



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:48 PM UTC

PDB ID : 1PX3 / pdb_00001px3
Title : E. COLI (LACZ) BETA-GALACTOSIDASE (G794A)
Authors : Juers, D.H.; Hakda, S.; Matthews, B.W.; Huber, R.E.
Deposited on : 2003-07-02
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

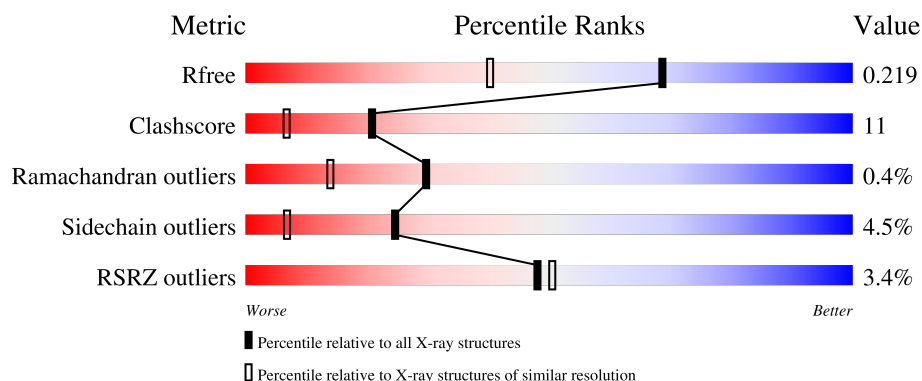
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1023	4% 71% 23% ..
1	B	1023	3% 72% 22% ..
1	C	1023	2% 73% 21% ...
1	D	1023	4% 71% 23% 5% ..

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	8404	-	-	X	-
4	DMS	A	8419	-	-	X	-
4	DMS	C	8425	-	-	X	-
4	DMS	D	8703	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36619 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	1010	Total	C	N	O	S	0	0	0
			8119	5135	1439	1507	38			
1	B	1009	Total	C	N	O	S	0	0	0
			8114	5132	1438	1506	38			
1	C	1007	Total	C	N	O	S	0	0	0
			8095	5120	1433	1504	38			
1	D	1008	Total	C	N	O	S	0	0	0
			8103	5126	1434	1505	38			

There are 36 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 4 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



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

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

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

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

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

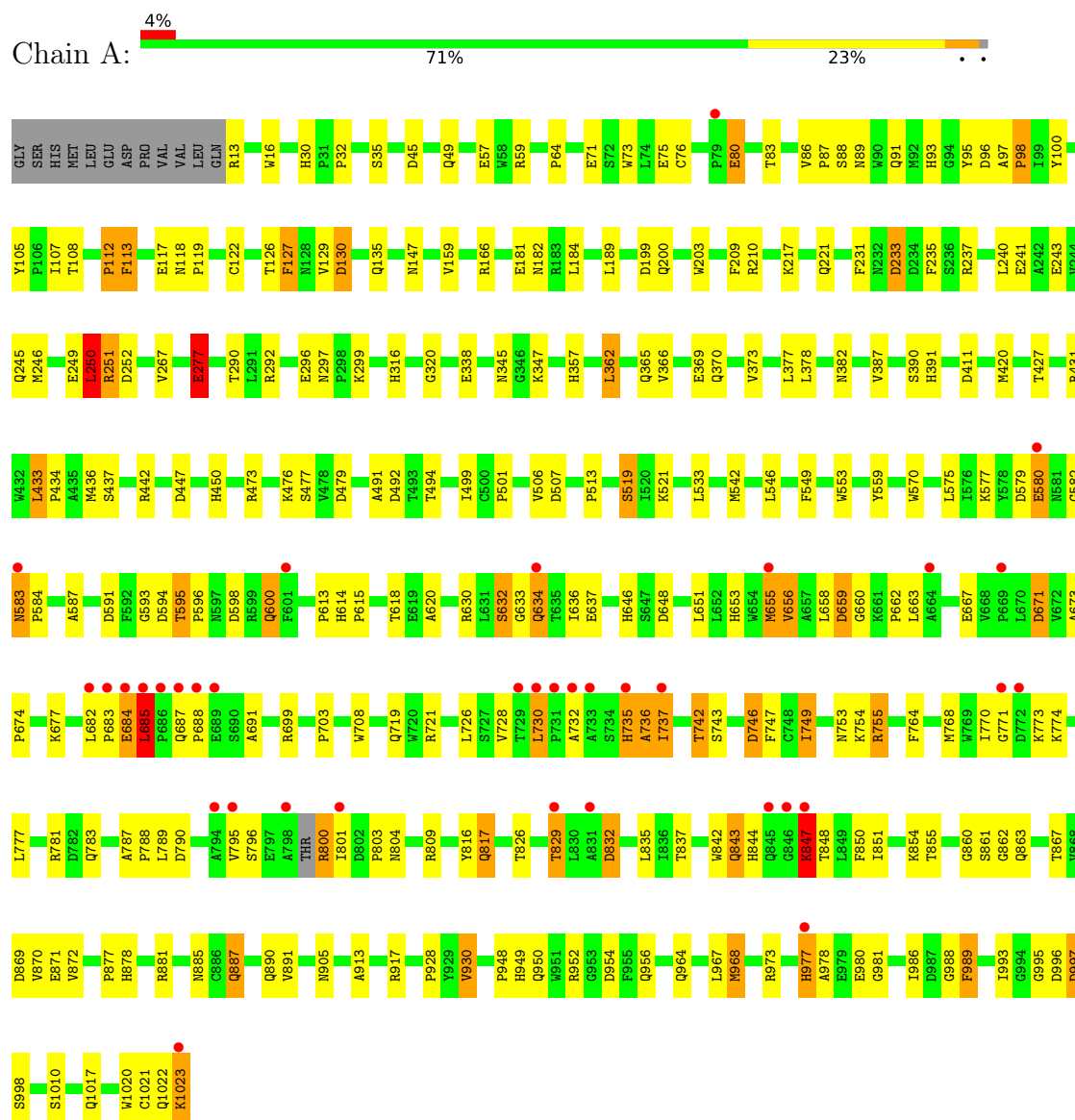
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	916	Total O 916 916	0	0
5	B	985	Total O 985 985	0	0
5	C	935	Total O 935 935	0	0
5	D	984	Total O 984 984	0	0

