PRO	CA-C-N	-6.87	111.61	122.73
1	B	738	PRO	C-N-CA	-6.87	111.61	122.73
1	D	728	VAL	N-CA-C	-6.87	105.95	113.43
1	A	251	ARG	NE-CZ-NH1	6.85	128.35	121.50
1	B	323	ILE	N-CA-C	-6.83	105.19	111.67
1	C	633	GLY	CA-C-N	-6.83	111.95	122.60
1	C	633	GLY	C-N-CA	-6.83	111.95	122.60
1	A	251	ARG	NE-CZ-NH2	-6.82	113.06	119.20
1	B	85	VAL	CB-CA-C	-6.81	101.68	111.34
1	A	809	ARG	CD-NE-CZ	-6.80	114.88	124.40
1	D	735	HIS	N-CA-CB	-6.79	99.01	110.49
1	A	176	PHE	CA-CB-CG	-6.79	107.01	113.80
1	B	357	HIS	CA-CB-CG	-6.79	107.01	113.80
1	B	345	ASN	CA-CB-CG	-6.78	105.82	112.60
1	A	627	PHE	CA-CB-CG	-6.77	107.03	113.80
1	B	479	ASP	CA-CB-CG	-6.77	105.83	112.60
1	D	878	HIS	CA-CB-CG	-6.76	107.04	113.80
1	C	702	GLN	CB-CA-C	-6.72	103.52	110.17
1	A	730	LEU	CA-C-N	6.71	126.69	119.78
1	A	730	LEU	C-N-CA	6.71	126.69	119.78
1	C	889	ALA	O-C-N	-6.68	114.05	122.27
1	B	52	ARG	CB-CA-C	-6.67	97.16	109.37
1	C	234	ASP	CA-CB-CG	-6.67	105.93	112.60
1	C	702	GLN	CA-C-O	6.67	124.96	119.36
1	B	363	HIS	CA-CB-CG	-6.65	107.15	113.80
1	C	178	ARG	CD-NE-CZ	6.64	133.70	124.40
1	C	988	GLY	N-CA-C	-6.63	104.48	113.37
1	B	646	HIS	ND1-CG-CD2	6.63	112.73	106.10
1	C	725	ASN	CA-CB-CG	-6.62	105.98	112.60
1	C	877	PRO	N-CA-CB	6.62	109.20	103.31
1	C	345	ASN	CA-CB-CG	-6.61	105.99	112.60
1	D	363	HIS	CA-CB-CG	-6.61	107.19	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	571	VAL	N-CA-C	6.60	117.63	108.12
1	D	651	LEU	CA-C-N	-6.59	113.62	122.72
1	D	651	LEU	C-N-CA	-6.59	113.62	122.72
1	D	958	ASN	N-CA-CB	6.59	123.36	111.37
1	A	233	ASP	CA-C-N	-6.58	112.16	122.49
1	A	233	ASP	C-N-CA	-6.58	112.16	122.49
1	D	559	TYR	CB-CA-C	-6.58	103.66	110.17
1	D	601	PHE	CA-CB-CG	-6.57	107.23	113.80
1	C	646	HIS	CA-CB-CG	-6.57	107.23	113.80
1	C	958	ASN	N-CA-CB	6.56	123.74	111.53
1	D	719	GLN	N-CA-CB	6.56	123.11	111.69
1	A	613	PRO	CB-CA-C	-6.53	102.43	110.98
1	C	997	ASP	CA-CB-CG	-6.53	106.07	112.60
1	B	699	ARG	CB-CA-C	-6.52	96.77	109.68
1	B	595	THR	O-C-N	6.51	126.91	121.83
1	D	128	ASN	CA-CB-CG	-6.49	106.11	112.60
1	D	1007	PHE	CA-CB-CG	-6.49	107.31	113.80
1	D	501	PRO	CB-CA-C	-6.49	102.75	111.12
1	A	592	PHE	CA-CB-CG	-6.49	107.31	113.80
1	B	232	ASN	CA-CB-CG	-6.49	106.11	112.60
1	C	711	ALA	CA-C-O	-6.46	114.09	121.19
1	D	324	GLU	N-CA-CB	6.46	122.60	111.69
1	C	298	PRO	CB-CA-C	-6.44	102.98	111.23
1	C	1022	GLN	CB-CG-CD	-6.43	101.67	112.60
1	A	164	ASP	CA-CB-CG	-6.42	106.19	112.60
1	C	519	SER	N-CA-C	-6.38	101.24	110.24
1	A	251	ARG	CD-NE-CZ	6.37	133.32	124.40
1	B	130	ASP	CA-CB-CG	-6.35	106.25	112.60
1	A	15	ASP	O-C-N	6.35	129.65	122.22
1	D	725	ASN	CA-CB-CG	-6.35	106.25	112.60
1	B	730	LEU	O-C-N	6.34	128.54	121.43
1	A	274	PHE	CA-CB-CG	-6.34	107.46	113.80
1	D	217	LYS	O-C-N	6.34	126.74	121.35
1	C	113	PHE	CA-CB-CG	-6.34	107.46	113.80
1	C	252	ASP	CA-CB-CG	-6.33	106.27	112.60
1	B	770	ILE	N-CA-CB	6.32	120.19	112.10
1	A	212	VAL	N-CA-CB	6.31	120.12	111.41
1	D	730	LEU	CA-C-O	6.31	125.37	119.76
1	D	128	ASN	OD1-CG-ND2	6.30	128.90	122.60
1	A	78	LEU	CA-C-N	6.29	126.20	119.28
1	A	78	LEU	C-N-CA	6.29	126.20	119.28
1	D	772	ASP	CA-C-N	-6.28	114.05	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	772	ASP	C-N-CA	-6.28	114.05	122.72
1	C	931	PHE	CA-C-O	6.28	124.64	119.36
1	A	634	GLN	N-CA-CB	6.27	121.55	111.20
1	A	601	PHE	CA-CB-CG	-6.27	107.53	113.80
1	C	809	ARG	CD-NE-CZ	6.26	133.16	124.40
1	D	734	SER	N-CA-C	6.25	119.73	108.17
1	C	494	THR	CA-C-N	-6.25	112.74	122.67
1	C	494	THR	C-N-CA	-6.25	112.74	122.67
1	C	917	ARG	CD-NE-CZ	-6.25	115.65	124.40
1	C	734	SER	N-CA-CB	6.25	119.49	110.06
1	D	499	ILE	CA-C-N	-6.23	115.91	122.89
1	D	499	ILE	C-N-CA	-6.23	115.91	122.89
1	C	884	LEU	CA-C-N	-6.23	110.98	121.75
1	C	884	LEU	C-N-CA	-6.23	110.98	121.75
1	C	247	CYS	CA-CB-SG	-6.22	100.09	114.40
1	D	817	GLN	N-CA-C	6.20	120.92	113.23
1	B	729	THR	CB-CA-C	6.18	121.69	111.31
1	B	829	THR	CB-CA-C	6.17	119.94	109.75
1	B	948	PRO	CB-CA-C	-6.17	102.18	110.88
1	A	97	ALA	N-CA-C	6.16	117.84	110.07
1	C	297	ASN	CB-CA-C	-6.16	106.82	111.20
1	A	19	PRO	N-CA-C	-6.16	106.65	114.35
1	A	504	ALA	N-CA-C	-6.13	101.20	110.28
1	C	447	ASP	N-CA-C	6.13	121.52	113.30
1	A	246	MET	CG-SD-CE	-6.13	87.41	100.90
1	D	809	ARG	NE-CZ-NH1	6.12	127.62	121.50
1	D	646	HIS	ND1-CG-CD2	6.12	112.22	106.10
1	B	734	SER	CA-C-O	6.10	126.81	120.40
1	A	113	PHE	CA-CB-CG	-6.10	107.70	113.80
1	D	339	ASN	CA-CB-CG	-6.07	106.53	112.60
1	D	47	PRO	N-CA-CB	6.06	108.62	103.35
1	A	90	TRP	CB-CA-C	6.05	121.82	110.63
1	C	209	PHE	N-CA-C	6.05	120.79	113.17
1	B	583	ASN	CA-CB-CG	-6.05	106.55	112.60
1	B	735	HIS	CB-CA-C	6.04	122.45	110.42
1	C	614	HIS	N-CA-C	-6.04	102.26	110.36
1	D	584	PRO	CB-CA-C	-6.04	103.06	110.98
1	B	370	GLN	CA-CB-CG	-6.04	102.03	114.10
1	C	249	GLU	N-CA-C	6.04	118.49	109.25
1	C	685	LEU	N-CA-C	6.03	118.23	110.39
1	C	571	VAL	N-CA-C	6.03	117.44	108.46
1	B	218	PRO	N-CA-CB	6.01	109.69	103.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	HIS	CB-CG-CD2	-6.01	123.39	131.20
1	B	509	ASP	CA-C-O	-6.01	114.15	121.36
1	B	973	ARG	NE-CZ-NH2	6.01	124.61	119.20
1	D	74	LEU	O-C-N	6.00	128.49	122.12
1	B	442	ARG	NE-CZ-NH2	-6.00	113.80	119.20
1	B	381	GLN	CA-CB-CG	-6.00	102.11	114.10
1	A	928	PRO	CB-CA-C	-5.98	105.05	112.89
1	B	650	GLU	CB-CA-C	-5.98	99.10	109.86
1	D	980	GLU	O-C-N	-5.98	115.81	122.86
1	A	320	GLY	CA-C-N	-5.97	113.77	122.19
1	A	320	GLY	C-N-CA	-5.97	113.77	122.19
1	D	360	HIS	CA-CB-CG	-5.97	107.83	113.80
1	C	116	THR	CA-C-N	-5.96	113.65	122.41
1	C	116	THR	C-N-CA	-5.96	113.65	122.41
1	C	323	ILE	N-CA-C	-5.96	106.01	111.67
1	A	155	ASN	CA-CB-CG	-5.95	106.66	112.60
1	A	431	ARG	CA-CB-CG	-5.94	102.22	114.10
1	C	869	ASP	CA-CB-CG	-5.94	106.66	112.60
1	B	685	LEU	N-CA-CB	5.93	120.92	110.37
1	A	699	ARG	CD-NE-CZ	5.92	132.69	124.40
1	B	144	ASP	CA-CB-CG	-5.91	106.69	112.60
1	C	274	PHE	CA-CB-CG	-5.91	107.89	113.80
1	B	519	SER	N-CA-C	-5.90	101.92	110.24
1	B	161	TYR	N-CA-CB	-5.90	100.55	111.52
1	B	731	PRO	CA-N-CD	-5.89	103.75	112.00
1	D	80	GLU	N-CA-C	5.88	120.32	113.20
1	A	264	GLU	CA-C-O	5.88	126.39	119.28
1	D	219	THR	CA-CB-OG1	-5.87	100.79	109.60
1	D	1022	GLN	CB-CG-CD	5.87	122.58	112.60
1	C	47	PRO	N-CA-CB	5.87	108.25	103.32
1	C	634	GLN	CB-CG-CD	-5.86	102.63	112.60
1	A	954	ASP	CA-CB-CG	-5.86	106.74	112.60
1	D	737	ILE	N-CA-CB	5.86	119.41	111.21
1	C	1022	GLN	CB-CA-C	-5.85	98.77	110.42
1	A	447	ASP	N-CA-C	5.85	120.54	113.17
1	A	507	ASP	N-CA-CB	-5.85	102.81	110.59
1	C	682	LEU	CA-C-O	5.84	125.10	120.19
1	A	845	GLN	CB-CA-C	-5.84	103.28	111.80
1	A	193	ASP	N-CA-C	-5.83	105.26	112.38
1	A	553	TRP	CA-CB-CG	-5.83	102.53	113.60
1	A	363	HIS	CA-CB-CG	-5.81	107.99	113.80
1	C	925	MET	N-CA-C	-5.81	106.05	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1010	SER	N-CA-CB	-5.80	101.74	110.73
1	D	553	TRP	CA-CB-CG	-5.80	102.59	113.60
1	A	360	HIS	CA-CB-CG	-5.79	108.01	113.80
1	B	464	HIS	CA-C-N	-5.79	116.96	121.82
1	B	464	HIS	C-N-CA	-5.79	116.96	121.82
1	A	653	HIS	CA-CB-CG	-5.78	108.03	113.80
1	B	75	GLU	CA-C-N	-5.77	111.63	121.85
1	B	75	GLU	C-N-CA	-5.77	111.63	121.85
1	B	296	GLU	CA-CB-CG	-5.77	102.56	114.10
1	B	688	PRO	N-CA-C	-5.76	102.21	111.38
1	D	735	HIS	CA-CB-CG	-5.76	108.04	113.80
1	A	816	TYR	CA-C-N	-5.75	113.57	122.49
1	A	816	TYR	C-N-CA	-5.75	113.57	122.49
1	D	247	CYS	N-CA-C	-5.75	100.60	109.52
1	C	161	TYR	N-CA-CB	-5.75	102.06	111.66
1	C	846	GLY	CA-C-N	-5.75	114.08	122.65
1	C	846	GLY	C-N-CA	-5.75	114.08	122.65
1	C	39	SER	N-CA-C	5.75	117.54	111.28
1	A	644	PHE	CA-CB-CG	-5.74	108.06	113.80
1	A	1018	LEU	CB-CA-C	-5.72	96.85	109.56
1	B	570	TRP	N-CA-C	5.72	117.38	111.03
1	B	842	TRP	CA-CB-CG	-5.72	102.72	113.60
1	D	699	ARG	NE-CZ-NH1	5.72	127.22	121.50
1	B	804	ASN	N-CA-CB	-5.72	101.52	110.44
1	B	920	LEU	CB-CA-C	-5.70	98.94	110.17
1	B	931	PHE	CA-C-O	5.69	124.14	119.36
1	D	1018	LEU	CA-C-O	-5.69	114.46	121.06
1	A	355	ASN	CA-C-N	-5.68	114.75	122.77
1	A	355	ASN	C-N-CA	-5.68	114.75	122.77
1	D	234	ASP	CA-CB-CG	-5.68	106.92	112.60
1	A	147	ASN	N-CA-CB	-5.67	101.66	110.55
1	C	352	ARG	O-C-N	5.67	128.65	122.64
1	C	889	ALA	CA-C-O	5.67	126.49	119.97
1	B	480	PRO	CB-CA-C	-5.67	101.52	111.21
1	C	690	SER	N-CA-C	5.66	115.86	107.88
1	C	788	PRO	N-CA-C	5.66	120.48	111.26
1	B	592	PHE	CA-CB-CG	-5.65	108.15	113.80
1	B	728	VAL	CB-CA-C	-5.62	104.71	111.85
1	A	938	ARG	N-CA-CB	5.62	120.53	110.80
1	B	1018	LEU	CB-CA-C	-5.62	97.97	109.38
1	C	69	VAL	CA-C-O	5.62	122.46	119.15
1	A	499	ILE	CA-C-N	-5.61	116.61	122.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	499	ILE	C-N-CA	-5.61	116.61	122.89
1	D	299	LYS	N-CA-C	-5.60	100.68	109.25
1	C	147	ASN	N-CA-CB	-5.60	101.76	110.55
1	D	332	PHE	CA-CB-CG	-5.60	108.20	113.80
1	A	790	ASP	CA-CB-CG	-5.59	107.01	112.60
1	A	489	GLY	CA-C-N	-5.58	113.42	122.30
1	A	489	GLY	C-N-CA	-5.58	113.42	122.30
1	A	464	HIS	CA-C-N	-5.58	117.50	122.47
1	A	464	HIS	C-N-CA	-5.58	117.50	122.47
1	A	280	ASP	CA-C-O	-5.58	115.15	120.56
1	B	98	PRO	N-CA-C	-5.57	102.37	111.68
1	B	844	HIS	CA-CB-CG	-5.56	108.24	113.80
1	A	267	VAL	CG1-CB-CG2	-5.55	98.59	110.80
1	B	352	ARG	CA-C-N	-5.55	116.69	122.69
1	B	352	ARG	C-N-CA	-5.55	116.69	122.69
1	C	1021	CYS	O-C-N	-5.55	116.45	123.17
1	D	648	ASP	N-CA-C	5.55	119.91	113.20
1	D	862	GLY	CA-C-O	5.54	125.27	119.06
1	A	329	ASP	CA-CB-CG	-5.54	107.06	112.60
1	B	371	THR	CA-C-N	-5.54	112.43	120.29
1	B	371	THR	C-N-CA	-5.54	112.43	120.29
1	A	809	ARG	NE-CZ-NH2	5.53	124.18	119.20
1	D	320	GLY	CA-C-N	-5.53	115.37	123.00
1	D	320	GLY	C-N-CA	-5.53	115.37	123.00
1	C	728	VAL	CA-C-O	5.53	123.96	118.98
1	D	605	GLY	N-CA-C	5.53	121.81	113.02