3 Residue-property plots

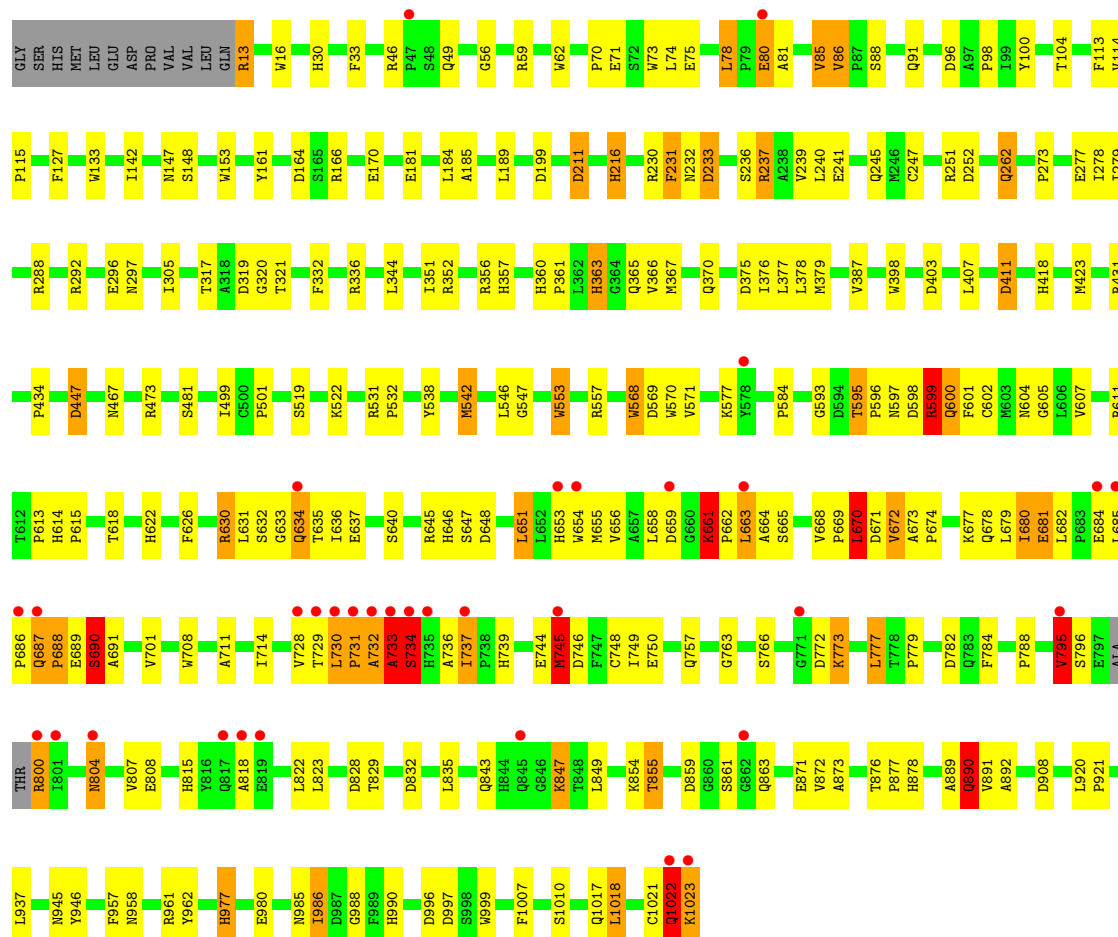
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: beta-galactosidase