1	B	1019	VAL	CA-C-N	-5.52	115.38	123.00
1	B	1019	VAL	C-N-CA	-5.52	115.38	123.00
1	D	52	ARG	N-CA-CB	-5.52	101.23	110.83
1	C	1018	LEU	CB-CA-C	-5.51	97.94	110.07
1	A	853	ARG	NE-CZ-NH2	-5.51	114.24	119.20
1	D	635	THR	CA-C-N	-5.51	115.98	122.93
1	D	635	THR	C-N-CA	-5.51	115.98	122.93
1	B	264	GLU	CA-C-N	-5.51	114.94	122.93
1	B	264	GLU	C-N-CA	-5.51	114.94	122.93
1	C	921	PRO	N-CA-CB	5.51	108.45	103.33
1	B	757	GLN	N-CA-C	5.50	117.37	108.41
1	D	76	CYS	N-CA-C	5.50	117.20	108.79
1	D	164	ASP	CA-CB-CG	-5.49	107.11	112.60
1	D	648	ASP	CA-CB-CG	-5.49	107.11	112.60
1	C	927	THR	CB-CA-C	-5.49	103.59	109.85
1	A	646	HIS	N-CA-C	-5.49	102.39	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	584	PRO	CB-CA-C	-5.49	102.78	110.63
1	C	802	ASP	CA-CB-CG	-5.49	107.11	112.60
1	A	685	LEU	CB-CA-C	5.49	117.25	109.08
1	C	680	ILE	CA-CB-CG1	-5.48	101.08	110.40
1	D	968	MET	N-CA-CB	-5.48	101.29	110.39
1	C	130	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	98	PRO	N-CA-C	-5.46	102.56	111.68
1	D	788	PRO	N-CA-C	5.46	119.66	111.14
1	D	211	ASP	N-CA-C	5.46	117.33	110.24
1	C	686	PRO	N-CA-C	-5.45	103.59	111.22
1	A	336	ARG	NE-CZ-NH1	5.44	126.94	121.50
1	B	919	ASP	CA-CB-CG	-5.44	107.16	112.60
1	D	592	PHE	CA-CB-CG	-5.44	108.36	113.80
1	B	516	PRO	CB-CA-C	-5.44	104.10	111.12
1	B	770	ILE	N-CA-C	-5.43	98.12	107.24
1	D	704	ASN	CA-CB-CG	-5.42	107.17	112.60
1	B	39	SER	N-CA-C	5.42	117.95	111.71
1	B	613	PRO	CB-CA-C	-5.42	102.88	110.63
1	D	1018	LEU	CB-CA-C	-5.42	97.53	109.56
1	C	546	LEU	N-CA-CB	5.42	122.58	113.10
1	A	235	PHE	CA-CB-CG	-5.41	108.39	113.80
1	A	735	HIS	N-CA-CB	-5.41	101.34	110.49
1	A	563	GLN	N-CA-C	5.41	118.89	112.72
1	D	404	ARG	N-CA-C	5.41	118.34	111.69
1	D	707	ALA	CA-C-N	-5.40	114.05	122.37
1	D	707	ALA	C-N-CA	-5.40	114.05	122.37
1	B	553	TRP	CA-CB-CG	-5.40	103.34	113.60
1	B	842	TRP	CA-C-N	-5.39	114.12	122.59
1	B	842	TRP	C-N-CA	-5.39	114.12	122.59
1	D	997	ASP	N-CA-CB	5.39	120.08	111.56
1	B	442	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	57	GLU	N-CA-C	5.38	117.49	109.25
1	A	1023	LYS	N-CA-CB	5.38	119.65	110.50
1	D	131	GLU	N-CA-CB	5.38	118.03	110.12
1	D	519	SER	N-CA-C	-5.38	102.65	110.24
1	B	731	PRO	N-CD-CG	5.38	111.27	103.20
1	C	184	LEU	CB-CA-C	-5.38	100.65	109.53
1	D	878	HIS	CA-C-O	5.38	124.23	119.71
1	C	781	ARG	N-CA-CB	-5.37	102.20	111.55
1	A	181	GLU	O-C-N	5.37	129.44	122.89
1	A	437	SER	CA-C-N	-5.37	111.75	120.72
1	A	437	SER	C-N-CA	-5.37	111.75	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1007	PHE	CA-CB-CG	-5.37	108.43	113.80
1	A	446	ARG	NE-CZ-NH1	5.36	126.86	121.50
1	C	279	ILE	N-CA-C	-5.36	107.56	111.90
1	D	166	ARG	N-CA-C	5.36	120.50	112.94
1	D	832	ASP	N-CA-CB	-5.36	100.94	111.60
1	C	210	ARG	N-CA-CB	5.36	119.09	111.05
1	D	220	THR	N-CA-C	-5.35	99.05	108.20
1	A	352	ARG	CA-C-N	-5.34	116.92	122.69
1	A	352	ARG	C-N-CA	-5.34	116.92	122.69
1	C	602	CYS	CA-C-N	-5.33	115.07	123.13
1	C	602	CYS	C-N-CA	-5.33	115.07	123.13
1	C	746	ASP	CB-CA-C	-5.33	98.98	111.09
1	B	735	HIS	N-CA-C	5.33	122.16	110.80
1	C	98	PRO	N-CA-C	-5.33	102.78	111.68
1	A	213	SER	O-C-N	5.33	129.23	123.10
1	A	324	GLU	N-CA-CB	5.33	119.65	111.56
1	A	352	ARG	N-CA-C	-5.33	98.60	108.24
1	B	440	VAL	CB-CA-C	-5.33	104.94	111.92
1	A	746	ASP	CB-CA-C	-5.32	100.72	110.62
1	D	843	GLN	OE1-CD-NE2	5.31	127.91	122.60
1	B	793	ILE	N-CA-C	5.30	117.20	111.58
1	C	512	PHE	CA-C-O	5.30	125.69	120.17
1	C	553	TRP	CA-CB-CG	-5.30	103.52	113.60
1	C	634	GLN	CA-C-N	-5.30	115.68	123.00
1	C	634	GLN	C-N-CA	-5.30	115.68	123.00
1	C	97	ALA	N-CA-C	5.30	116.75	110.07
1	D	49	GLN	CB-CG-CD	-5.30	103.59	112.60
1	C	613	PRO	N-CA-C	5.30	119.80	111.38
1	B	941	THR	CA-CB-OG1	-5.29	101.67	109.60
1	A	719	GLN	CA-CB-CG	5.29	124.68	114.10
1	A	650	GLU	CB-CA-C	-5.29	99.21	109.68
1	B	787	ALA	N-CA-C	-5.29	99.87	109.44
1	C	384	PHE	CA-CB-CG	-5.29	108.52	113.80
1	D	986	ILE	CB-CG1-CD1	-5.28	102.71	113.80
1	B	830	LEU	CA-C-N	-5.28	113.68	120.65
1	B	830	LEU	C-N-CA	-5.28	113.68	120.65
1	D	613	PRO	CB-CA-C	-5.28	104.06	110.98
1	A	719	GLN	CB-CA-C	-5.27	98.47	110.07
1	A	477	SER	CB-CA-C	-5.27	101.94	110.79
1	C	363	HIS	N-CA-C	5.27	119.69	113.16
1	D	479	ASP	CB-CA-C	-5.27	103.55	110.87
1	A	604	ASN	CA-C-N	-5.26	114.02	121.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	604	ASN	C-N-CA	-5.26	114.02	121.13
1	D	161	TYR	CA-C-N	-5.26	114.96	121.38
1	D	161	TYR	C-N-CA	-5.26	114.96	121.38
1	A	277	GLU	CB-CG-CD	5.26	121.55	112.60
1	A	777	LEU	N-CA-CB	5.25	118.14	110.47
1	B	565	GLY	CA-C-O	-5.25	116.64	121.63
1	B	14	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	B	843	GLN	CA-C-N	-5.25	114.62	122.39
1	B	843	GLN	C-N-CA	-5.25	114.62	122.39
1	C	719	GLN	CG-CD-NE2	-5.25	108.53	116.40
1	B	642	TYR	N-CA-C	-5.24	102.72	110.48
1	B	956	GLN	CB-CG-CD	-5.24	103.69	112.60
1	A	661	LYS	N-CA-CB	-5.24	102.37	110.07
1	D	966	GLN	CB-CG-CD	5.24	121.50	112.60
1	A	761	GLN	CB-CG-CD	5.24	121.50	112.60
1	B	63	PHE	CA-CB-CG	-5.24	108.56	113.80
1	D	453	VAL	O-C-N	5.23	128.50	122.64
1	B	360	HIS	CA-CB-CG	-5.22	108.58	113.80
1	A	172	ASP	CA-C-N	-5.22	114.46	122.60
1	A	172	ASP	C-N-CA	-5.22	114.46	122.60
1	B	989	PHE	CA-CB-CG	-5.22	108.58	113.80
1	B	42	ALA	CA-C-O	5.22	126.30	120.82
1	C	418	ASN	N-CA-C	5.21	117.64	111.33
1	A	605	GLY	N-CA-C	5.21	121.31	113.02
1	D	143	PHE	CA-CB-CG	-5.21	108.59	113.80
1	C	418	ASN	CA-CB-CG	5.20	117.80	112.60
1	C	15	ASP	CA-CB-CG	-5.20	107.41	112.60
1	A	968	MET	N-CA-CB	-5.19	102.23	110.28
1	A	668	VAL	CA-C-N	-5.18	114.61	119.85
1	A	668	VAL	C-N-CA	-5.18	114.61	119.85
1	B	977	HIS	CA-CB-CG	-5.18	108.62	113.80
1	D	303	ALA	N-CA-C	-5.18	106.21	112.54
1	A	721	ARG	CB-CA-C	-5.18	101.30	109.80
1	C	693	GLN	CA-C-O	5.18	125.90	120.36
1	B	448	ARG	CA-C-N	-5.18	114.00	122.54
1	B	448	ARG	C-N-CA	-5.18	114.00	122.54
1	D	75	GLU	N-CA-C	5.18	118.06	111.69
1	D	319	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	220	THR	N-CA-C	-5.17	100.30	108.73
1	D	770	ILE	N-CA-C	-5.17	98.50	106.72
1	C	889	ALA	N-CA-CB	-5.17	102.27	110.28
1	A	431	ARG	NE-CZ-NH2	-5.17	114.55	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	742	THR	N-CA-C	5.16	117.98	109.72
1	B	209	PHE	O-C-N	5.16	128.79	122.34
1	B	491	ALA	N-CA-CB	-5.16	106.06	113.65
1	B	731	PRO	N-CA-CB	5.16	108.67	103.25
1	C	927	THR	CA-CB-OG1	-5.16	101.86	109.60
1	D	277	GLU	N-CA-CB	-5.16	102.88	110.26
1	C	730	LEU	N-CA-CB	-5.16	101.88	109.98
1	B	746	ASP	CA-CB-CG	-5.16	107.44	112.60
1	D	512	PHE	CA-C-O	5.15	125.53	120.17
1	A	218	PRO	N-CA-CB	5.15	108.78	103.38
1	B	865	ALA	CA-C-O	5.14	126.04	120.43
1	D	730	LEU	N-CA-C	5.14	116.13	109.65
1	D	423	MET	N-CA-C	5.14	117.62	111.71
1	B	876	THR	N-CA-C	-5.14	103.71	110.39
1	D	69	VAL	CA-C-N	5.13	125.93	120.13
1	D	69	VAL	C-N-CA	5.13	125.93	120.13
1	D	651	LEU	N-CA-CB	-5.13	101.92	110.80
1	A	323	ILE	N-CA-C	-5.13	106.68	111.45
1	D	787	ALA	N-CA-C	-5.13	100.60	109.58
1	B	118	ASN	O-C-N	5.13	125.99	121.32
1	D	418	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	669	PRO	N-CA-CB	5.12	108.10	103.33
1	A	167	LEU	O-C-N	5.12	126.21	121.80
1	B	964	GLN	N-CA-C	-5.12	105.82	111.71
1	D	777	LEU	N-CA-CB	5.12	117.94	110.47
1	A	890	GLN	N-CA-C	5.12	117.46	110.55
1	B	734	SER	CA-C-N	5.12	131.31	121.54
1	B	734	SER	C-N-CA	5.12	131.31	121.54
1	C	54	LEU	N-CA-C	-5.11	106.35	112.59
1	A	111	PRO	N-CA-CB	5.11	108.04	103.08
1	B	878	HIS	CA-CB-CG	-5.11	108.69	113.80
1	A	247	CYS	N-CA-C	-5.11	101.43	109.50
1	B	315	LEU	N-CA-C	-5.11	100.92	109.24
1	B	421	VAL	CA-C-O	-5.11	117.28	119.94
1	D	266	GLN	CA-C-N	-5.11	114.30	121.55
1	D	266	GLN	C-N-CA	-5.11	114.30	121.55
1	C	117	GLU	CB-CG-CD	-5.11	103.92	112.60
1	C	789	LEU	CB-CA-C	-5.11	99.83	110.40
1	D	176	PHE	CA-C-N	-5.10	111.78	122.03
1	D	176	PHE	C-N-CA	-5.10	111.78	122.03
1	A	956	GLN	N-CA-C	-5.10	101.56	109.72
1	B	415	ILE	CB-CA-C	-5.10	104.60	110.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	237	ARG	NE-CZ-NH2	-5.09	114.61	119.20
1	D	980	GLU	CA-C-O	5.09	127.11	121.56
1	A	319	ASP	CB-CA-C	5.09	119.43	110.37
1	B	566	PHE	CA-CB-CG	-5.09	108.71	113.80
1	B	473	ARG	CD-NE-CZ	5.09	131.52	124.40
1	D	297	ASN	CA-C-O	-5.09	116.96	120.47
1	B	512	PHE	CA-C-N	-5.08	114.67	119.76
1	B	512	PHE	C-N-CA	-5.08	114.67	119.76
1	C	710	GLU	CB-CA-C	-5.08	99.64	109.76
1	A	913	ALA	CA-C-O	-5.08	116.02	121.56
1	B	986	ILE	CB-CA-C	5.08	117.28	110.42
1	D	436	MET	CB-CA-C	-5.08	102.35	110.79
1	A	319	ASP	CB-CG-OD2	-5.08	106.72	118.40
1	B	635	THR	N-CA-C	5.08	117.52	109.24
1	D	854	LYS	N-CA-C	5.08	116.90	109.24
1	A	685	LEU	N-CA-CB	5.07	117.83	110.32
1	B	576	ILE	CB-CA-C	-5.07	104.55	111.15
1	C	857	ARG	CA-C-N	-5.07	116.90	123.19
1	C	857	ARG	C-N-CA	-5.07	116.90	123.19
1	A	779	PRO	CB-CA-C	-5.07	104.58	111.12
1	B	559	TYR	CB-CA-C	-5.07	104.54	110.17
1	D	736	ALA	N-CA-C	5.07	116.23	108.52
1	B	846	GLY	CA-C-N	-5.07	115.10	122.65
1	B	846	GLY	C-N-CA	-5.07	115.10	122.65
1	A	198	GLU	O-C-N	5.07	128.57	121.83
1	A	667	GLU	CB-CA-C	-5.07	98.31	109.56
1	C	770	ILE	N-CA-C	-5.06	98.67	106.72
1	A	310	ARG	CA-C-N	-5.06	116.02	123.00
1	A	310	ARG	C-N-CA	-5.06	116.02	123.00
1	B	572	ASP	CA-CB-CG	5.06	117.66	112.60
1	A	446	ARG	NE-CZ-NH2	-5.05	114.65	119.20
1	A	917	ARG	CD-NE-CZ	-5.05	117.33	124.40
1	A	303	ALA	N-CA-C	-5.05	106.38	112.54
1	A	765	LEU	N-CA-C	-5.05	101.88	109.15
1	B	742	THR	N-CA-C	5.04	117.19	109.07
1	C	590	GLY	O-C-N	-5.04	116.26	122.46
1	A	545	SER	N-CA-C	5.04	115.03	108.07
1	A	516	PRO	CB-CA-C	-5.04	104.78	111.23
1	D	279	ILE	CA-C-O	5.04	123.52	119.29
1	A	184	LEU	CB-CA-C	-5.03	101.00	109.50
1	D	746	ASP	CB-CA-C	-5.03	99.64	110.45
1	C	842	TRP	CA-CB-CG	-5.02	104.06	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	PHE	N-CA-CB	5.02	118.48	110.65
1	B	208	ILE	N-CA-CB	-5.02	107.19	112.06
1	D	177	LEU	CA-C-N	-5.02	114.45	122.53
1	D	177	LEU	C-N-CA	-5.02	114.45	122.53
1	C	913	ALA	CA-C-N	-5.02	114.93	122.81
1	C	913	ALA	C-N-CA	-5.02	114.93	122.81
1	D	556	PHE	O-C-N	-5.02	116.80	122.12
1	A	318	ALA	CA-C-N	-5.01	113.94	122.56
1	A	318	ALA	C-N-CA	-5.01	113.94	122.56
1	B	601	PHE	CA-CB-CG	-5.01	108.79	113.80
1	C	303	ALA	N-CA-CB	5.01	118.71	110.39
1	C	278	ILE	CB-CA-C	-5.01	103.42	111.59
1	B	362	LEU	N-CA-CB	-5.01	102.76	110.42
1	A	737	ILE	CA-C-N	-5.01	114.62	119.78
1	A	737	ILE	C-N-CA	-5.01	114.62	119.78
1	D	432	TRP	CA-C-O	5.00	125.34	119.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8123	0	7715	230	0
1	B	8123	0	7715	158	0
1	C	8123	0	7715	142	0
1	D	8123	0	7715	173	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
3	D	4	0	0	0	0
4	A	45	0	53	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	45	0	53	4	0
4	C	45	0	53	2	0
4	D	45	0	53	1	0
5	A	96	0	144	21	0
5	B	104	0	156	28	0
5	C	96	0	144	30	0
5	D	92	0	138	16	0
6	A	862	0	0	21	0
6	B	995	0	0	22	0
6	C	974	0	0	15	0
6	D	897	0	0	13	0
All	All	36820	0	31654	717	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (717) 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)
5:D:8403:DMS:S	5:D:8403:DMS:C2	2.08	1.41
1:A:1017:GLN:HE21	1:A:1018:LEU:N	1.46	1.11
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.16	1.08
1:D:750:GLU:HG3	1:D:755:ARG:HG3	1.37	1.06
1:A:730:LEU:HD22	1:A:731:PRO:HD2	1.36	1.05
1:B:369:GLU:HG2	1:B:370:GLN:HE22	1.16	1.05
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.44	0.99
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.45	0.99
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.43	0.99
1:B:809:ARG:HG2	1:B:809:ARG:HH11	1.30	0.95
1:A:600:GLN:H	1:A:600:GLN:HE21	0.95	0.94
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.03	0.92
1:C:643:LEU:HD23	1:C:675:GLN:NE2	1.87	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.14	0.89
1:A:1017:GLN:HE21	1:A:1018:LEU:H	1.09	0.89
1:D:735:HIS:ND1	1:D:735:HIS:N	2.16	0.89
1:C:737:ILE:CD1	1:C:738:PRO:HD2	2.03	0.89
1:B:804:ASN:HD22	1:B:809:ARG:NH2	1.71	0.88
1:B:804:ASN:ND2	1:B:809:ARG:HH21	1.74	0.86
1:B:369:GLU:HG2	1:B:370:GLN:NE2	1.90	0.86
1:A:241:GLU:HG2	1:A:292:ARG:HG2	1.57	0.84
1:C:277:GLU:HG2	6:C:4832:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.14	0.82
1:D:777:LEU:HD13	1:D:980:GLU:HG3	1.60	0.82
6:B:4763:HOH:O	5:C:8420:DMS:H22	1.80	0.82
1:D:730:LEU:HG	1:D:731:PRO:HD2	1.61	0.82
1:A:1017:GLN:NE2	1:A:1018:LEU:N	2.27	0.82
1:B:102:ASN:ND2	5:B:8506:DMS:H11	1.94	0.82
1:B:777:LEU:CD1	1:B:980:GLU:HG2	2.10	0.82
1:C:251:ARG:HB3	1:C:251:ARG:HH11	1.44	0.81
1:A:579:ASP:OD2	1:A:583:ASN:HB2	1.81	0.81
5:C:8502:DMS:H21	6:C:4944:HOH:O	1.81	0.81
1:D:750:GLU:CG	1:D:755:ARG:HG3	2.09	0.81
1:A:231:PHE:O	5:A:8417:DMS:H23	1.79	0.81
1:D:730:LEU:CD2	1:D:731:PRO:HD2	2.10	0.81
1:B:730:LEU:HD13	1:B:730:LEU:O	1.81	0.80
1:D:750:GLU:HG3	1:D:755:ARG:CG	2.10	0.80
1:B:251:ARG:HD2	5:B:8416:DMS:O	1.82	0.80
1:C:653:HIS:ND1	1:C:667:GLU:HG2	1.97	0.80
1:A:290:THR:O	5:A:8412:DMS:H23	1.82	0.80
1:C:653:HIS:CE1	1:C:667:GLU:HG2	2.17	0.79
1:A:890:GLN:OE1	1:A:947:GLY:HA3	1.82	0.79
1:D:730:LEU:CG	1:D:731:PRO:HD2	2.13	0.79
1:A:131:GLU:O	1:A:135:GLN:HG2	1.83	0.78
1:C:630:ARG:HB3	1:C:630:ARG:HH11	1.49	0.78
1:B:1023:LYS:HA	6:B:4995:HOH:O	1.83	0.78
1:A:730:LEU:CD2	1:A:731:PRO:HD2	2.14	0.78
1:D:797:GLU:O	1:D:801:ILE:HD13	1.84	0.78
1:A:655:MET:HE3	1:A:664:ALA:O	1.83	0.78
1:B:777:LEU:HD11	1:B:980:GLU:HG2	1.64	0.77
1:B:251:ARG:HA	5:B:8416:DMS:O	1.83	0.77
1:D:262:GLN:HE22	1:D:299:LYS:HD2	1.48	0.77
1:A:279:ILE:HD11	1:D:422:PRO:HG3	1.66	0.77
1:D:759:ASN:OD1	1:D:761:GLN:HG3	1.83	0.77
1:D:730:LEU:HD23	1:D:731:PRO:HD2	1.65	0.77
1:C:251:ARG:HB3	1:C:251:ARG:NH1	2.00	0.76
1:B:844:HIS:CE1	1:B:845:GLN:HG3	2.21	0.76
1:D:1022:GLN:HG3	1:D:1023:LYS:HG3	1.67	0.76
1:C:685:LEU:HD23	1:C:686:PRO:HD2	1.65	0.76
1:A:655:MET:HE2	1:A:656:VAL:O	1.86	0.76
1:C:685:LEU:HD23	1:C:686:PRO:CD	2.17	0.75
1:D:750:GLU:HG2	1:D:754:LYS:O	1.87	0.75
1:A:431:ARG:HG3	6:A:4683:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:TRP:NE1	1:A:774:LYS:HD3	2.01	0.75
1:B:292:ARG:HH12	5:B:8412:DMS:C2	1.99	0.75
1:A:634:GLN:HB2	1:A:682:LEU:HB2	1.69	0.74
1:B:809:ARG:HG2	1:B:809:ARG:NH1	2.00	0.74
1:A:600:GLN:H	1:A:600:GLN:NE2	1.79	0.74
1:D:130:ASP:OD1	1:D:132:SER:N	2.20	0.74
1:C:251:ARG:HA	5:C:8416:DMS:O	1.87	0.73
1:D:699:ARG:HH12	5:D:8415:DMS:H11	1.54	0.73
1:A:581:ASN:HD22	1:A:583:ASN:HD22	1.36	0.73
1:A:600:GLN:HE21	1:A:600:GLN:N	1.80	0.73
1:B:216:HIS:CG	5:B:8504:DMS:H11	2.24	0.72
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.19	0.72
1:A:797:GLU:O	1:A:801:ILE:HD13	1.89	0.72
1:D:128:ASN:HB3	1:D:180:GLY:O	1.90	0.72
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.24	0.71
1:D:651:LEU:CD2	1:D:653:HIS:HE1	2.04	0.71
1:A:684:GLU:O	1:A:686:PRO:HD3	1.90	0.71
1:A:965:GLN:O	1:A:969:GLU:HG3	1.89	0.71
1:A:655:MET:HG3	1:A:656:VAL:N	1.96	0.71
1:B:757:GLN:NE2	1:B:766:SER:OG	2.23	0.71
1:B:744:GLU:HB2	1:B:745:MET:HE3	1.72	0.71
1:C:576:ILE:N	1:C:576:ILE:HD13	2.05	0.71
1:D:618:THR:HG23	6:D:4358:HOH:O	1.89	0.71
1:D:1016:TYR:C	1:D:1017:GLN:HG3	2.14	0.71
1:B:370:GLN:N	1:B:370:GLN:HE21	1.88	0.71
1:A:634:GLN:HG2	1:A:682:LEU:O	1.91	0.70
1:D:233:ASP:HA	5:D:8417:DMS:H13	1.72	0.70
1:B:804:ASN:ND2	1:B:809:ARG:NH2	2.35	0.70
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.17	0.69
1:D:749:ILE:HD12	1:D:749:ILE:N	2.06	0.69
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.74	0.69
4:B:2001:IPT:C3'	5:B:8506:DMS:H21	2.22	0.69
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.27	0.69
1:A:130:ASP:OD1	1:A:130:ASP:C	2.36	0.69
1:B:249:GLU:CG	1:B:251:ARG:HD3	2.23	0.69
1:B:370:GLN:NE2	1:B:370:GLN:N	2.40	0.69
1:D:316:HIS:HA	1:D:323:ILE:CD1	2.20	0.69
1:A:800:ARG:HB2	1:A:800:ARG:CZ	2.22	0.69
5:A:8415:DMS:H11	6:A:4769:HOH:O	1.92	0.69
1:C:737:ILE:HD13	1:C:832:ASP:HA	1.75	0.69
1:B:847:LYS:HG3	1:B:848:THR:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:GLU:OE2	5:C:8412:DMS:H22	1.93	0.68
1:A:808:GLU:OE1	1:A:811:LYS:NZ	2.25	0.68
1:A:656:VAL:HG21	1:A:685:LEU:CD1	2.23	0.68
1:A:367:MET:HB3	1:A:372:MET:HE2	1.76	0.68
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.76	0.68
1:B:102:ASN:HD22	5:B:8506:DMS:H11	1.57	0.68
1:A:130:ASP:OD1	1:A:132:SER:N	2.26	0.67
1:A:430:PRO:HD3	5:A:8420:DMS:H21	1.77	0.67
1:A:686:PRO:O	1:A:687:GLN:NE2	2.28	0.67
1:D:708:TRP:CE3	1:D:709:SER:HB3	2.30	0.66
1:C:685:LEU:CD2	1:C:686:PRO:HD2	2.24	0.66
1:A:292:ARG:HH12	5:A:8412:DMS:H22	1.60	0.66
1:D:78:LEU:HB3	1:D:80:GLU:OE2	1.96	0.66
1:A:754:LYS:NZ	6:A:4752:HOH:O	2.28	0.66
5:A:8420:DMS:H22	6:D:4743:HOH:O	1.96	0.66
1:D:755:ARG:NH1	1:D:771:GLY:O	2.28	0.66
1:A:608:PHE:CE1	1:A:614:HIS:HD2	2.14	0.66
1:A:863:GLN:HE22	1:A:952:ARG:HH22	1.44	0.66
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:A:730:LEU:HD22	1:A:731:PRO:CD	2.21	0.66
1:D:984:LEU:HD21	1:D:986:ILE:HG13	1.78	0.66
1:B:249:GLU:HG2	1:B:251:ARG:HD3	1.76	0.65
1:C:45:ASP:OD1	5:C:8501:DMS:H11	1.96	0.65
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.79	0.65
1:D:777:LEU:CD1	1:D:980:GLU:HG3	2.26	0.65
1:D:262:GLN:NE2	1:D:299:LYS:HD2	2.10	0.65
1:A:135:GLN:HG3	6:A:4816:HOH:O	1.96	0.65
1:C:576:ILE:CD1	5:C:8411:DMS:H13	2.27	0.65
1:D:131:GLU:OE1	1:D:134:LEU:HB2	1.97	0.65
1:A:1017:GLN:NE2	1:A:1018:LEU:H	1.90	0.65
1:A:770:ILE:O	1:A:773:LYS:HE2	1.96	0.64
1:C:251:ARG:HH11	1:C:251:ARG:CB	2.09	0.64
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.79	0.64
1:B:708:TRP:CH2	5:B:8403:DMS:H22	2.33	0.64
1:D:580:GLU:OE1	1:D:580:GLU:HA	1.97	0.64
1:D:277:GLU:CD	1:D:277:GLU:H	2.03	0.64
1:C:651:LEU:HD11	1:C:653:HIS:ND1	2.12	0.64
1:B:75:GLU:HA	1:B:75:GLU:OE1	1.98	0.64
1:C:576:ILE:HD12	5:C:8411:DMS:H13	1.80	0.64
1:A:72:SER:OG	6:A:4467:HOH:O	2.15	0.64
1:D:71:GLU:H	1:D:71:GLU:CD	2.07	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:CB	6:A:4830:HOH:O	2.47	0.63
1:B:795:VAL:HG12	5:B:8506:DMS:H23	1.81	0.63
1:A:778:THR:HG21	6:A:4708:HOH:O	1.99	0.63
1:A:579:ASP:O	1:A:582:GLY:N	2.29	0.63
1:C:576:ILE:HD12	5:C:8411:DMS:C1	2.29	0.63
1:A:474:TRP:O	1:A:478:VAL:HG22	1.99	0.63
1:D:65:ALA:HB1	1:D:66:PRO:HD2	1.81	0.63
1:C:696:LEU:HB2	1:C:722:LEU:HD11	1.81	0.62
1:A:360:HIS:CE1	1:A:362:LEU:HB2	2.34	0.62
1:B:687:GLN:HB3	1:B:688:PRO:HD2	1.80	0.62
1:A:737:ILE:O	1:A:737:ILE:HD13	1.99	0.62
1:A:319:ASP:HB2	6:A:4830:HOH:O	1.99	0.62
1:D:416:GLU:OE2	1:D:418:ASN:HB2	2.00	0.62
1:A:759:ASN:OD1	1:A:762:SER:N	2.32	0.62
1:C:643:LEU:HD23	1:C:675:GLN:HE22	1.61	0.62
1:B:54:LEU:HD11	1:B:214:LEU:HG	1.82	0.61
1:A:73:TRP:HA	1:A:76:CYS:O	1.99	0.61
1:C:890:GLN:HG3	1:C:891:VAL:N	2.14	0.61
1:A:292:ARG:HH12	5:A:8412:DMS:C2	2.12	0.61
1:A:595:THR:HA	1:A:596:PRO:C	2.25	0.61
1:D:618:THR:HG21	6:D:4343:HOH:O	2.00	0.61
1:A:251:ARG:HD3	5:A:8416:DMS:H23	1.83	0.61
1:A:441:THR:O	1:A:445:GLN:HG3	2.00	0.61
1:A:581:ASN:HD22	1:A:583:ASN:ND2	1.97	0.61
1:B:950:GLN:OE1	1:B:952:ARG:HD3	2.00	0.61
1:C:43:ARG:NH1	1:C:264:GLU:OE1	2.28	0.61
1:A:93:HIS:CE1	5:A:8414:DMS:H12	2.36	0.61
1:A:130:ASP:OD1	1:A:131:GLU:N	2.34	0.61
1:B:656:VAL:CG1	1:B:694:LEU:HD22	2.31	0.60
5:B:8427:DMS:H21	6:B:4437:HOH:O	2.00	0.60
1:D:878:HIS:HD2	6:D:4105:HOH:O	1.83	0.60
5:B:8504:DMS:H13	6:B:4832:HOH:O	2.00	0.60
1:C:292:ARG:HH12	5:C:8412:DMS:C2	2.13	0.60