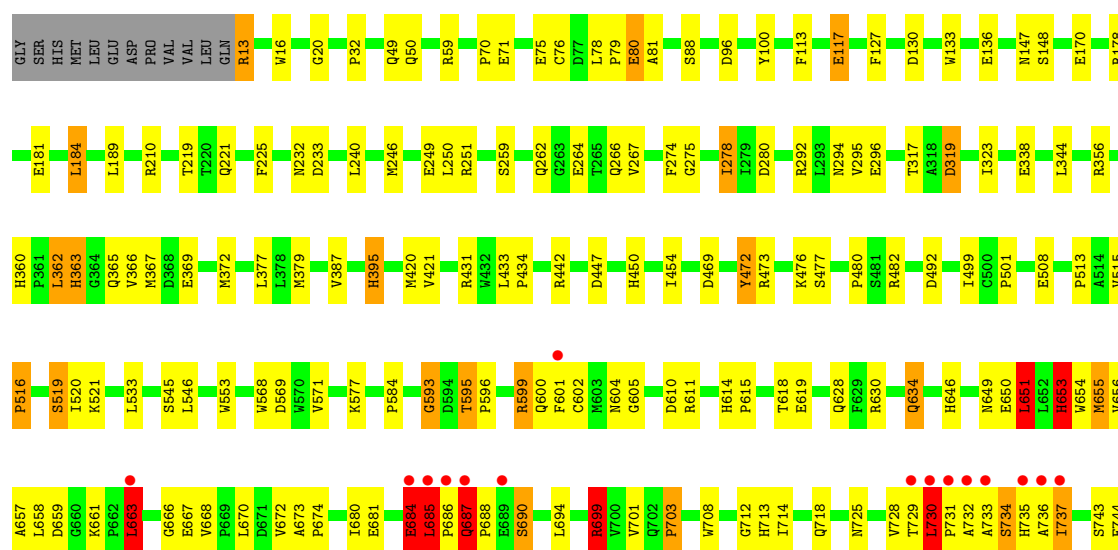


• Molecule 1: beta-galactosidase





• Molecule 1: beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.70Å 168.59Å 200.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.70 – 1.60 21.70 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.70-1.60) 88.3 (21.70-1.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.60Å)	Xtrriage
Refinement program	TNT	Depositor
R, R_{free}	0.192 , 0.243 (Not available) , 0.219	Depositor DCC
R_{free} test set	8858 reflections (1.45%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtrriage
Anisotropy	0.138	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36619	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.46 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8122e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	1.34	7/8360 (0.1%)	1.81	123/11404 (1.1%)
1	B	1.34	10/8355 (0.1%)	1.77	113/11397 (1.0%)
1	C	1.33	13/8336 (0.2%)	1.78	119/11372 (1.0%)
1	D	1.34	13/8344 (0.2%)	1.80	136/11383 (1.2%)
All	All	1.34	43/33395 (0.1%)	1.79	491/45556 (1.1%)

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

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	56	GLY	C-O	7.48	1.28	1.23
1	D	297	ASN	CA-C	-7.46	1.48	1.53
1	A	479	ASP	C-N	-7.22	1.26	1.34
1	C	450	HIS	CE1-NE2	6.70	1.39	1.32
1	B	418	HIS	CE1-NE2	6.20	1.38	1.32
1	A	656	VAL	CA-CB	-6.18	1.47	1.54
1	A	928	PRO	N-CA	-5.93	1.40	1.47
1	D	537	GLU	CD-OE2	5.87	1.36	1.25
1	D	122	CYS	CA-C	-5.81	1.45	1.52
1	A	249	GLU	CD-OE2	5.79	1.36	1.25
1	B	547	GLY	C-O	5.72	1.29	1.24
1	B	398	TRP	C-O	5.70	1.30	1.24
1	B	199	ASP	CG-OD2	5.67	1.36	1.25
1	B	538	TYR	C-O	5.67	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	909	ARG	CA-CB	5.63	1.57	1.53
1	D	940	GLY	CA-C	5.52	1.57	1.51
1	D	86	VAL	CA-CB	-5.47	1.50	1.54
1	D	280	ASP	CG-OD2	5.45	1.35	1.25
1	C	492	ASP	CG-OD2	5.44	1.35	1.25
1	C	117	GLU	C-N	-5.44	1.28	1.33
1	C	482	ARG	CZ-NH1	5.43	1.40	1.32
1	C	421	VAL	CA-CB	5.42	1.58	1.54
1	A	450	HIS	CE1-NE2	5.41	1.38	1.32
1	D	136	GLU	CD-OE2	5.33	1.35	1.25
1	B	990	HIS	CG-ND1	5.33	1.44	1.38
1	D	893	GLU	CD-OE2	5.30	1.35	1.25
1	C	650	GLU	CD-OE2	5.27	1.35	1.25
1	D	681	GLU	CD-OE2	5.25	1.35	1.25
1	D	31	PRO	CA-C	5.24	1.57	1.52
1	C	684	GLU	CD-OE2	5.21	1.35	1.25
1	A	492	ASP	CG-OD2	5.21	1.35	1.25
1	C	454	ILE	C-O	-5.15	1.19	1.24
1	A	507	ASP	CG-OD2	5.14	1.35	1.25
1	B	980	GLU	CD-OE2	5.14	1.35	1.25
1	C	170	GLU	CD-OE2	5.08	1.35	1.25
1	D	297	ASN	C-O	-5.08	1.21	1.23
1	C	280	ASP	CG-OD2	5.06	1.34	1.25
1	B	411	ASP	CA-C	5.04	1.59	1.52
1	B	711	ALA	CA-C	-5.03	1.46	1.52
1	D	650	GLU	CD-OE2	5.02	1.34	1.25
1	C	969	GLU	CD-OE2	5.02	1.34	1.25
1	C	442	ARG	CZ-NH1	5.02	1.39	1.32
1	D	391	HIS	ND1-CE1	5.00	1.37	1.32