1:A:685:LEU:HD23	1:A:686:PRO:CD	2.28	0.60
1:C:708:TRP:CH2	5:C:8403:DMS:H22	2.36	0.60
1:A:93:HIS:CD2	5:A:8414:DMS:H12	2.37	0.60
1:B:795:VAL:HG12	5:B:8506:DMS:C2	2.32	0.60
1:A:771:GLY:O	1:A:773:LYS:HD3	2.01	0.60
1:B:675:GLN:HG3	6:B:4808:HOH:O	2.00	0.60
1:C:292:ARG:HH12	5:C:8412:DMS:H23	1.66	0.60
1:A:887:GLN:NE2	1:A:980:GLU:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:GLU:HG2	1:D:292:ARG:HG2	1.83	0.60
1:D:800:ARG:NH1	1:D:800:ARG:HB2	2.16	0.60
1:B:639:THR:OG1	1:B:677:LYS:HE3	2.02	0.60
1:C:920:LEU:HB3	1:C:921:PRO:HD2	1.84	0.60
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.84	0.60
1:A:476:LYS:NZ	6:A:4050:HOH:O	2.35	0.59
1:D:655:MET:HE3	1:D:697:THR:HB	1.82	0.59
1:A:778:THR:HG23	1:A:887:GLN:HB3	1.84	0.59
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.84	0.59
1:C:125:LEU:HD11	5:C:8408:DMS:H12	1.83	0.59
1:B:369:GLU:CG	1:B:370:GLN:HE22	2.04	0.59
1:A:599:ARG:HD2	1:A:600:GLN:HE22	1.68	0.59
1:A:651:LEU:CD2	1:A:703:PRO:HG3	2.27	0.59
1:A:656:VAL:HG21	1:A:685:LEU:HD13	1.84	0.59
1:C:750:GLU:HG3	6:C:4736:HOH:O	2.02	0.59
1:B:730:LEU:HD13	1:B:730:LEU:C	2.24	0.59
1:B:844:HIS:ND1	1:B:845:GLN:HG3	2.17	0.59
1:A:93:HIS:CG	5:A:8414:DMS:H12	2.38	0.59
1:B:37:ARG:HH12	5:B:8504:DMS:H21	1.68	0.58
1:C:844:HIS:HD2	6:C:4824:HOH:O	1.86	0.58
1:C:554:GLN:HG3	6:C:4934:HOH:O	2.01	0.58
1:A:54:LEU:HD11	1:A:214:LEU:HD13	1.86	0.58
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.85	0.58
1:B:277:GLU:HG2	6:B:4822:HOH:O	2.02	0.58
1:A:649:ASN:OD1	1:A:703:PRO:HD2	2.04	0.57
1:A:777:LEU:HG	1:A:889:ALA:HA	1.86	0.57
1:A:984:LEU:HD21	1:A:986:ILE:HG13	1.86	0.57
1:B:890:GLN:OE1	1:B:947:GLY:HA3	2.04	0.57
1:D:36:TRP:O	1:D:37:ARG:HD3	2.04	0.57
1:A:878:HIS:HD2	6:A:4073:HOH:O	1.86	0.57
1:B:363:HIS:HD2	6:B:4596:HOH:O	1.87	0.57
1:C:878:HIS:HD2	6:C:4098:HOH:O	1.87	0.57
1:D:130:ASP:OD1	1:D:130:ASP:C	2.46	0.57
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.57
1:A:742:THR:HG22	1:A:743:SER:N	2.19	0.57
5:D:8503:DMS:O	6:D:4264:HOH:O	2.15	0.57
1:B:689:GLU:O	1:B:690:SER:HB2	2.04	0.57
1:B:128:ASN:HB2	6:B:4847:HOH:O	2.05	0.57
1:C:367:MET:HE2	1:C:372:MET:HG2	1.86	0.57
1:D:773:LYS:HD2	1:D:774:LYS:O	2.05	0.57
1:A:685:LEU:O	1:A:687:GLN:OE1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:TRP:HE1	1:A:774:LYS:HD3	1.70	0.57
1:A:128:ASN:HB2	1:A:180:GLY:C	2.31	0.56
1:B:635:THR:HG23	1:B:681:GLU:OE2	2.04	0.56
1:A:656:VAL:HG21	1:A:685:LEU:HD11	1.86	0.56
1:A:277:GLU:H	1:A:277:GLU:CD	2.12	0.56
1:B:370:GLN:HB2	6:B:4525:HOH:O	2.05	0.56
1:C:662:PRO:O	1:C:663:LEU:HD23	2.06	0.56
1:D:231:PHE:O	5:D:8417:DMS:H23	2.06	0.56
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.40	0.56
1:C:319:ASP:C	1:C:319:ASP:OD1	2.49	0.56
1:C:45:ASP:O	5:C:8501:DMS:H13	2.05	0.55
1:D:131:GLU:HG3	1:D:135:GLN:OE1	2.05	0.55
1:B:1023:LYS:HD3	1:B:1023:LYS:N	2.21	0.55
1:C:595:THR:HA	1:C:596:PRO:C	2.32	0.55
1:A:252:ASP:HB2	5:A:8416:DMS:O	2.07	0.55
1:D:673:ALA:HB1	1:D:674:PRO:HD2	1.89	0.55
1:D:844:HIS:CE1	1:D:845:GLN:HG2	2.42	0.55
1:A:655:MET:HB3	1:A:699:ARG:HH22	1.72	0.55
1:B:754:LYS:HE2	1:B:1022:GLN:HG2	1.88	0.55
1:C:363:HIS:HD2	6:C:4598:HOH:O	1.90	0.55
1:C:595:THR:O	5:C:8413:DMS:H12	2.07	0.55
1:D:131:GLU:OE2	1:D:135:GLN:HG2	2.07	0.55
1:A:146:VAL:HG11	1:A:150:PHE:CD2	2.41	0.54
1:C:378:LEU:HG	6:C:4568:HOH:O	2.08	0.54
1:D:625:GLN:NE2	6:D:4231:HOH:O	2.41	0.54
1:D:730:LEU:HD23	1:D:731:PRO:CD	2.35	0.54
1:D:777:LEU:HD13	1:D:980:GLU:CG	2.36	0.54
1:C:131:GLU:OE2	1:C:135:GLN:HG3	2.07	0.54
1:D:595:THR:HA	1:D:596:PRO:C	2.32	0.54
1:A:579:ASP:CG	1:A:583:ASN:HB2	2.31	0.54
1:B:292:ARG:NH1	5:B:8412:DMS:H23	2.23	0.54
1:B:473:ARG:NH1	6:B:4701:HOH:O	2.24	0.54
1:A:664:ALA:HB3	1:A:685:LEU:HD21	1.88	0.54
1:B:878:HIS:HD2	6:B:4098:HOH:O	1.89	0.54
5:C:8404:DMS:H23	6:C:4153:HOH:O	2.07	0.54
5:C:8421:DMS:H23	6:C:4539:HOH:O	2.08	0.54
1:B:655:MET:HE2	1:B:665:SER:HB3	1.90	0.54
1:C:251:ARG:HD2	5:C:8416:DMS:O	2.08	0.54
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.23	0.54
1:A:130:ASP:OD2	1:A:132:SER:OG	2.22	0.54
1:D:734:SER:OG	1:D:860:GLY:HA3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1022:GLN:HE21	1:D:1023:LYS:CG	2.21	0.54
1:D:508:GLU:OE2	5:D:8407:DMS:H11	2.07	0.54
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.90	0.53
1:C:630:ARG:HB3	1:C:630:ARG:NH1	2.21	0.53
1:D:675:GLN:HG3	6:D:4777:HOH:O	2.07	0.53
1:B:292:ARG:HH12	5:B:8412:DMS:H23	1.70	0.53
1:C:88:SER:HA	1:C:366:VAL:HG21	1.89	0.53
1:A:866:ILE:O	1:A:1017:GLN:NE2	2.42	0.52
1:B:687:GLN:NE2	1:B:687:GLN:HA	2.23	0.52
1:C:646:HIS:HB3	6:C:4836:HOH:O	2.08	0.52
1:D:651:LEU:HD21	1:D:653:HIS:HE1	1.74	0.52
5:A:8403:DMS:H12	6:A:4076:HOH:O	2.08	0.52
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.91	0.52
1:B:581:ASN:HB2	6:B:4827:HOH:O	2.10	0.52
5:D:8410:DMS:H22	6:D:4292:HOH:O	2.10	0.52
1:D:131:GLU:HA	1:D:134:LEU:HD12	1.90	0.52
1:D:1022:GLN:HG3	1:D:1023:LYS:CG	2.39	0.52
1:B:655:MET:HG2	6:B:4962:HOH:O	2.09	0.52
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.92	0.52
1:B:16:TRP:CG	1:B:189:LEU:HD13	2.45	0.52
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.92	0.52
5:A:8413:DMS:H23	6:A:4361:HOH:O	2.08	0.52
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.92	0.52
1:A:79:PRO:HD2	1:A:80:GLU:HG3	1.92	0.52
1:A:502:MET:O	1:A:517:LYS:HE3	2.10	0.52
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.35	0.51
1:A:608:PHE:CE1	1:A:614:HIS:CD2	2.96	0.51
1:A:577:LYS:O	1:A:584:PRO:HA	2.10	0.51
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.73	0.51
1:D:725:ASN:HB2	6:D:4779:HOH:O	2.10	0.51
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.93	0.51
1:A:769:TRP:CE2	1:A:774:LYS:HD3	2.45	0.51
1:C:640:SER:O	1:C:675:GLN:HA	2.10	0.51
1:C:687:GLN:HG3	1:C:688:PRO:HD2	1.91	0.51
1:A:1017:GLN:HE21	1:A:1017:GLN:C	2.12	0.51
1:C:859:ASP:OD1	1:C:861:SER:OG	2.25	0.51
1:D:748:CYS:C	1:D:749:ILE:HD12	2.36	0.51
5:D:8403:DMS:H21	6:D:4316:HOH:O	2.10	0.51
1:C:50:GLN:HG3	5:C:8504:DMS:H23	1.93	0.51
1:B:292:ARG:NH1	5:B:8412:DMS:C2	2.73	0.51
1:D:579:ASP:O	1:D:582:GLY:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.26	0.51
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.41	0.50
1:C:651:LEU:HD11	1:C:667:GLU:HG2	1.92	0.50
1:D:76:CYS:O	1:D:77:ASP:C	2.53	0.50
1:D:338:GLU:HG2	6:D:4707:HOH:O	2.10	0.50
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.92	0.50
1:B:817:GLN:HG2	6:B:4364:HOH:O	2.11	0.50
1:C:13:ARG:O	1:C:14:ARG:C	2.53	0.50
1:C:131:GLU:OE1	1:C:131:GLU:O	2.29	0.50
1:C:809:ARG:NH2	1:C:1001:PRO:CG	2.74	0.50
1:A:737:ILE:HD13	1:A:737:ILE:C	2.37	0.50
1:A:131:GLU:HG2	1:A:135:GLN:NE2	2.26	0.50
1:C:772:ASP:OD1	1:C:772:ASP:N	2.40	0.50
1:B:685:LEU:O	1:B:686:PRO:O	2.29	0.50
1:C:428:ASP:O	5:C:8420:DMS:H11	2.12	0.50
1:C:431:ARG:HD2	6:C:4776:HOH:O	2.12	0.50
1:C:105:TYR:CE2	1:C:199:ASP:HB2	2.46	0.50
1:A:16:TRP:CD2	1:A:189:LEU:CD1	2.94	0.50
1:B:88:SER:HA	1:B:366:VAL:HG21	1.94	0.50
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.12	0.50
1:C:730:LEU:O	1:C:731:PRO:O	2.30	0.50
1:A:863:GLN:HE22	1:A:952:ARG:NH2	2.10	0.49
1:B:370:GLN:NE2	1:B:370:GLN:CA	2.74	0.49
1:B:1013:ARG:NH1	6:B:4014:HOH:O	2.28	0.49
1:A:26:ARG:NH1	1:A:169:SER:OG	2.37	0.49
1:B:583:ASN:ND2	6:B:4827:HOH:O	2.27	0.49
1:D:130:ASP:OD1	1:D:132:SER:OG	2.25	0.49
5:A:8420:DMS:H12	1:D:478:VAL:HG22	1.94	0.49
1:C:685:LEU:HD23	1:C:686:PRO:HD3	1.91	0.49
1:C:717:TRP:CH2	5:C:8415:DMS:H12	2.48	0.49
1:D:1022:GLN:HE21	1:D:1023:LYS:HG2	1.78	0.49
1:D:1022:GLN:CG	1:D:1023:LYS:HG3	2.40	0.49
1:B:730:LEU:CD1	1:B:730:LEU:N	2.76	0.49
1:B:777:LEU:HD13	1:B:980:GLU:HG2	1.91	0.49
1:D:292:ARG:C	1:D:293:LEU:HD12	2.37	0.49
1:A:77:ASP:HB2	6:A:4314:HOH:O	2.12	0.49
1:C:622:HIS:O	5:C:8402:DMS:H12	2.11	0.49
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.94	0.49
1:A:653:HIS:HD2	1:A:667:GLU:HG2	1.77	0.49
1:A:691:ALA:HA	1:A:725:ASN:HB2	1.93	0.49
1:B:708:TRP:HH2	5:B:8403:DMS:H22	1.74	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.48	0.49
1:A:658:LEU:O	1:A:661:LYS:HE2	2.12	0.49
1:A:338:GLU:HG2	6:A:4661:HOH:O	2.12	0.49
1:B:646:HIS:ND1	6:B:4823:HOH:O	2.33	0.49
1:A:655:MET:HE1	1:A:662:PRO:CB	2.42	0.49
1:B:600:GLN:HE21	1:B:600:GLN:N	1.97	0.49
1:B:753:ASN:OD1	1:B:753:ASN:N	2.42	0.49
1:B:367:MET:HA	1:B:367:MET:HE3	1.94	0.49
1:B:696:LEU:HB2	1:B:722:LEU:HD11	1.94	0.49
1:C:251:ARG:NH1	5:C:8416:DMS:O	2.46	0.49
1:C:682:LEU:CB	1:C:683:PRO:HD2	2.42	0.49
1:B:658:LEU:O	1:B:659:ASP:C	2.54	0.48
1:C:147:ASN:HA	1:C:148:SER:HA	1.67	0.48
1:C:653:HIS:CE1	1:C:667:GLU:CG	2.91	0.48
1:D:37:ARG:NH2	1:D:218:PRO:HD3	2.27	0.48
1:D:290:THR:O	5:D:8412:DMS:H23	2.13	0.48
1:D:973:ARG:O	5:D:8423:DMS:H12	2.13	0.48
1:A:85:VAL:O	1:A:88:SER:HB3	2.12	0.48
1:A:319:ASP:HB3	6:A:4830:HOH:O	2.10	0.48
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.47	0.48
1:D:730:LEU:HG	1:D:731:PRO:CD	2.39	0.48
1:D:800:ARG:NH1	1:D:800:ARG:CB	2.75	0.48
1:A:255:ARG:HB2	1:A:316:HIS:CE1	2.48	0.48
1:A:264:GLU:HG3	6:A:4747:HOH:O	2.12	0.48
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.48	0.48
1:B:37:ARG:NH1	5:B:8504:DMS:H21	2.29	0.48
1:C:830:LEU:N	1:C:833:ALA:O	2.34	0.48
1:B:251:ARG:HA	5:B:8416:DMS:S	2.53	0.48
1:B:801:ILE:HD12	1:B:808:GLU:CD	2.39	0.48
1:A:63:PHE:HB3	1:A:64:PRO:HD2	1.95	0.48
1:A:73:TRP:CD1	1:A:183:ARG:HH22	2.31	0.48
1:A:78:LEU:HB2	1:A:81:ALA:HB2	1.95	0.48
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.94	0.48
1:D:734:SER:HA	1:D:735:HIS:CE1	2.49	0.48
1:A:173:LEU:O	1:A:176:PHE:N	2.42	0.48
1:B:847:LYS:NZ	6:B:4929:HOH:O	2.47	0.48
1:D:965:GLN:O	1:D:969:GLU:HG3	2.14	0.48
1:D:79:PRO:HG2	1:D:80:GLU:OE2	2.14	0.47
1:D:821:ALA:N	1:D:841:ALA:O	2.43	0.47
1:A:844:HIS:ND1	1:A:845:GLN:HG2	2.30	0.47
1:D:373:VAL:O	1:D:377:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:8410:DMS:H22	6:A:4260:HOH:O	2.14	0.47
1:A:416:GLU:OE2	1:A:418:ASN:HB2	2.15	0.47
1:A:580:GLU:OE2	1:A:580:GLU:HA	2.13	0.47
1:D:26:ARG:HD2	1:D:169:SER:HA	1.95	0.47
1:A:824:GLN:HG2	1:A:825:CYS:N	2.28	0.47
1:C:533:LEU:C	1:C:533:LEU:HD23	2.40	0.47
1:C:687:GLN:CG	1:C:688:PRO:HD2	2.44	0.47
1:D:37:ARG:HG2	1:D:50:GLN:NE2	2.29	0.47
1:D:742:THR:CG2	1:D:743:SER:N	2.78	0.47
1:C:689:GLU:O	1:C:690:SER:HB3	2.15	0.47
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.49	0.47
1:D:734:SER:HA	1:D:735:HIS:ND1	2.29	0.47
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.97	0.47
1:B:71:GLU:N	1:B:71:GLU:OE1	2.48	0.47
1:B:732:ALA:O	1:B:734:SER:HB3	2.15	0.47
1:C:619:GLU:HA	1:C:912:ALA:HB2	1.96	0.47
1:D:762:SER:OG	1:D:763:GLY:N	2.46	0.47
1:A:635:THR:OG1	1:A:681:GLU:OE2	2.25	0.47
1:B:730:LEU:C	1:B:730:LEU:HD22	2.40	0.47
1:D:367:MET:HE2	1:D:372:MET:HG2	1.97	0.47
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.96	0.46
1:A:664:ALA:CB	1:A:685:LEU:HD21	2.45	0.46
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.97	0.46
1:B:770:ILE:HD12	1:B:775:GLN:CD	2.41	0.46
1:A:16:TRP:CG	1:A:189:LEU:CD1	2.98	0.46
1:A:708:TRP:CH2	5:A:8403:DMS:H22	2.50	0.46
1:B:372:MET:HE1	1:B:395:HIS:CG	2.51	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.44	0.46
1:A:687:GLN:HA	1:A:688:PRO:HD3	1.78	0.46
1:A:253:TYR:CD1	1:A:253:TYR:C	2.94	0.46
1:B:367:MET:HE3	1:B:367:MET:CA	2.46	0.46
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.15	0.46
1:D:920:LEU:HB3	1:D:921:PRO:HD2	1.97	0.46
1:A:167:LEU:HB3	1:A:168:PRO:HD2	1.98	0.46
1:A:71:GLU:O	1:A:72:SER:C	2.58	0.46
1:A:607:VAL:HG12	1:A:613:PRO:HA	1.96	0.46
1:B:682:LEU:HD12	1:B:682:LEU:HA	1.59	0.46
1:D:824:GLN:HG2	1:D:825:CYS:N	2.26	0.46
1:A:521:LYS:HE3	6:A:4416:HOH:O	2.16	0.46
1:D:230:ARG:NH2	4:D:2003:IPT:O6	2.42	0.46
1:D:93:HIS:CD2	5:D:8414:DMS:H23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:A:145:GLY:N	1:A:210:ARG:HB2	2.31	0.46
1:D:246:MET:SD	1:D:246:MET:C	3.00	0.46
1:D:749:ILE:N	1:D:749:ILE:CD1	2.78	0.46
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.50	0.45
1:A:599:ARG:HB2	1:A:600:GLN:HE21	1.82	0.45
1:B:658:LEU:O	1:B:661:LYS:HE3	2.16	0.45
1:C:367:MET:HB3	1:C:372:MET:HE2	1.97	0.45
1:B:1022:GLN:O	1:B:1022:GLN:HG3	2.12	0.45
4:B:2001:IPT:H3'2	5:B:8506:DMS:H21	1.97	0.45
1:C:673:ALA:O	1:C:674:PRO:C	2.56	0.45
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.98	0.45
4:C:2004:IPT:H3'3	4:C:2004:IPT:H1	1.55	0.45
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.34	0.45
1:B:369:GLU:CG	1:B:370:GLN:NE2	2.73	0.45
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.98	0.45
1:C:670:LEU:HD23	1:C:670:LEU:HA	1.63	0.45
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.97	0.45
1:D:147:ASN:HA	1:D:148:SER:HA	1.64	0.45
1:A:832:ASP:OD1	1:A:832:ASP:N	2.48	0.45
1:B:595:THR:HG22	5:B:8413:DMS:S	2.56	0.45
1:C:251:ARG:HA	1:C:251:ARG:HD2	1.76	0.45
1:C:1022:GLN:NE2	1:C:1022:GLN:N	2.65	0.45
1:D:984:LEU:CD2	1:D:986:ILE:HG13	2.46	0.45
1:B:518:TRP:O	1:B:519:SER:C	2.60	0.45
1:B:867:THR:HG23	6:B:4435:HOH:O	2.17	0.45
1:B:906:TYR:CZ	1:B:937:LEU:HB2	2.52	0.45
1:C:131:GLU:HG3	1:C:135:GLN:NE2	2.31	0.45
1:C:608:PHE:CZ	1:C:614:HIS:CD2	3.05	0.45
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.76	0.45
1:A:59:ARG:NH2	1:A:81:ALA:O	2.50	0.45
1:B:369:GLU:C	1:B:370:GLN:NE2	2.75	0.45
1:D:78:LEU:O	1:D:79:PRO:C	2.59	0.45
1:D:734:SER:C	1:D:736:ALA:H	2.24	0.45
1:B:687:GLN:N	1:B:687:GLN:CD	2.75	0.45
1:C:55:ASN:O	5:C:8408:DMS:H21	2.16	0.45
5:C:8403:DMS:H12	6:C:4101:HOH:O	2.17	0.45
1:D:809:ARG:NH2	1:D:1001:PRO:CG	2.80	0.45
1:A:92:MET:HE3	1:A:205:MET:CE	2.47	0.45
1:A:742:THR:CG2	1:A:743:SER:N	2.80	0.45
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ASN:HB3	1:B:945:ASN:HB2	1.98	0.45
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.52	0.45
1:C:630:ARG:NH1	1:C:630:ARG:CB	2.79	0.45
1:C:802:ASP:C	1:C:802:ASP:OD1	2.57	0.45
1:A:739:HIS:CD2	6:A:4777:HOH:O	2.69	0.45
1:B:542:MET:HA	1:B:604:ASN:HA	1.98	0.45
1:B:640:SER:O	1:B:675:GLN:HA	2.17	0.45
1:D:651:LEU:HD23	1:D:653:HIS:HE1	1.80	0.45
1:D:696:LEU:O	1:D:719:GLN:HB3	2.17	0.45
1:A:80:GLU:HG3	1:A:80:GLU:H	1.36	0.44
1:A:581:ASN:ND2	1:A:583:ASN:HD22	2.11	0.44
1:C:457:SER:HA	1:C:485:GLN:O	2.17	0.44
1:A:299:LYS:HE2	1:A:299:LYS:HA	1.98	0.44
1:A:769:TRP:HA	1:A:773:LYS:O	2.17	0.44
1:B:291:LEU:N	1:B:291:LEU:HD22	2.32	0.44
1:B:1000:SER:O	1:B:1001:PRO:C	2.58	0.44
1:C:906:TYR:CZ	1:C:937:LEU:HB2	2.52	0.44
1:D:800:ARG:CB	1:D:800:ARG:HH11	2.31	0.44
1:A:724:GLU:O	1:B:847:LYS:NZ	2.50	0.44
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.11	0.44
1:A:18:ASN:C	1:A:20:GLY:H	2.24	0.44
1:A:973:ARG:O	5:A:8423:DMS:H12	2.18	0.44
1:B:730:LEU:O	1:B:731:PRO:O	2.36	0.44
1:C:768:MET:CE	1:C:776:LEU:HD11	2.47	0.44
1:C:524:LEU:HD11	1:C:562:LEU:HG	1.99	0.44
1:D:241:GLU:HG3	6:D:4835:HOH:O	2.16	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.62	0.44
1:A:240:LEU:C	1:A:240:LEU:HD23	2.42	0.44
1:B:513:PRO:O	1:B:514:ALA:HB3	2.17	0.44
1:D:139:THR:OG1	1:D:216:HIS:HD2	2.00	0.44
1:B:383:ASN:HA	5:B:8403:DMS:H11	1.99	0.44
1:B:728:VAL:O	1:B:728:VAL:HG23	2.14	0.44
1:C:54:LEU:HD11	1:C:214:LEU:HD13	1.98	0.44
1:D:619:GLU:HA	1:D:912:ALA:HB2	1.99	0.44
1:A:817:GLN:HE21	1:A:817:GLN:HB3	1.47	0.44
1:A:920:LEU:HB3	1:A:921:PRO:HD2	1.99	0.44
1:B:133:TRP:NE1	5:B:8504:DMS:H12	2.32	0.44
1:B:372:MET:HE1	1:B:395:HIS:HB3	1.99	0.44
1:B:873:ALA:O	1:B:876:THR:HG22	2.17	0.44
1:C:682:LEU:HA	1:C:683:PRO:HD3	1.64	0.44
1:D:215:LEU:HD21	1:D:217:LYS:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:458:LEU:HD11	1:D:472:TYR:HB2	2.00	0.44
1:A:634:GLN:CB	1:A:682:LEU:HB2	2.42	0.44
1:A:654:TRP:CZ3	1:A:665:SER:HA	2.53	0.44
1:A:739:HIS:HD2	6:A:4777:HOH:O	2.00	0.44
1:B:508:GLU:OE2	5:B:8407:DMS:H11	2.17	0.44
1:C:576:ILE:CD1	5:C:8411:DMS:C1	2.92	0.44
1:D:630:ARG:NE	1:D:637:GLU:OE1	2.50	0.44
1:B:102:ASN:HD22	5:B:8506:DMS:C1	2.28	0.43
1:B:216:HIS:ND1	5:B:8504:DMS:H11	2.32	0.43
1:B:651:LEU:HD13	1:B:703:PRO:HG3	2.00	0.43
1:B:754:LYS:CE	1:B:1022:GLN:HG2	2.48	0.43
1:D:111:PRO:HA	1:D:112:PRO:HA	1.64	0.43
1:D:356:ARG:NH2	1:D:367:MET:HE2	2.32	0.43
1:D:737:ILE:HG13	1:D:738:PRO:O	2.18	0.43
1:A:518:TRP:O	1:A:519:SER:C	2.61	0.43
1:A:192:SER:C	1:A:194:GLY:N	2.76	0.43
1:B:373:VAL:O	1:B:377:LEU:HG	2.18	0.43
1:B:416:GLU:OE2	1:B:418:ASN:HB2	2.19	0.43
1:C:824:GLN:O	1:C:838:THR:HA	2.18	0.43
1:D:577:LYS:O	1:D:584:PRO:HA	2.17	0.43
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.32	0.43
1:B:533:LEU:HD23	1:B:533:LEU:C	2.42	0.43
1:C:873:ALA:O	1:C:876:THR:HG22	2.18	0.43
1:D:651:LEU:CD2	1:D:653:HIS:CE1	2.93	0.43
1:A:91:GLN:OE1	1:A:205:MET:HB3	2.18	0.43
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.54	0.43
1:C:375:ASP:O	1:C:379:MET:HG3	2.19	0.43
1:C:847:LYS:NZ	1:D:724:GLU:O	2.52	0.43
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.00	0.43
1:A:768:MET:CE	1:A:1020:TRP:CH2	3.00	0.43
1:C:292:ARG:NH1	5:C:8412:DMS:H23	2.32	0.43
1:D:88:SER:HA	1:D:366:VAL:HG21	2.01	0.43
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.83	0.43
1:D:380:LYS:O	5:D:8403:DMS:H11	2.18	0.43
1:A:70:PRO:O	1:A:71:GLU:C	2.61	0.43
1:A:93:HIS:NE2	5:A:8414:DMS:H12	2.33	0.43
1:A:141:ILE:HA	1:A:213:SER:O	2.19	0.43
1:C:128:ASN:HA	1:C:180:GLY:O	2.19	0.43
1:C:554:GLN:CD	4:C:2004:IPT:H3	2.43	0.43
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.53	0.43
1:A:608:PHE:CD1	1:A:614:HIS:HD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.53	0.43
1:B:730:LEU:HD12	1:B:730:LEU:H	1.84	0.43
1:C:246:MET:SD	1:C:246:MET:C	3.02	0.43
1:C:577:LYS:HB3	1:C:577:LYS:HE3	1.61	0.43
1:C:579:ASP:HB2	1:C:580:GLU:OE2	2.18	0.43
1:D:613:PRO:HB3	1:D:617:LEU:HD23	2.01	0.43
1:D:802:ASP:OD1	1:D:802:ASP:C	2.62	0.43
1:A:107:ILE:O	1:A:108:THR:C	2.60	0.43
1:A:147:ASN:HA	1:A:165:SER:OG	2.19	0.43
1:D:859:ASP:OD1	1:D:861:SER:OG	2.28	0.43
1:A:599:ARG:HD2	1:A:600:GLN:NE2	2.34	0.43
1:A:806:TRP:CD2	1:A:991:MET:HE1	2.53	0.43
1:D:734:SER:C	1:D:735:HIS:ND1	2.76	0.43
1:B:809:ARG:NH1	1:B:809:ARG:CG	2.73	0.42
1:D:102:ASN:OD1	1:D:102:ASN:C	2.60	0.42
1:D:742:THR:HG22	1:D:743:SER:N	2.34	0.42
1:A:143:PHE:O	1:A:168:PRO:HA	2.20	0.42
1:A:777:LEU:HA	1:A:777:LEU:HD23	1.83	0.42
1:C:576:ILE:HD11	5:C:8411:DMS:H13	2.00	0.42
1:D:74:LEU:HA	1:D:74:LEU:HD23	1.68	0.42
1:D:910:LEU:HD12	1:D:910:LEU:C	2.45	0.42
1:B:890:GLN:O	1:B:890:GLN:HG3	2.02	0.42
1:D:93:HIS:CD2	5:D:8414:DMS:C2	3.02	0.42
1:D:379:MET:HE1	1:D:387:VAL:HB	2.00	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.42
1:A:901:GLY:HA3	1:A:902:PRO:HA	1.73	0.42
1:C:240:LEU:C	1:C:240:LEU:HD23	2.44	0.42
1:A:47:PRO:HA	5:A:8501:DMS:O	2.19	0.42
1:A:339:ASN:O	1:B:527:PRO:HB3	2.20	0.42
1:A:379:MET:CE	1:A:407:LEU:HD13	2.50	0.42
1:A:640:SER:O	1:A:675:GLN:HA	2.20	0.42
1:A:771:GLY:O	1:A:772:ASP:HB2	2.20	0.42
1:B:13:ARG:NH2	1:C:13:ARG:HB2	2.35	0.42
1:C:390:SER:HA	1:C:391:HIS:HA	1.90	0.42
1:B:224:ASP:OD2	6:B:4836:HOH:O	2.22	0.42
4:B:2001:IPT:C3'	5:B:8506:DMS:C2	2.96	0.42
1:C:733:ALA:O	1:C:735:HIS:CE1	2.73	0.42
1:A:50:GLN:N	1:A:50:GLN:CD	2.78	0.42
1:A:843:GLN:HB3	1:A:847:LYS:O	2.19	0.42
1:A:984:LEU:HD11	1:A:986:ILE:HG12	2.01	0.42
1:B:181:GLU:CB	6:B:4882:HOH:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:LEU:O	1:B:345:ASN:C	2.61	0.42