All (491) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	804	ASN	CA-CB-CG	-12.02	100.58	112.60
1	D	601	PHE	CA-CB-CG	-11.83	101.97	113.80
1	C	699	ARG	NE-CZ-NH1	11.15	132.65	121.50
1	A	771	GLY	N-CA-C	-10.27	91.96	110.86
1	C	699	ARG	NE-CZ-NH2	-10.07	110.14	119.20
1	B	78	LEU	CA-C-O	9.54	126.38	119.32
1	A	997	ASP	CA-CB-CG	-8.99	103.61	112.60
1	B	804	ASN	N-CA-CB	8.79	123.89	110.44
1	C	685	LEU	CA-C-N	8.79	130.06	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	685	LEU	C-N-CA	8.79	130.06	120.13
1	C	473	ARG	CD-NE-CZ	8.58	136.41	124.40
1	C	113	PHE	CA-CB-CG	-8.45	105.35	113.80
1	A	954	ASP	CA-CB-CG	-8.41	104.19	112.60
1	A	209	PHE	CA-CB-CG	-8.34	105.47	113.80
1	C	680	ILE	CA-C-N	-8.28	111.75	122.77
1	C	680	ILE	C-N-CA	-8.28	111.75	122.77
1	C	249	GLU	N-CA-C	8.27	121.91	109.25
1	C	614	HIS	N-CA-C	-8.21	100.69	110.13
1	A	277	GLU	CB-CG-CD	8.16	126.47	112.60
1	C	730	LEU	N-CA-CB	8.09	119.12	109.74
1	B	614	HIS	N-CA-CB	8.05	119.07	109.74
1	B	661	LYS	CA-C-N	8.02	128.49	119.83
1	B	661	LYS	C-N-CA	8.02	128.49	119.83
1	D	770	ILE	N-CA-C	-8.01	96.06	107.75
1	C	593	GLY	CA-C-O	8.00	128.02	119.06
1	B	804	ASN	CA-CB-CG	8.00	120.60	112.60
1	B	737	ILE	N-CA-CB	7.87	120.03	111.61
1	D	980	GLU	CA-C-N	-7.86	107.25	121.32
1	D	980	GLU	C-N-CA	-7.86	107.25	121.32
1	A	634	GLN	CB-CG-CD	7.83	125.91	112.60
1	B	691	ALA	N-CA-C	-7.82	100.79	110.41
1	A	685	LEU	CB-CA-C	7.77	119.41	108.76
1	A	770	ILE	N-CA-CB	7.69	122.28	111.82
1	D	687	GLN	N-CA-CB	7.69	118.49	109.72
1	A	431	ARG	NE-CZ-NH2	-7.68	112.29	119.20
1	B	216	HIS	CA-CB-CG	-7.67	106.13	113.80
1	C	733	ALA	N-CA-C	7.67	121.62	110.42
1	B	634	GLN	N-CA-C	-7.65	103.01	112.88
1	D	829	THR	N-CA-CB	7.64	123.13	110.52
1	A	804	ASN	CA-CB-CG	-7.64	104.96	112.60
1	D	844	HIS	CA-CB-CG	-7.61	106.19	113.80
1	D	1022	GLN	N-CA-CB	7.58	122.48	110.57
1	B	86	VAL	CA-C-O	-7.56	114.83	119.51
1	A	730	LEU	CB-CA-C	7.53	121.61	109.41
1	D	784	PHE	CA-CB-CG	-7.50	106.30	113.80
1	A	598	ASP	CA-CB-CG	-7.48	105.12	112.60
1	A	997	ASP	N-CA-CB	7.47	123.37	111.56
1	B	363	HIS	CA-CB-CG	-7.42	106.38	113.80
1	B	977	HIS	CA-CB-CG	-7.42	106.38	113.80
1	A	95	TYR	N-CA-C	7.38	120.38	111.82
1	A	130	ASP	CA-CB-CG	-7.33	105.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	PHE	CA-CB-CG	-7.30	106.50	113.80
1	D	583	ASN	CA-C-N	7.28	127.21	119.85
1	D	583	ASN	C-N-CA	7.28	127.21	119.85
1	B	233	ASP	CA-C-N	-7.27	111.07	122.49
1	B	233	ASP	C-N-CA	-7.27	111.07	122.49
1	C	750	GLU	N-CA-CB	7.23	124.08	111.00
1	C	661	LYS	CA-C-O	7.20	123.97	119.29
1	D	687	GLN	C-N-CD	-7.20	95.50	125.00
1	C	599	ARG	NE-CZ-NH1	7.19	128.69	121.50
1	D	752	GLY	CA-C-N	-7.18	111.77	122.83
1	D	752	GLY	C-N-CA	-7.18	111.77	122.83
1	B	671	ASP	CA-CB-CG	-7.13	105.47	112.60
1	C	442	ARG	NE-CZ-NH2	-7.12	112.80	119.20
1	D	997	ASP	N-CA-CB	7.08	122.75	111.56
1	C	931	PHE	CB-CA-C	7.06	117.16	110.17
1	B	570	TRP	N-CA-C	7.05	118.65	110.97
1	A	75	GLU	CB-CA-C	7.04	121.56	109.24
1	D	869	ASP	CA-CB-CG	-7.02	105.58	112.60
1	A	235	PHE	CA-CB-CG	-7.02	106.78	113.80
1	B	557	ARG	NE-CZ-NH2	-7.01	112.89	119.20
1	D	878	HIS	CA-CB-CG	-7.01	106.78	113.80
1	D	519	SER	N-CA-C	-6.98	100.40	110.24
1	D	685	LEU	N-CA-C	6.97	119.93	110.31
1	B	871	GLU	CB-CG-CD	-6.96	100.76	112.60
1	C	76	CYS	N-CA-CB	-6.93	98.63	111.53
1	A	113	PHE	CA-CB-CG	-6.93	106.87	113.80
1	C	599	ARG	CD-NE-CZ	6.92	134.09	124.40
1	C	773	LYS	N-CA-C	6.92	119.96	108.96