1:A:579:ASP:OD1	1:A:579:ASP:C	2.62	0.42
1:A:708:TRP:CE3	1:A:709:SER:HB3	2.55	0.42
1:A:784:PHE:HA	1:A:881:ARG:O	2.20	0.42
1:C:739:HIS:HE1	1:C:741:THR:OG1	2.03	0.42
1:C:910:LEU:C	1:C:910:LEU:HD12	2.45	0.42
1:C:986:ILE:HD12	1:C:986:ILE:HG21	1.69	0.42
5:C:8408:DMS:H13	6:C:4685:HOH:O	2.20	0.42
1:D:100:TYR:HB3	1:D:589:GLY:HA2	2.02	0.42
1:D:240:LEU:HD23	1:D:240:LEU:C	2.45	0.42
1:D:699:ARG:NH1	5:D:8415:DMS:H11	2.30	0.42
1:A:131:GLU:HB3	1:A:135:GLN:NE2	2.35	0.42
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.54	0.42
1:B:231:PHE:O	5:B:8417:DMS:H23	2.19	0.42
1:B:749:ILE:HD13	1:B:858:ILE:HD12	2.00	0.42
1:B:901:GLY:HA3	1:B:902:PRO:HA	1.77	0.42
1:C:131:GLU:OE2	1:C:135:GLN:NE2	2.49	0.42
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.49	0.42
1:C:908:ASP:HB3	1:C:1007:PHE:CD1	2.55	0.42
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.01	0.42
1:D:256:VAL:O	1:D:271:THR:HA	2.20	0.42
1:D:584:PRO:HD2	6:D:4693:HOH:O	2.19	0.42
1:D:777:LEU:HD23	1:D:777:LEU:HA	1.90	0.42
1:B:784:PHE:HA	1:B:881:ARG:O	2.20	0.42
1:B:1020:TRP:CD1	1:B:1020:TRP:C	2.98	0.42
1:D:995:GLY:C	1:D:997:ASP:N	2.76	0.42
1:A:301:TRP:CH2	1:A:452:SER:HA	2.55	0.41
1:A:952:ARG:HG3	1:A:952:ARG:HH11	1.84	0.41
1:B:147:ASN:HA	1:B:148:SER:HA	1.74	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.94	0.41
1:C:45:ASP:CG	5:C:8501:DMS:H11	2.45	0.41
1:C:615:PRO:O	1:C:618:THR:HG22	2.19	0.41
1:D:79:PRO:CD	1:D:80:GLU:OE2	2.68	0.41
1:D:316:HIS:HB2	1:D:321:THR:O	2.19	0.41
1:A:673:ALA:O	1:A:674:PRO:C	2.63	0.41
1:A:984:LEU:CD2	1:A:986:ILE:HG13	2.49	0.41
1:B:824:GLN:O	1:B:838:THR:HA	2.19	0.41
5:C:8427:DMS:H22	6:C:4463:HOH:O	2.20	0.41
1:D:800:ARG:HB2	1:D:800:ARG:CZ	2.50	0.41
1:A:319:ASP:OD2	6:A:4764:HOH:O	2.22	0.41
1:A:593:GLY:O	1:A:595:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:ARG:HB2	1:A:600:GLN:NE2	2.35	0.41
1:B:804:ASN:HD21	1:B:809:ARG:HH21	1.64	0.41
1:C:977:HIS:O	1:C:977:HIS:CD2	2.73	0.41
1:D:85:VAL:HG12	1:D:86:VAL:N	2.35	0.41
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.55	0.41
1:A:118:ASN:O	1:A:119:PRO:C	2.63	0.41
1:D:576:ILE:HD13	1:D:576:ILE:HA	1.77	0.41
1:D:799:THR:O	1:D:799:THR:HG23	2.18	0.41
1:A:102:ASN:OD1	1:A:102:ASN:C	2.63	0.41
1:A:125:LEU:O	1:A:183:ARG:HA	2.21	0.41
1:A:127:PHE:N	1:A:127:PHE:CD2	2.88	0.41
1:A:132:SER:HA	1:A:135:GLN:CG	2.50	0.41
1:A:804:ASN:O	1:A:809:ARG:HD2	2.20	0.41
1:A:861:SER:OG	1:A:863:GLN:HG3	2.21	0.41
1:D:138:GLN:O	1:D:216:HIS:HA	2.21	0.41
1:D:464:HIS:HB2	1:D:489:GLY:HA3	2.02	0.41
1:A:844:HIS:CE1	1:A:845:GLN:HG2	2.54	0.41
1:B:291:LEU:N	1:B:291:LEU:CD2	2.83	0.41
1:C:989:PHE:CD1	1:C:989:PHE:N	2.89	0.41
1:D:18:ASN:C	1:D:20:GLY:H	2.26	0.41
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.38	0.41
1:D:581:ASN:HD22	1:D:583:ASN:ND2	2.18	0.41
1:A:140:ARG:HG2	1:A:215:LEU:HB3	2.01	0.41
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.01	0.41
1:A:986:ILE:HG23	1:A:986:ILE:HD13	1.63	0.41
1:B:817:GLN:HG2	1:B:817:GLN:H	1.52	0.41
1:C:246:MET:HB3	1:C:274:PHE:CZ	2.55	0.41
1:C:784:PHE:HA	1:C:881:ARG:O	2.20	0.41
1:C:800:ARG:CZ	1:C:801:ILE:O	2.69	0.41
1:C:907:PRO:HG2	1:C:990:HIS:O	2.21	0.41
1:C:977:HIS:O	1:C:977:HIS:CG	2.74	0.41
1:D:262:GLN:NE2	1:D:299:LYS:CD	2.82	0.41
1:D:362:LEU:HA	1:D:362:LEU:HD23	1.84	0.41
1:A:262:GLN:OE1	1:A:262:GLN:HA	2.21	0.41
1:A:800:ARG:CZ	1:A:800:ARG:CB	2.97	0.41
1:B:277:GLU:HG2	1:B:277:GLU:H	1.53	0.41
1:A:246:MET:HE1	1:A:254:LEU:HD13	2.03	0.41
1:A:703:PRO:O	1:A:711:ALA:HB1	2.20	0.41
1:A:782:ASP:HA	1:A:884:LEU:HD23	2.02	0.41
1:A:883:GLY:HA3	1:A:987:ASP:HA	2.03	0.41
1:B:652:LEU:O	1:B:667:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:806:TRP:CD2	1:B:991:MET:HE1	2.56	0.41
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.56	0.41
1:C:24:LEU:HB2	1:C:161:TYR:HB3	2.01	0.41
1:C:988:GLY:C	1:C:989:PHE:CD1	2.99	0.41
1:D:36:TRP:C	1:D:37:ARG:HD3	2.45	0.41
1:D:78:LEU:HA	1:D:79:PRO:HD2	1.81	0.41
1:D:737:ILE:HD12	1:D:738:PRO:HD2	2.03	0.41
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.56	0.41
1:A:142:ILE:HG23	1:A:170:GLU:HG2	2.01	0.41
1:A:576:ILE:CD1	5:A:8411:DMS:S	3.09	0.41
1:B:844:HIS:CE1	1:B:845:GLN:CG	3.00	0.41
1:A:30:HIS:HB2	1:A:31:PRO:HD2	2.04	0.40
1:A:460:ASN:O	1:A:461:GLU:C	2.65	0.40
1:A:507:ASP:O	4:B:2004:IPT:H2	2.21	0.40
1:A:635:THR:HA	1:A:680:ILE:O	2.21	0.40
1:B:746:ASP:HA	1:B:760:ARG:HG3	2.03	0.40
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.57	0.40
1:C:658:LEU:O	1:C:659:ASP:C	2.64	0.40
1:A:608:PHE:CD1	1:A:614:HIS:CD2	3.09	0.40
1:B:651:LEU:C	1:B:651:LEU:CD2	2.94	0.40
1:C:882:ILE:CD1	1:C:1014:TYR:CD1	3.04	0.40
1:A:18:ASN:C	1:A:20:GLY:N	2.78	0.40
1:A:131:GLU:HB3	1:A:135:GLN:HE21	1.86	0.40
1:B:778:THR:HG23	1:B:779:PRO:HD2	2.02	0.40
1:B:825:CYS:HA	1:B:837:THR:O	2.21	0.40
1:B:1023:LYS:N	1:B:1023:LYS:CD	2.84	0.40
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.87	0.40
1:D:424:ASN:OD1	1:D:424:ASN:C	2.64	0.40
1:D:708:TRP:CZ2	5:D:8403:DMS:H13	2.55	0.40
1:A:225:PHE:HA	1:A:243:GLU:O	2.21	0.40
1:A:279:ILE:HD13	1:A:284:GLY:HA2	2.03	0.40
1:A:658:LEU:O	1:A:659:ASP:C	2.64	0.40
1:A:686:PRO:C	1:A:687:GLN:NE2	2.79	0.40
1:B:655:MET:HB3	6:B:4962:HOH:O	2.21	0.40
1:B:767:GLN:HG3	1:B:768:MET:N	2.37	0.40
1:D:19:PRO:HA	1:D:193:ASP:OD1	2.22	0.40
1:A:379:MET:HE1	1:A:387:VAL:HB	2.03	0.40
1:B:732:ALA:O	1:B:733:ALA:C	2.65	0.40
1:D:71:GLU:CD	1:D:71:GLU:N	2.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	959 (95%)	49 (5%)	1 (0%)	48	34
1	B	1009/1023 (99%)	967 (96%)	35 (4%)	7 (1%)	18	8
1	C	1009/1023 (99%)	973 (96%)	34 (3%)	2 (0%)	43	31
1	D	1009/1023 (99%)	976 (97%)	30 (3%)	3 (0%)	36	25
All	All	4036/4092 (99%)	3875 (96%)	148 (4%)	13 (0%)	36	25

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	686	PRO
1	B	731	PRO
1	B	735	HIS
1	C	731	PRO
1	D	688	PRO
1	B	732	ALA
1	B	733	ALA
1	A	688	PRO
1	C	164	ASP
1	D	735	HIS
1	B	690	SER
1	D	164	ASP
1	B	164	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	864/875 (99%)	815 (94%)	49 (6%)	18	8
1	B	864/875 (99%)	824 (95%)	40 (5%)	24	12
1	C	864/875 (99%)	834 (96%)	30 (4%)	32	19
1	D	864/875 (99%)	820 (95%)	44 (5%)	21	9
All	All	3456/3500 (99%)	3293 (95%)	163 (5%)	23	11

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	72	SER
1	A	75	GLU
1	A	76	CYS
1	A	80	GLU
1	A	128	ASN
1	A	130	ASP
1	A	177	LEU
1	A	178	ARG
1	A	246	MET
1	A	262	GLN
1	A	279	ILE
1	A	319	ASP
1	A	437	SER
1	A	473	ARG
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	581	ASN
1	A	595	THR
1	A	600	GLN
1	A	634	GLN
1	A	651	LEU
1	A	655	MET
1	A	663	LEU
1	A	672	VAL
1	A	684	GLU
1	A	689	GLU
1	A	699	ARG
1	A	725	ASN
1	A	729	THR
1	A	730	LEU
1	A	735	HIS

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Mol	Chain	Res	Type
1	A	737	ILE
1	A	741	THR
1	A	761	GLN
1	A	774	LYS
1	A	778	THR
1	A	799	THR
1	A	800	ARG
1	A	809	ARG
1	A	817	GLN
1	A	819	GLU
1	A	843	GLN
1	A	890	GLN
1	A	910	LEU
1	A	986	ILE
1	A	1017	GLN
1	A	1023	LYS
1	B	40	GLU
1	B	49	GLN
1	B	71	GLU
1	B	75	GLU
1	B	80	GLU
1	B	117	GLU
1	B	251	ARG
1	B	291	LEU
1	B	344	LEU
1	B	370	GLN
1	B	477	SER
1	B	519	SER
1	B	546	LEU
1	B	600	GLN
1	B	646	HIS
1	B	651	LEU
1	B	655	MET
1	B	663	LEU
1	B	681	GLU
1	B	682	LEU
1	B	685	LEU
1	B	687	GLN
1	B	689	GLU
1	B	730	LEU
1	B	737	ILE
1	B	745	MET

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Mol	Chain	Res	Type
1	B	755	ARG
1	B	773	LYS
1	B	799	THR
1	B	817	GLN
1	B	819	GLU
1	B	829	THR
1	B	857	ARG
1	B	866	ILE
1	B	867	THR
1	B	890	GLN
1	B	893	GLU
1	B	956	GLN
1	B	1022	GLN
1	B	1023	LYS
1	C	71	GLU
1	C	80	GLU
1	C	131	GLU
1	C	214	LEU
1	C	251	ARG
1	C	262	GLN
1	C	264	GLU
1	C	277	GLU
1	C	344	LEU
1	C	370	GLN
1	C	546	LEU
1	C	576	ILE
1	C	580	GLU
1	C	634	GLN
1	C	651	LEU
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	728	VAL
1	C	730	LEU
1	C	737	ILE
1	C	772	ASP
1	C	773	LYS
1	C	800	ARG
1	C	824	GLN

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Mol	Chain	Res	Type
1	C	986	ILE
1	C	1023	LYS
1	D	49	GLN
1	D	75	GLU
1	D	80	GLU
1	D	128	ASN
1	D	129	VAL
1	D	130	ASP
1	D	135	GLN
1	D	177	LEU
1	D	217	LYS
1	D	277	GLU
1	D	279	ILE
1	D	299	LYS
1	D	319	ASP
1	D	344	LEU
1	D	370	GLN
1	D	546	LEU
1	D	580	GLU
1	D	581	ASN
1	D	634	GLN
1	D	655	MET
1	D	685	LEU
1	D	687	GLN
1	D	699	ARG
1	D	719	GLN
1	D	730	LEU
1	D	734	SER
1	D	735	HIS
1	D	737	ILE
1	D	741	THR
1	D	743	SER
1	D	744	GLU
1	D	745	MET
1	D	750	GLU
1	D	761	GLN
1	D	773	LYS
1	D	797	GLU
1	D	799	THR
1	D	801	ILE
1	D	845	GLN
1	D	847	LYS

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Mol	Chain	Res	Type
1	D	986	ILE
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 (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	135	GLN
1	A	163	GLN
1	A	266	GLN
1	A	485	GLN
1	A	581	ASN
1	A	600	GLN
1	A	653	HIS
1	A	687	GLN
1	A	702	GLN
1	A	739	HIS
1	A	761	GLN
1	A	804	ASN
1	A	817	GLN
1	A	863	GLN
1	A	878	HIS
1	A	977	HIS
1	A	1017	GLN
1	B	163	GLN
1	B	363	HIS
1	B	370	GLN
1	B	485	GLN
1	B	510	GLN
1	B	600	GLN
1	B	624	GLN
1	B	704	ASN
1	B	739	HIS
1	B	757	GLN
1	B	804	ASN
1	B	817	GLN
1	B	843	GLN
1	B	878	HIS
1	B	1022	GLN
1	C	49	GLN

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Mol	Chain	Res	Type
1	C	163	GLN
1	C	266	GLN
1	C	363	HIS
1	C	370	GLN
1	C	394	ASN
1	C	485	GLN
1	C	675	GLN
1	C	735	HIS
1	C	739	HIS
1	C	817	GLN
1	C	824	GLN
1	C	878	HIS
1	C	903	GLN
1	C	1017	GLN
1	D	49	GLN
1	D	50	GLN
1	D	163	GLN
1	D	216	HIS
1	D	262	GLN
1	D	363	HIS
1	D	485	GLN
1	D	581	ASN
1	D	583	ASN
1	D	628	GLN
1	D	653	HIS
1	D	675	GLN
1	D	702	GLN
1	D	739	HIS
1	D	757	GLN
1	D	761	GLN
1	D	824	GLN
1	D	878	HIS
1	D	903	GLN
1	D	977	HIS
1	D	1017	GLN
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 141 ligands modelled in this entry, 32 are monoatomic - leaving 109 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	A	8413	-	3,3,3	2.25	1 (33%)	3,3,3	0.31	0
5	DMS	C	8423	-	3,3,3	1.53	0	3,3,3	0.46	0
5	DMS	D	8403	-	3,3,3	2.65	1 (33%)	3,3,3	0.43	0
5	DMS	C	8503	-	3,3,3	1.08	0	3,3,3	0.24	0
5	DMS	C	8504	-	3,3,3	0.69	0	3,3,3	0.25	0
5	DMS	D	8402	-	3,3,3	2.02	1 (33%)	3,3,3	0.30	0
5	DMS	B	8403	-	3,3,3	1.48	1 (33%)	3,3,3	0.78	0
5	DMS	C	8401	-	3,3,3	1.26	0	3,3,3	0.70	0
5	DMS	D	8411	-	3,3,3	1.47	1 (33%)	3,3,3	0.64	0
5	DMS	D	8414	-	3,3,3	0.82	0	3,3,3	0.38	0
4	IPT	C	2003	-	15,15,15	0.69	0	18,21,21	1.37	3 (16%)
5	DMS	A	8411	-	3,3,3	0.80	0	3,3,3	0.20	0
5	DMS	B	8417	-	3,3,3	1.59	1 (33%)	3,3,3	1.82	1 (33%)
4	IPT	C	2004	-	15,15,15	0.44	0	18,21,21	1.66	2 (11%)
5	DMS	C	8405	-	3,3,3	0.85	0	3,3,3	0.19	0
5	DMS	A	8420	-	3,3,3	0.94	0	3,3,3	0.23	0
5	DMS	C	8402	-	3,3,3	1.62	1 (33%)	3,3,3	0.53	0
5	DMS	B	8416	-	3,3,3	0.71	0	3,3,3	0.74	0
5	DMS	A	8501	-	3,3,3	0.89	0	3,3,3	0.31	0
5	DMS	A	8412	-	3,3,3	0.44	0	3,3,3	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	B	8410	-	3,3,3	1.76	1 (33%)	3,3,3	0.58	0
5	DMS	A	8421	-	3,3,3	0.93	0	3,3,3	0.21	0
5	DMS	D	8408	-	3,3,3	1.06	0	3,3,3	0.51	0
4	IPT	A	2001	3	15,15,15	0.75	0	18,21,21	1.00	0
5	DMS	A	8407	-	3,3,3	1.27	0	3,3,3	0.24	0
5	DMS	A	8401	-	3,3,3	0.61	0	3,3,3	0.19	0
5	DMS	B	8506	-	3,3,3	1.65	1 (33%)	3,3,3	0.42	0
5	DMS	C	8413	-	3,3,3	1.80	1 (33%)	3,3,3	0.16	0
5	DMS	A	8504	-	3,3,3	0.69	0	3,3,3	0.12	0
5	DMS	D	8413	-	3,3,3	1.25	0	3,3,3	0.06	0
5	DMS	C	8420	-	3,3,3	1.06	0	3,3,3	0.20	0
5	DMS	A	8409	-	3,3,3	2.48	2 (66%)	3,3,3	0.27	0
5	DMS	D	8404	-	3,3,3	1.31	0	3,3,3	0.20	0
4	IPT	A	2003	-	15,15,15	0.67	0	18,21,21	2.05	3 (16%)
5	DMS	C	8403	-	3,3,3	1.77	1 (33%)	3,3,3	0.46	0
5	DMS	B	8405	-	3,3,3	1.48	1 (33%)	3,3,3	0.53	0
5	DMS	B	8411	-	3,3,3	0.97	0	3,3,3	0.64	0
5	DMS	B	8502	-	3,3,3	1.35	1 (33%)	3,3,3	1.09	0
5	DMS	B	8402	-	3,3,3	0.85	0	3,3,3	0.36	0
5	DMS	C	8412	-	3,3,3	1.18	0	3,3,3	0.42	0
5	DMS	B	8501	-	3,3,3	1.53	1 (33%)	3,3,3	0.38	0
5	DMS	D	8412	-	3,3,3	1.48	1 (33%)	3,3,3	0.53	0
5	DMS	B	8421	-	3,3,3	0.56	0	3,3,3	0.51	0
5	DMS	D	8501	-	3,3,3	0.15	0	3,3,3	0.56	0
5	DMS	A	8414	-	3,3,3	0.99	0	3,3,3	0.52	0
5	DMS	C	8408	-	3,3,3	0.50	0	3,3,3	1.25	1 (33%)
5	DMS	A	8406	-	3,3,3	0.53	0	3,3,3	0.40	0
5	DMS	B	8401	-	3,3,3	0.85	0	3,3,3	1.30	1 (33%)
5	DMS	D	8407	-	3,3,3	1.50	1 (33%)	3,3,3	0.40	0
5	DMS	D	8705	-	3,3,3	0.77	0	3,3,3	0.51	0
5	DMS	D	8406	-	3,3,3	1.03	0	3,3,3	0.76	0
4	IPT	D	2003	-	15,15,15	0.59	0	18,21,21	1.52	4 (22%)
4	IPT	D	2001	3	15,15,15	0.50	0	18,21,21	1.37	4 (22%)
5	DMS	A	8416	-	3,3,3	0.92	0	3,3,3	0.25	0
5	DMS	B	8425	3	3,3,3	1.12	0	3,3,3	0.20	0
5	DMS	C	8502	-	3,3,3	0.67	0	3,3,3	1.26	1 (33%)
5	DMS	B	8423	-	3,3,3	1.80	1 (33%)	3,3,3	0.54	0
5	DMS	A	8408	-	3,3,3	0.52	0	3,3,3	0.19	0
5	DMS	A	8417	-	3,3,3	1.08	0	3,3,3	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	A	8423	-	3,3,3	1.71	1 (33%)	3,3,3	0.16	0
4	IPT	B	2001	3	15,15,15	0.76	0	18,21,21	0.93	1 (5%)
5	DMS	B	8504	-	3,3,3	0.44	0	3,3,3	0.19	0
5	DMS	D	8409	-	3,3,3	2.38	1 (33%)	3,3,3	0.89	0
5	DMS	A	8410	-	3,3,3	0.77	0	3,3,3	0.16	0
5	DMS	B	8427	-	3,3,3	0.79	0	3,3,3	0.21	0
4	IPT	A	2002	-	15,15,15	1.07	1 (6%)	18,21,21	1.37	3 (16%)
5	DMS	C	8416	-	3,3,3	0.82	0	3,3,3	0.14	0
5	DMS	B	8413	-	3,3,3	1.22	0	3,3,3	0.60	0
5	DMS	C	8414	-	3,3,3	0.98	0	3,3,3	1.00	0
5	DMS	A	8403	-	3,3,3	1.82	1 (33%)	3,3,3	1.20	1 (33%)
5	DMS	A	8502	-	3,3,3	2.09	1 (33%)	3,3,3	0.66	0
5	DMS	C	8407	-	3,3,3	1.65	1 (33%)	3,3,3	0.54	0
5	DMS	D	8417	-	3,3,3	1.27	0	3,3,3	0.86	0
5	DMS	A	8405	-	3,3,3	0.65	0	3,3,3	0.14	0
5	DMS	A	8415	-	3,3,3	1.44	0	3,3,3	0.59	0
5	DMS	B	8404	-	3,3,3	1.33	1 (33%)	3,3,3	1.30	1 (33%)
5	DMS	D	8421	-	3,3,3	1.23	1 (33%)	3,3,3	0.34	0
5	DMS	D	8416	-	3,3,3	1.20	0	3,3,3	0.09	0
5	DMS	D	8415	-	3,3,3	1.86	1 (33%)	3,3,3	0.33	0
5	DMS	C	8425	3	3,3,3	1.69	1 (33%)	3,3,3	0.16	0
5	DMS	B	8409	-	3,3,3	2.44	1 (33%)	3,3,3	0.49	0
5	DMS	D	8419	-	3,3,3	0.56	0	3,3,3	0.24	0
5	DMS	B	8420	-	3,3,3	2.58	2 (66%)	3,3,3	0.55	0
5	DMS	C	8421	-	3,3,3	0.41	0	3,3,3	0.32	0
5	DMS	A	8402	-	3,3,3	1.73	1 (33%)	3,3,3	0.31	0
5	DMS	A	8404	-	3,3,3	0.66	0	3,3,3	0.57	0
5	DMS	C	8427	-	3,3,3	0.13	0	3,3,3	0.46	0
5	DMS	C	8415	-	3,3,3	1.96	1 (33%)	3,3,3	0.21	0
5	DMS	B	8412	-	3,3,3	0.90	0	3,3,3	0.55	0
5	DMS	A	8419	-	3,3,3	0.61	0	3,3,3	0.34	0
4	IPT	C	2001	3	15,15,15	0.68	0	18,21,21	1.18	2 (11%)
5	DMS	D	8410	-	3,3,3	1.34	0	3,3,3	0.43	0
5	DMS	D	8423	-	3,3,3	0.66	0	3,3,3	0.19	0
5	DMS	B	8407	-	3,3,3	1.91	2 (66%)	3,3,3	0.48	0
4	IPT	D	2002	-	15,15,15	0.94	1 (6%)	18,21,21	1.19	2 (11%)
5	DMS	B	8406	-	3,3,3	0.84	0	3,3,3	0.17	0
5	DMS	C	8404	-	3,3,3	1.53	1 (33%)	3,3,3	1.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	8503	-	3,3,3	0.85	0	3,3,3	0.18	0
5	DMS	C	8501	-	3,3,3	1.34	1 (33%)	3,3,3	0.96	0
4	IPT	B	2003	-	15,15,15	0.81	0	18,21,21	1.18	1 (5%)
5	DMS	D	8405	-	3,3,3	1.03	0	3,3,3	0.38	0
5	DMS	B	8414	-	3,3,3	1.39	1 (33%)	3,3,3	1.07	0
5	DMS	C	8409	-	3,3,3	1.14	0	3,3,3	0.26	0
4	IPT	B	2004	-	15,15,15	0.65	0	18,21,21	1.66	2 (11%)
5	DMS	D	8401	-	3,3,3	2.33	2 (66%)	3,3,3	0.96	0
5	DMS	B	8415	-	3,3,3	1.73	1 (33%)	3,3,3	0.46	0
5	DMS	C	8410	-	3,3,3	1.87	1 (33%)	3,3,3	0.54	0
5	DMS	B	8408	-	3,3,3	1.36	0	3,3,3	0.39	0
5	DMS	C	8411	-	3,3,3	2.29	2 (66%)	3,3,3	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	IPT	A	2002	-	-	0/6/26/26	0/1/1/1
4	IPT	C	2004	-	-	3/6/26/26	0/1/1/1
4	IPT	B	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	D	2003	-	-	0/6/26/26	0/1/1/1
4	IPT	A	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	A	2003	-	-	0/6/26/26	0/1/1/1
4	IPT	B	2004	-	-	2/6/26/26	0/1/1/1
4	IPT	D	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	C	2003	-	-	1/6/26/26	0/1/1/1
4	IPT	C	2001	3	-	1/6/26/26	0/1/1/1
4	IPT	B	2003	-	-	0/6/26/26	0/1/1/1
4	IPT	D	2002	-	-	0/6/26/26	0/1/1/1

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8403	DMS	C2-S	4.51	2.08	1.76
5	B	8409	DMS	O-S	3.88	1.75	1.50
5	A	8409	DMS	O-S	3.67	1.74	1.50
5	A	8413	DMS	O-S	3.67	1.74	1.50
5	D	8409	DMS	O-S	3.63	1.74	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	8401	DMS	C1-S	3.26	1.99	1.76
5	B	8420	DMS	C1-S	3.11	1.98	1.76
5	C	8411	DMS	C2-S	3.10	1.98	1.76
5	A	8403	DMS	C2-S	3.07	1.98	1.76
5	A	8502	DMS	O-S	3.05	1.70	1.50
5	B	8420	DMS	C2-S	2.92	1.96	1.76
5	D	8402	DMS	C2-S	2.91	1.96	1.76
5	C	8425	DMS	O-S	2.87	1.69	1.50
5	C	8403	DMS	C2-S	2.86	1.96	1.76
5	C	8413	DMS	O-S	2.77	1.68	1.50
5	A	8423	DMS	C1-S	2.74	1.95	1.76
5	C	8410	DMS	C1-S	2.69	1.95	1.76
5	B	8506	DMS	O-S	2.69	1.68	1.50
4	A	2002	IPT	O5-C1	2.68	1.46	1.42
5	A	8402	DMS	O-S	2.59	1.67	1.50
5	C	8404	DMS	C2-S	2.54	1.94	1.76
5	B	8423	DMS	O-S	2.53	1.66	1.50
5	B	8407	DMS	C2-S	2.52	1.94	1.76
5	B	8405	DMS	O-S	2.50	1.66	1.50
4	D	2002	IPT	O4-C4	2.46	1.49	1.43
5	B	8410	DMS	C1-S	2.44	1.93	1.76
5	C	8415	DMS	O-S	2.43	1.66	1.50
5	B	8403	DMS	C2-S	2.35	1.92	1.76
5	C	8501	DMS	C2-S	2.32	1.92	1.76
5	C	8407	DMS	C2-S	2.32	1.92	1.76
5	D	8407	DMS	O-S	2.30	1.65	1.50
5	B	8404	DMS	C2-S	2.27	1.92	1.76
5	D	8412	DMS	O-S	2.26	1.65	1.50
5	B	8501	DMS	O-S	2.25	1.65	1.50
5	C	8402	DMS	O-S	2.24	1.65	1.50
5	C	8411	DMS	C1-S	2.21	1.91	1.76
5	B	8414	DMS	O-S	-2.18	1.35	1.50
5	B	8415	DMS	C1-S	2.16	1.91	1.76
5	B	8417	DMS	C2-S	2.15	1.91	1.76
5	D	8411	DMS	C1-S	2.14	1.91	1.76
5	B	8502	DMS	C1-S	2.13	1.91	1.76
5	D	8401	DMS	O-S	2.12	1.64	1.50
5	A	8409	DMS	C1-S	2.06	1.90	1.76
5	B	8407	DMS	O-S	2.06	1.63	1.50
5	D	8421	DMS	C1-S	2.06	1.90	1.76
5	D	8415	DMS	O-S	2.03	1.63	1.50

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2003	IPT	C3-C4-C5	-6.03	99.31	110.23
4	C	2004	IPT	C4-C3-C2	4.55	118.82	110.83
4	B	2004	IPT	C4-C3-C2	4.37	118.50	110.83
4	D	2003	IPT	C3-C4-C5	-3.80	103.34	110.23
4	C	2003	IPT	C1-O5-C5	-3.30	106.64	112.56
4	D	2001	IPT	C6-C5-C4	3.25	120.99	113.02
4	B	2004	IPT	O5-C5-C4	3.13	115.34	109.70
5	B	8417	DMS	C2-S-C1	3.12	114.39	98.42
4	A	2002	IPT	C1-C2-C3	-3.07	104.55	110.55
4	C	2003	IPT	O6-C6-C5	-2.88	101.52	111.33
4	A	2003	IPT	O2-C2-C3	-2.88	103.58	110.38
4	C	2004	IPT	C1-O5-C5	-2.82	107.51	112.56
4	A	2003	IPT	O3-C3-C4	2.79	116.95	110.38
4	D	2002	IPT	C2'-C1'-S1	2.42	117.09	110.12
4	D	2003	IPT	O6-C6-C5	-2.37	103.27	111.33
4	D	2001	IPT	O2-C2-C3	-2.35	104.84	110.38
4	B	2003	IPT	C1-O5-C5	-2.33	108.38	112.56
4	D	2003	IPT	O3-C3-C4	2.25	115.68	110.38
4	D	2003	IPT	O2-C2-C3	-2.22	105.15	110.38
4	A	2002	IPT	C3'-C1'-S1	-2.21	103.78	110.12
4	C	2001	IPT	C3'-C1'-S1	2.20	116.46	110.12
4	C	2003	IPT	C3'-C1'-S1	-2.20	103.80	110.12
5	B	8401	DMS	C2-S-C1	2.19	109.64	98.42
5	C	8502	DMS	C2-S-C1	2.18	109.58	98.42
5	B	8404	DMS	C2-S-C1	2.13	109.35	98.42
4	C	2001	IPT	C6-C5-C4	2.11	118.21	113.02
4	D	2002	IPT	O4-C4-C3	2.10	115.33	110.38
5	C	8408	DMS	C2-S-C1	2.07	109.05	98.42
5	A	8403	DMS	C2-S-C1	2.07	109.00	98.42
4	B	2001	IPT	C1-O5-C5	-2.05	108.88	112.56
4	A	2002	IPT	C1-O5-C5	-2.04	108.90	112.56
4	D	2001	IPT	O4-C4-C5	2.01	114.28	109.32
4	D	2001	IPT	C1-C2-C3	-2.01	106.62	110.55

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2003	IPT	C2'-C1'-S1-C1
4	C	2004	IPT	C3'-C1'-S1-C1
4	B	2004	IPT	C4-C5-C6-O6
4	C	2004	IPT	C4-C5-C6-O6
4	C	2004	IPT	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	2001	IPT	O5-C5-C6-O6
4	A	2001	IPT	O5-C5-C6-O6
4	D	2001	IPT	O5-C5-C6-O6
4	B	2001	IPT	O5-C5-C6-O6
4	B	2004	IPT	O5-C5-C6-O6

There are no ring outliers.