1	A	803	PRO	N-CA-CB	6.91	110.09	103.52
1	D	630	ARG	NE-CZ-NH1	6.91	128.41	121.50
1	C	699	ARG	CD-NE-CZ	6.88	134.03	124.40
1	C	690	SER	N-CA-C	6.86	117.33	108.34
1	A	76	CYS	N-CA-C	6.85	119.48	109.07
1	A	996	ASP	N-CA-C	-6.83	103.00	111.75
1	C	473	ARG	NE-CZ-NH1	6.83	128.33	121.50
1	A	736	ALA	N-CA-C	6.81	118.91	108.42
1	C	804	ASN	N-CA-C	-6.80	104.98	113.28
1	C	917	ARG	CD-NE-CZ	-6.80	114.88	124.40
1	A	691	ALA	N-CA-C	6.80	120.08	110.50
1	C	71	GLU	CB-CG-CD	6.75	124.08	112.60
1	A	659	ASP	CB-CA-C	-6.74	101.85	111.95
1	C	917	ARG	NE-CZ-NH2	6.71	125.24	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	725	ASN	CA-CB-CG	-6.71	105.89	112.60
1	D	931	PHE	CA-CB-CG	-6.67	107.13	113.80
1	A	968	MET	N-CA-CB	-6.66	99.33	110.39
1	A	431	ARG	NE-CZ-NH1	6.64	128.14	121.50
1	C	728	VAL	CA-C-N	-6.64	113.31	122.93
1	C	728	VAL	C-N-CA	-6.64	113.31	122.93
1	A	989	PHE	CA-CB-CG	-6.62	107.18	113.80
1	B	736	ALA	CA-C-O	-6.60	113.90	121.68
1	A	297	ASN	CA-C-O	6.57	125.54	120.48
1	A	209	PHE	N-CA-C	6.56	121.44	113.17
1	B	611	ARG	CB-CA-C	6.53	116.29	109.83
1	C	687	GLN	N-CA-C	6.51	124.20	109.81
1	C	735	HIS	CA-CB-CG	6.49	120.29	113.80
1	A	221	GLN	N-CA-CB	-6.49	101.11	111.62
1	B	832	ASP	CB-CA-C	-6.48	100.52	111.02
1	B	231	PHE	CA-CB-CG	-6.46	107.33	113.80
1	C	753	ASN	CA-CB-CG	-6.46	106.14	112.60
1	B	473	ARG	CD-NE-CZ	6.45	133.43	124.40
1	A	184	LEU	CB-CA-C	-6.45	98.49	109.51
1	B	744	GLU	CA-C-N	-6.44	111.92	122.54
1	B	744	GLU	C-N-CA	-6.44	111.92	122.54
1	C	733	ALA	N-CA-CB	6.43	119.18	109.34
1	D	320	GLY	N-CA-C	6.43	124.34	115.27
1	D	845	GLN	CA-C-N	-6.43	111.97	122.20
1	D	845	GLN	C-N-CA	-6.43	111.97	122.20
1	D	681	GLU	CB-CA-C	6.43	121.42	110.81
1	D	299	LYS	CA-CB-CG	-6.41	101.28	114.10
1	B	729	THR	CB-CA-C	6.38	120.24	109.84
1	A	147	ASN	OD1-CG-ND2	6.36	128.96	122.60
1	D	439	ARG	NE-CZ-NH2	-6.35	113.48	119.20
1	A	788	PRO	N-CA-CB	6.34	108.96	103.31
1	A	181	GLU	N-CA-C	6.33	119.45	109.96
1	C	958	ASN	N-CA-CB	6.33	123.30	111.53
1	C	733	ALA	CB-CA-C	6.33	118.50	109.71
1	C	20	GLY	N-CA-C	-6.31	107.06	115.32
1	B	653	HIS	CA-CB-CG	-6.30	107.50	113.80
1	C	653	HIS	N-CA-CB	6.28	120.44	110.57
1	A	632	SER	CB-CA-C	6.26	120.07	110.62
1	A	233	ASP	N-CA-C	6.25	118.89	111.33
1	D	403	ASP	CA-CB-CG	6.25	118.85	112.60
1	D	968	MET	N-CA-CB	-6.22	100.63	110.28
1	A	320	GLY	N-CA-C	6.21	123.71	114.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	996	ASP	CA-CB-CG	-6.21	106.39	112.60
1	D	661	LYS	CA-C-N	6.20	127.17	119.98
1	D	661	LYS	C-N-CA	6.20	127.17	119.98
1	C	924	ASP	CA-CB-CG	-6.20	106.40	112.60
1	C	685	LEU	O-C-N	6.19	127.43	120.68
1	B	729	THR	N-CA-CB	6.18	119.54	109.95
1	A	570	TRP	N-CA-C	6.17	117.88	111.03
1	D	431	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	A	829	THR	CB-CA-C	6.17	120.31	110.19
1	C	736	ALA	N-CA-C	6.17	117.94	109.18
1	B	239	VAL	N-CA-CB	6.16	119.65	111.64
1	C	219	THR	CA-CB-OG1	-6.15	100.37	109.60
1	A	614	HIS	N-CA-C	-6.15	102.12	110.36
1	D	746	ASP	N-CA-C	6.14	118.51	109.24
1	D	77	ASP	N-CA-C	6.13	119.38	110.42
1	A	166	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	B	997	ASP	N-CA-CB	6.13	121.24	111.56
1	D	728	VAL	CA-C-O	6.13	124.71	119.38
1	D	155	ASN	CA-CB-CG	-6.12	106.48	112.60
1	C	363	HIS	CA-CB-CG	-6.12	107.68	113.80
1	B	1018	LEU	CB-CA-C	-6.11	96.92	109.94
1	C	431	ARG	CA-CB-CG	-6.11	101.87	114.10
1	D	630	ARG	NE-CZ-NH2	-6.11	113.70	119.20
1	C	803	PRO	N-CA-C	-6.11	106.71	114.35
1	C	553	TRP	CA-CB-CG	-6.11	101.99	113.60
1	A	796	SER	N-CA-CB	6.11	119.12	111.00
1	A	861	SER	CB-CA-C	-6.10	99.90	110.09
1	A	746	ASP	N-CA-C	6.10	118.45	109.24
1	D	893	GLU	CB-CG-CD	6.09	122.96	112.60
1	B	85	VAL	CB-CA-C	-6.08	102.87	111.21
1	D	323	ILE	N-CA-C	-6.08	105.79	111.45
1	D	924	ASP	CA-CB-CG	-6.07	106.53	112.60
1	C	267	VAL	CA-CB-CG2	-6.06	100.11	110.40
1	C	447	ASP	N-CA-C	6.06	120.80	113.17
1	C	508	GLU	N-CA-CB	-6.05	100.17	110.16
1	B	986	ILE	CB-CA-C	6.05	118.59	110.42
1	C	729	THR	N-CA-CB	6.05	120.43	110.69
1	C	989	PHE	CA-CB-CG	-6.05	107.75	113.80
1	C	997	ASP	N-CA-CB	6.04	121.10	111.56
1	B	633	GLY	CA-C-N	-6.04	113.18	122.60
1	B	633	GLY	C-N-CA	-6.04	113.18	122.60
1	B	599	ARG	NE-CZ-NH1	6.02	127.52	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	PHE	CA-CB-CG	-6.02	107.78	113.80
1	D	781	ARG	CD-NE-CZ	6.00	132.79	124.40
1	C	685	LEU	CB-CA-C	5.99	116.88	110.65
1	D	948	PRO	CA-C-O	5.99	126.44	118.90
1	D	193	ASP	CA-CB-CG	-5.98	106.62	112.60
1	D	479	ASP	CA-CB-CG	-5.97	106.63	112.60
1	A	829	THR	CA-CB-OG1	5.97	118.55	109.60
1	A	97	ALA	N-CA-C	5.96	117.32	109.93
1	A	967	LEU	O-C-N	-5.96	115.81	122.12
1	B	784	PHE	CA-CB-CG	-5.94	107.86	113.80
1	B	598	ASP	CA-CB-CG	-5.93	106.67	112.60
1	C	931	PHE	CA-CB-CG	-5.93	107.87	113.80
1	D	915	PHE	CA-CB-CG	-5.93	107.87	113.80
1	B	161	TYR	N-CA-CB	-5.92	100.51	111.53
1	B	958	ASN	N-CA-CB	5.92	122.55	111.53
1	D	570	TRP	N-CA-C	5.92	117.61	111.03
1	D	274	PHE	CA-CB-CG	-5.92	107.88	113.80
1	B	640	SER	CB-CA-C	-5.91	100.11	109.80
1	B	599	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	D	948	PRO	CA-C-N	-5.89	112.02	122.74
1	D	948	PRO	C-N-CA	-5.89	112.02	122.74
1	A	100	TYR	N-CA-CB	5.88	120.40	110.46
1	A	129	VAL	N-CA-CB	5.88	119.28	111.64
1	A	433	LEU	CA-C-O	5.88	124.04	118.34
1	D	183	ARG	N-CA-C	5.87	117.97	108.34
1	A	842	TRP	CE2-CD2-CE3	5.86	124.66	118.80
1	D	395	HIS	N-CA-CB	-5.85	100.79	109.98
1	A	553	TRP	CA-CB-CG	-5.84	102.50	113.60
1	B	447	ASP	N-CA-C	5.84	120.53	113.17
1	C	210	ARG	N-CA-CB	5.84	119.80	111.05
1	B	279	ILE	CA-CB-CG2	5.82	120.39	110.50
1	B	211	ASP	N-CA-C	5.81	118.25	110.35
1	A	872	VAL	CB-CA-C	-5.80	102.53	110.77
1	B	626	PHE	CA-CB-CG	-5.80	108.00	113.80
1	D	117	GLU	N-CA-CB	-5.79	101.84	110.24
1	D	948	PRO	CB-CA-C	-5.79	102.30	111.04
1	A	118	ASN	O-C-N	5.78	126.24	121.44
1	C	520	ILE	N-CA-C	5.78	116.52	110.62
1	A	64	PRO	CB-CA-C	-5.78	102.01	111.31
1	B	680	ILE	CA-C-N	-5.77	114.05	122.19
1	B	680	ILE	C-N-CA	-5.77	114.05	122.19
1	C	96	ASP	N-CA-CB	5.77	120.35	111.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	473	ARG	NE-CZ-NH1	5.75	127.25	121.50
1	C	728	VAL	CB-CA-C	-5.74	104.50	112.36
1	C	232	ASN	N-CA-C	-5.73	102.44	110.35
1	D	464	HIS	CA-CB-CG	-5.73	108.07	113.80
1	D	949	HIS	N-CA-CB	-5.72	101.64	110.56
1	B	737	ILE	CA-C-O	5.71	123.27	119.38
1	D	750	GLU	CA-C-N	-5.71	113.13	121.76
1	D	750	GLU	C-N-CA	-5.71	113.13	121.76
1	B	670	LEU	CA-C-N	-5.71	112.93	122.92
1	B	670	LEU	C-N-CA	-5.71	112.93	122.92
1	D	319	ASP	CA-CB-CG	-5.70	106.90	112.60
1	D	395	HIS	ND1-CG-CD2	5.70	111.80	106.10
1	A	112	PRO	N-CA-CB	-5.69	96.34	102.60
1	B	568	TRP	CA-CB-CG	-5.69	102.78	113.60
1	A	513	PRO	CB-CA-C	-5.69	103.64	111.21
1	A	345	ASN	CA-CB-CG	-5.69	106.91	112.60
1	A	977	HIS	CA-C-N	-5.68	112.64	120.71
1	A	977	HIS	C-N-CA	-5.68	112.64	120.71
1	D	278	ILE	CA-C-N	-5.68	114.89	121.71