49 monomers are involved in 99 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8413	DMS	1	0
5	D	8403	DMS	4	0
5	C	8504	DMS	1	0
5	B	8403	DMS	3	0
5	D	8414	DMS	2	0
5	A	8411	DMS	1	0
5	B	8417	DMS	1	0
4	C	2004	IPT	2	0
5	A	8420	DMS	3	0
5	C	8402	DMS	1	0
5	B	8416	DMS	3	0
5	A	8501	DMS	1	0
5	A	8412	DMS	3	0
5	B	8506	DMS	8	0
5	C	8413	DMS	1	0
5	C	8420	DMS	2	0
5	C	8403	DMS	2	0
5	C	8412	DMS	4	0
5	D	8412	DMS	2	0
5	A	8414	DMS	4	0
5	C	8408	DMS	3	0
5	D	8407	DMS	1	0
4	D	2003	IPT	1	0
5	A	8416	DMS	2	0
5	C	8502	DMS	1	0
5	A	8417	DMS	1	0
5	A	8423	DMS	1	0
4	B	2001	IPT	3	0
5	B	8504	DMS	6	0
5	A	8410	DMS	1	0
5	B	8427	DMS	1	0
5	C	8416	DMS	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	8413	DMS	1	0
5	A	8403	DMS	2	0
5	D	8417	DMS	2	0
5	A	8415	DMS	1	0
5	D	8415	DMS	2	0
5	C	8421	DMS	1	0
5	C	8427	DMS	1	0
5	C	8415	DMS	1	0
5	B	8412	DMS	4	0
5	D	8410	DMS	1	0
5	D	8423	DMS	1	0
5	B	8407	DMS	1	0
5	C	8404	DMS	1	0
5	D	8503	DMS	1	0
5	C	8501	DMS	3	0
4	B	2004	IPT	1	0
5	C	8411	DMS	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.16	31 (3%) 51 51	11, 22, 52, 99	0
1	B	1011/1023 (98%)	-0.41	25 (2%) 58 58	10, 19, 49, 100	0
1	C	1011/1023 (98%)	-0.50	22 (2%) 62 62	11, 18, 46, 99	0
1	D	1011/1023 (98%)	-0.22	23 (2%) 61 61	13, 23, 51, 99	0
All	All	4044/4092 (98%)	-0.33	101 (2%) 58 58	10, 20, 50, 100	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	732	ALA	5.2
1	B	686	PRO	5.0
1	C	732	ALA	4.8
1	A	732	ALA	4.5
1	C	733	ALA	4.5
1	D	730	LEU	4.4
1	B	733	ALA	4.4
1	C	731	PRO	4.2
1	C	730	LEU	4.2
1	D	733	ALA	4.1
1	C	688	PRO	4.0
1	B	734	SER	4.0
1	C	735	HIS	4.0
1	A	735	HIS	3.9
1	B	745	MET	3.9
1	C	685	LEU	3.8
1	B	685	LEU	3.7
1	D	735	HIS	3.6
1	D	655	MET	3.6
1	D	685	LEU	3.6
1	B	731	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	687	GLN	3.5
1	A	731	PRO	3.5
1	A	686	PRO	3.5
1	A	685	LEU	3.4
1	D	734	SER	3.4
1	B	735	HIS	3.3
1	C	1023	LYS	3.2
1	A	76	CYS	3.2
1	A	733	ALA	3.2
1	B	687	GLN	3.2
1	B	1022	GLN	3.2
1	D	688	PRO	3.2
1	A	687	GLN	3.1
1	A	730	LEU	3.1
1	C	1022	GLN	3.1
1	C	686	PRO	3.0
1	D	686	PRO	3.0
1	A	688	PRO	2.9
1	A	78	LEU	2.9
1	A	729	THR	2.9
1	B	634	GLN	2.9
1	B	688	PRO	2.8
1	B	1023	LYS	2.8
1	B	730	LEU	2.8
1	A	799	THR	2.8
1	B	768	MET	2.8
1	C	131	GLU	2.7
1	D	1023	LYS	2.7
1	D	732	ALA	2.7
1	A	180	GLY	2.7
1	B	683	PRO	2.7
1	A	725	ASN	2.7
1	C	687	GLN	2.6
1	A	737	ILE	2.6
1	A	69	VAL	2.6
1	A	262	GLN	2.6
1	C	737	ILE	2.6
1	D	1022	GLN	2.6
1	A	80	GLU	2.6
1	B	682	LEU	2.5
1	C	581	ASN	2.5
1	A	82	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	74	LEU	2.5
1	C	800	ARG	2.4
1	D	262	GLN	2.4
1	A	279	ILE	2.4
1	D	773	LYS	2.4
1	A	634	GLN	2.3
1	D	731	PRO	2.3
1	D	76	CYS	2.3
1	A	131	GLU	2.3
1	C	71	GLU	2.3
1	B	669	PRO	2.3
1	A	117	GLU	2.3
1	C	580	GLU	2.3
1	C	689	GLU	2.3
1	D	737	ILE	2.2
1	A	128	ASN	2.2
1	B	739	HIS	2.2
1	A	181	GLU	2.2
1	B	1018	LEU	2.2
1	D	131	GLU	2.2
1	D	977	HIS	2.2
1	C	582	GLY	2.2
1	B	755	ARG	2.2
1	A	689	GLU	2.1
1	D	799	THR	2.1
1	B	860	GLY	2.1
1	A	75	GLU	2.1
1	A	64	PRO	2.1
1	C	683	PRO	2.1
1	D	729	THR	2.1
1	B	689	GLU	2.0
1	B	655	MET	2.0
1	B	725	ASN	2.0
1	D	761	GLN	2.0
1	A	319	ASP	2.0
1	C	772	ASP	2.0
1	D	580	GLU	2.0
1	C	773	LYS	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	B	8420	4/4	0.78	0.26	56,57,69,82	0
5	DMS	B	8417	4/4	0.79	0.21	28,29,73,100	0
5	DMS	B	8416	4/4	0.79	0.26	21,75,100,100	0
5	DMS	A	8421	4/4	0.80	0.19	28,62,80,100	0
5	DMS	C	8416	4/4	0.82	0.21	22,78,100,100	0
5	DMS	A	8423	4/4	0.83	0.24	58,63,65,100	0
5	DMS	D	8416	4/4	0.84	0.19	36,61,87,100	0
5	DMS	D	8421	4/4	0.84	0.16	47,55,65,100	0
5	DMS	D	8423	4/4	0.84	0.18	49,50,66,96	0
5	DMS	D	8705	4/4	0.84	0.20	38,47,100,100	0
5	DMS	D	8406	4/4	0.85	0.24	36,57,85,100	0
4	IPT	C	2004	15/15	0.86	0.17	29,55,100,100	0
3	NA	C	3105	1/1	0.87	0.13	48,48,48,48	0
5	DMS	D	8417	4/4	0.88	0.17	30,35,64,98	0
3	NA	D	3105	1/1	0.88	0.16	64,64,64,64	0
2	MG	A	3003	1/1	0.89	0.10	52,52,52,52	0
5	DMS	B	8427	4/4	0.89	0.17	41,68,100,100	0
5	DMS	A	8416	4/4	0.89	0.22	43,44,100,100	0
5	DMS	A	8414	4/4	0.90	0.16	38,40,91,100	0
5	DMS	B	8506	4/4	0.90	0.23	44,50,100,100	0
5	DMS	A	8502	4/4	0.90	0.17	36,41,54,100	0
5	DMS	C	8421	4/4	0.90	0.12	38,46,62,68	0
5	DMS	C	8427	4/4	0.90	0.11	38,49,72,73	0
5	DMS	C	8503	4/4	0.90	0.15	38,47,52,55	0
5	DMS	C	8504	4/4	0.90	0.18	37,66,69,100	0
5	DMS	A	8504	4/4	0.90	0.16	58,65,69,89	0
5	DMS	B	8415	4/4	0.90	0.17	28,32,48,100	0
4	IPT	B	2004	15/15	0.90	0.13	31,45,99,100	0
5	DMS	A	8420	4/4	0.90	0.17	45,55,55,65	0
5	DMS	A	8403	4/4	0.90	0.20	24,26,36,100	0
5	DMS	B	8423	4/4	0.90	0.19	35,58,73,80	0
5	DMS	D	8414	4/4	0.91	0.21	30,61,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8417	4/4	0.91	0.13	30,36,38,100	0
5	DMS	A	8419	4/4	0.91	0.20	38,62,71,100	0
5	DMS	B	8421	4/4	0.91	0.17	36,47,100,100	0
3	NA	B	3105	1/1	0.91	0.12	48,48,48,48	0
5	DMS	D	8413	4/4	0.91	0.12	39,40,52,56	0
5	DMS	C	8423	4/4	0.92	0.16	27,40,47,77	0
5	DMS	D	8419	4/4	0.92	0.17	55,62,64,72	0
5	DMS	A	8410	4/4	0.92	0.12	40,45,58,61	0
5	DMS	C	8420	4/4	0.92	0.18	47,52,67,79	0
5	DMS	D	8503	4/4	0.92	0.16	25,47,53,100	0
5	DMS	B	8403	4/4	0.92	0.18	26,33,38,100	0
5	DMS	C	8414	4/4	0.93	0.14	23,41,47,52	0
5	DMS	B	8504	4/4	0.93	0.13	53,54,60,65	0
5	DMS	A	8413	4/4	0.93	0.12	44,46,52,52	0
5	DMS	D	8501	4/4	0.93	0.14	31,37,48,74	0
5	DMS	C	8403	4/4	0.93	0.18	23,33,36,100	0
5	DMS	D	8403	4/4	0.93	0.12	28,33,42,42	0
5	DMS	C	8413	4/4	0.94	0.15	28,48,50,100	0
5	DMS	D	8409	4/4	0.94	0.10	28,31,34,46	0
5	DMS	A	8409	4/4	0.94	0.12	38,39,50,66	0
5	DMS	B	8404	4/4	0.94	0.08	19,20,32,38	0
5	DMS	B	8413	4/4	0.94	0.12	32,42,44,69	0
5	DMS	B	8425	4/4	0.94	0.14	41,42,43,50	0
5	DMS	B	8414	4/4	0.94	0.15	24,42,50,100	0
5	DMS	A	8501	4/4	0.94	0.11	36,53,54,57	0
5	DMS	C	8501	4/4	0.94	0.11	25,48,53,60	0
4	IPT	D	2003	15/15	0.94	0.10	28,36,55,63	0
4	IPT	A	2003	15/15	0.94	0.12	26,35,77,100	0
5	DMS	C	8410	4/4	0.94	0.13	17,33,39,100	0
5	DMS	D	8408	4/4	0.95	0.09	26,34,43,47	0
5	DMS	B	8502	4/4	0.95	0.09	19,29,62,68	0
5	DMS	D	8410	4/4	0.95	0.11	32,41,45,71	0
5	DMS	A	8408	4/4	0.95	0.09	31,37,48,82	0
3	NA	B	3103	1/1	0.95	0.07	31,31,31,31	0
5	DMS	D	8415	4/4	0.95	0.09	26,30,37,48	0
5	DMS	C	8425	4/4	0.95	0.14	34,36,52,57	0
5	DMS	B	8406	4/4	0.95	0.13	35,36,44,100	0
5	DMS	C	8409	4/4	0.95	0.11	33,38,43,51	0
5	DMS	B	8407	4/4	0.95	0.11	25,39,43,50	0
5	DMS	A	8404	4/4	0.95	0.09	24,33,36,44	0
5	DMS	A	8412	4/4	0.95	0.10	36,51,51,65	0
5	DMS	A	8407	4/4	0.95	0.10	32,34,40,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	D	8407	4/4	0.95	0.10	25,34,40,44	0
5	DMS	C	8402	4/4	0.96	0.11	20,21,32,34	0
5	DMS	A	8406	4/4	0.96	0.10	28,51,52,61	0
5	DMS	C	8404	4/4	0.96	0.10	20,23,40,53	0
5	DMS	C	8407	4/4	0.96	0.10	28,28,36,43	0
5	DMS	C	8408	4/4	0.96	0.12	31,35,41,100	0
5	DMS	A	8415	4/4	0.96	0.11	27,31,48,49	0
4	IPT	B	2003	15/15	0.96	0.07	23,30,38,42	0
5	DMS	C	8412	4/4	0.96	0.11	31,35,37,54	0
5	DMS	D	8412	4/4	0.96	0.10	30,39,46,62	0
4	IPT	C	2003	15/15	0.96	0.09	18,28,47,67	0
3	NA	D	3103	1/1	0.96	0.08	31,31,31,31	0
5	DMS	C	8415	4/4	0.96	0.10	21,26,37,46	0
2	MG	A	3012	1/1	0.96	0.07	40,40,40,40	0
2	MG	D	3003	1/1	0.96	0.07	48,48,48,48	0
5	DMS	B	8408	4/4	0.96	0.10	39,42,42,56	0
5	DMS	B	8409	4/4	0.96	0.08	24,34,36,41	0
5	DMS	B	8410	4/4	0.96	0.09	22,35,44,48	0
5	DMS	B	8412	4/4	0.96	0.11	34,35,39,57	0
3	NA	A	3105	1/1	0.96	0.07	46,46,46,46	0
5	DMS	C	8502	4/4	0.96	0.08	28,29,41,44	0
3	NA	B	3104	1/1	0.97	0.07	29,29,29,29	0
4	IPT	B	2001	15/15	0.97	0.07	16,20,28,33	0
5	DMS	D	8411	4/4	0.97	0.13	27,35,38,100	0
2	MG	B	3011	1/1	0.97	0.06	41,41,41,41	0
4	IPT	A	2001	15/15	0.97	0.07	17,25,58,60	0
5	DMS	B	8402	4/4	0.97	0.07	19,20,32,36	0
4	IPT	A	2002	15/15	0.97	0.07	15,22,30,34	0
2	MG	A	3002	1/1	0.97	0.06	23,23,23,23	0
5	DMS	D	8402	4/4	0.97	0.10	12,25,29,42	0
5	DMS	B	8405	4/4	0.97	0.09	28,32,33,38	0
5	DMS	D	8404	4/4	0.97	0.08	18,30,34,35	0
5	DMS	D	8405	4/4	0.97	0.09	33,33,39,39	0
4	IPT	D	2001	15/15	0.97	0.07	20,30,34,52	0
4	IPT	D	2002	15/15	0.97	0.07	13,22,31,32	0
5	DMS	C	8405	4/4	0.97	0.08	28,29,32,33	0
3	NA	A	3103	1/1	0.98	0.06	33,33,33,33	0
5	DMS	D	8401	4/4	0.98	0.06	14,22,23,26	0
2	MG	D	3002	1/1	0.98	0.06	27,27,27,27	0
3	NA	C	3104	1/1	0.98	0.10	26,26,26,26	0
5	DMS	B	8411	4/4	0.98	0.10	23,27,36,47	0
2	MG	C	3003	1/1	0.98	0.03	15,15,15,15	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	8411	4/4	0.98	0.08	28,29,36,43	0
5	DMS	B	8501	4/4	0.98	0.06	21,24,32,32	0
4	IPT	C	2001	15/15	0.98	0.05	14,19,31,37	0
5	DMS	C	8411	4/4	0.98	0.06	21,23,23,27	0
5	DMS	A	8405	4/4	0.98	0.07	33,34,34,35	0
3	NA	D	3102	1/1	0.98	0.05	17,17,17,17	0
2	MG	C	3001	1/1	0.99	0.05	15,15,15,15	0
5	DMS	A	8401	4/4	0.99	0.04	15,24,25,26	0
5	DMS	A	8402	4/4	0.99	0.07	18,25,26,31	0
3	NA	B	3101	1/1	0.99	0.04	17,17,17,17	0
5	DMS	C	8401	4/4	0.99	0.05	15,15,21,22	0
3	NA	B	3102	1/1	0.99	0.04	15,15,15,15	0
2	MG	C	3002	1/1	0.99	0.04	18,18,18,18	0
2	MG	B	3001	1/1	0.99	0.03	16,16,16,16	0
2	MG	D	3001	1/1	0.99	0.03	18,18,18,18	0
3	NA	C	3101	1/1	0.99	0.02	15,15,15,15	0
3	NA	C	3102	1/1	0.99	0.03	16,16,16,16	0
5	DMS	B	8401	4/4	0.99	0.05	16,22,22,24	0
3	NA	C	3103	1/1	0.99	0.04	30,30,30,30	0
2	MG	B	3002	1/1	0.99	0.05	19,19,19,19	0
2	MG	B	3007	1/1	0.99	0.07	26,26,26,26	0
3	NA	D	3101	1/1	0.99	0.04	19,19,19,19	0
2	MG	A	3001	1/1	0.99	0.04	17,17,17,17	0
3	NA	A	3102	1/1	1.00	0.03	15,15,15,15	0
3	NA	A	3101	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.