1	D	278	ILE	C-N-CA	-5.68	114.89	121.71
1	C	737	ILE	CA-CB-CG2	5.67	120.14	110.50
1	C	319	ASP	CA-C-N	-5.67	113.43	122.10
1	C	319	ASP	C-N-CA	-5.67	113.43	122.10
1	D	845	GLN	CB-CA-C	-5.66	102.77	111.66
1	A	728	VAL	CA-C-O	5.66	125.29	119.35
1	C	571	VAL	N-CA-C	5.66	116.89	108.46
1	A	832	ASP	CA-CB-CG	-5.66	106.94	112.60
1	A	80	GLU	N-CA-C	5.65	120.02	113.18
1	A	127	PHE	CA-CB-CG	-5.65	108.15	113.80
1	D	781	ARG	NE-CZ-NH1	5.64	127.14	121.50
1	B	481	SER	N-CA-C	5.64	120.01	113.18
1	D	630	ARG	CD-NE-CZ	5.64	132.30	124.40
1	B	252	ASP	CA-CB-CG	-5.63	106.97	112.60
1	C	1011	ALA	N-CA-C	5.63	119.77	113.01
1	D	772	ASP	CA-CB-CG	-5.62	106.97	112.60
1	D	209	PHE	N-CA-C	5.62	120.25	113.17
1	D	329	ASP	CA-CB-CG	-5.62	106.98	112.60
1	A	613	PRO	CB-CA-C	-5.61	102.86	110.60
1	C	323	ILE	N-CA-C	-5.61	106.23	111.45
1	D	33	PHE	CA-CB-CG	5.61	119.41	113.80
1	B	30	HIS	CA-CB-CG	-5.61	108.19	113.80
1	D	651	LEU	N-CA-CB	-5.61	100.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	ASN	N-CA-C	-5.60	100.05	109.07
1	D	23	GLN	CA-C-O	-5.60	114.84	121.06
1	A	98	PRO	N-CA-C	-5.60	102.33	111.68
1	A	519	SER	N-CA-C	-5.59	102.36	110.24
1	A	998	SER	CA-C-N	-5.59	110.81	121.15
1	A	998	SER	C-N-CA	-5.59	110.81	121.15
1	B	571	VAL	N-CA-C	5.58	116.78	108.46
1	B	33	PHE	CB-CA-C	-5.58	98.84	109.66
1	C	790	ASP	CA-CB-CG	-5.58	107.02	112.60
1	D	221	GLN	N-CA-CB	-5.58	102.75	111.56
1	C	663	LEU	CB-CA-C	-5.58	100.60	111.03
1	D	77	ASP	CA-CB-CG	-5.57	107.03	112.60
1	A	477	SER	N-CA-CB	5.57	118.37	110.13
1	D	116	THR	CA-CB-OG1	-5.57	101.25	109.60
1	A	13	ARG	NE-CZ-NH2	-5.57	114.19	119.20
1	A	917	ARG	NE-CZ-NH1	-5.57	115.94	121.50
1	A	96	ASP	N-CA-CB	5.56	120.03	111.46
1	B	733	ALA	N-CA-C	5.55	122.63	110.80
1	A	30	HIS	N-CA-CB	-5.54	105.58	111.29
1	D	787	ALA	N-CA-C	-5.54	99.42	109.44
1	D	210	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	C	13	ARG	N-CA-CB	5.53	119.90	110.50
1	C	737	ILE	N-CA-CB	5.51	118.92	111.21
1	B	332	PHE	CA-CB-CG	-5.51	108.29	113.80
1	B	828	ASP	CA-CB-CG	-5.51	107.09	112.60
1	C	365	GLN	CA-CB-CG	-5.50	103.09	114.10
1	C	472	TYR	N-CA-C	-5.50	105.18	111.07
1	D	997	ASP	CA-C-O	-5.50	115.56	121.45
1	A	491	ALA	N-CA-C	5.50	122.07	113.72
1	A	905	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	B	519	SER	N-CA-C	-5.49	102.50	110.24
1	B	661	LYS	CA-C-O	5.49	125.47	119.32
1	B	351	ILE	N-CA-CB	-5.49	104.80	110.95
1	C	842	TRP	CE2-CD2-CE3	5.49	124.29	118.80
1	C	338	GLU	CB-CG-CD	-5.49	103.27	112.60
1	B	467	ASN	CA-C-O	5.48	126.36	120.55
1	A	636	ILE	N-CA-CB	5.48	117.57	110.99
1	D	958	ASN	N-CA-CB	5.48	121.23	111.69
1	A	147	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	890	GLN	O-C-N	5.48	129.19	122.84
1	C	32	PRO	N-CA-CB	5.47	109.00	103.25
1	B	75	GLU	CA-C-N	-5.47	112.28	121.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	75	GLU	C-N-CA	-5.47	112.28	121.75
1	D	245	GLN	CA-CB-CG	-5.47	103.16	114.10
1	D	687	GLN	O-C-N	5.47	126.19	120.99
1	C	519	SER	N-CA-C	-5.47	102.30	110.23
1	D	736	ALA	N-CA-C	5.47	118.33	109.86
1	A	816	TYR	CA-C-N	-5.46	114.02	122.49
1	A	816	TYR	C-N-CA	-5.46	114.02	122.49
1	B	357	HIS	ND1-CG-CD2	5.46	111.56	106.10
1	B	239	VAL	CA-CB-CG2	-5.46	101.12	110.40
1	C	796	SER	CA-C-O	5.46	124.90	118.90
1	A	431	ARG	CD-NE-CZ	5.45	132.03	124.40
1	D	719	GLN	CB-CG-CD	-5.44	103.36	112.60
1	D	184	LEU	CB-CA-C	-5.43	100.35	109.48
1	C	685	LEU	N-CA-CB	5.42	119.43	110.38
1	D	956	GLN	N-CA-C	-5.42	101.05	109.72
1	A	869	ASP	CA-CB-CG	-5.42	107.18	112.60
1	C	829	THR	N-CA-CB	5.42	119.08	110.57
1	D	100	TYR	N-CA-CB	5.41	119.61	110.46
1	D	689	GLU	N-CA-C	-5.41	105.55	111.82
1	D	949	HIS	N-CA-C	5.40	118.79	110.42
1	B	622	HIS	ND1-CE1-NE2	5.40	113.80	108.40
1	C	516	PRO	CB-CA-C	-5.40	104.16	111.12
1	C	703	PRO	N-CA-CB	5.39	109.23	103.52
1	C	420	MET	CA-C-N	-5.38	118.17	122.85
1	C	420	MET	C-N-CA	-5.38	118.17	122.85
1	A	583	ASN	N-CA-CB	5.38	118.19	109.90
1	D	598	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	853	ARG	NE-CZ-NH2	-5.38	114.36	119.20
1	D	272	ALA	N-CA-C	5.37	113.06	108.22
1	B	553	TRP	CA-CB-CG	-5.37	103.39	113.60
1	C	130	ASP	CA-CB-CG	-5.37	107.23	112.60
1	D	923	SER	CA-CB-OG	-5.37	100.37	111.10
1	B	636	ILE	N-CA-CB	5.36	118.22	111.46
1	C	818	ALA	CA-C-N	5.36	130.40	123.00
1	C	818	ALA	C-N-CA	5.36	130.40	123.00
1	B	297	ASN	CA-CB-CG	-5.36	107.24	112.60
1	A	742	THR	CB-CA-C	-5.36	98.77	109.33
1	C	854	LYS	N-CA-CB	-5.36	102.36	111.69
1	D	760	ARG	N-CA-CB	5.36	119.13	110.40
1	D	954	ASP	CA-CB-CG	-5.36	107.24	112.60
1	A	118	ASN	N-CA-CB	-5.35	102.29	111.39
1	D	309	TYR	N-CA-C	-5.35	101.98	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	136	GLU	N-CA-CB	-5.35	103.11	111.56
1	B	843	GLN	O-C-N	5.35	130.26	122.94
1	D	447	ASP	N-CA-C	5.34	119.90	113.17
1	B	62	TRP	O-C-N	-5.34	116.95	123.19
1	A	91	GLN	OE1-CD-NE2	5.33	127.93	122.60
1	D	376	ILE	CA-CB-CG2	5.33	119.56	110.50
1	A	671	ASP	CA-C-N	-5.33	115.71	123.06
1	A	671	ASP	C-N-CA	-5.33	115.71	123.06
1	A	210	ARG	N-CA-CB	5.33	119.04	111.05
1	D	673	ALA	N-CA-CB	-5.33	102.43	109.78
1	B	745	MET	N-CA-C	5.32	119.88	113.17
1	B	779	PRO	N-CA-CB	5.31	108.38	103.39
1	C	651	LEU	N-CA-CB	5.31	121.03	111.37
1	B	728	VAL	N-CA-C	-5.31	107.95	113.10
1	B	818	ALA	CA-C-N	-5.31	114.98	122.94
1	B	818	ALA	C-N-CA	-5.31	114.98	122.94
1	C	604	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	D	446	ARG	NE-CZ-NH1	5.30	126.81	121.50
1	D	559	TYR	CB-CA-C	-5.30	104.92	110.17
1	D	136	GLU	N-CA-C	5.30	116.86	108.96
1	D	855	THR	N-CA-CB	5.30	120.62	111.13
1	C	842	TRP	N-CA-CB	5.30	118.87	110.55
1	D	599	ARG	CA-CB-CG	-5.30	103.51	114.10
1	A	726	LEU	O-C-N	-5.29	116.37	122.87
1	A	365	GLN	CA-CB-CG	-5.28	103.53	114.10
1	D	575	LEU	O-C-N	-5.28	116.33	123.19
1	C	735	HIS	N-CA-C	-5.27	106.11	112.54
1	A	787	ALA	N-CA-C	-5.26	99.02	109.60
1	B	166	ARG	NE-CZ-NH2	-5.26	114.46	119.20
1	C	225	PHE	N-CA-CB	5.26	119.47	110.57
1	A	147	ASN	N-CA-CB	-5.26	102.29	110.55
1	D	134	LEU	N-CA-C	-5.26	105.60	112.23
1	D	164	ASP	CA-CB-CG	-5.26	107.34	112.60
1	D	226	HIS	ND1-CG-CD2	5.25	111.35	106.10
1	D	669	PRO	CA-C-N	-5.25	115.47	122.72
1	D	669	PRO	C-N-CA	-5.25	115.47	122.72
1	B	593	GLY	N-CA-C	-5.25	108.39	115.36
1	D	39	SER	N-CA-C	5.25	117.00	111.28
1	C	687	GLN	CA-C-O	5.24	127.34	120.16
1	D	1000	SER	N-CA-C	-5.24	103.41	108.07
1	C	794	ALA	N-CA-C	5.24	118.86	111.52
1	D	739	HIS	CA-CB-CG	-5.24	108.56	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	423	MET	N-CA-C	5.24	117.73	111.71
1	C	221	GLN	N-CA-C	5.24	117.03	109.07
1	D	614	HIS	N-CA-C	-5.24	102.54	110.39
1	B	634	GLN	CA-C-N	-5.23	115.51	122.72
1	B	634	GLN	C-N-CA	-5.23	115.51	122.72
1	D	681	GLU	CB-CG-CD	5.23	121.49	112.60
1	D	807	VAL	N-CA-C	5.22	115.94	110.62
1	A	862	GLY	CA-C-O	5.21	124.90	119.06
1	A	930	VAL	N-CA-CB	5.21	116.29	110.51
1	D	220	THR	CA-CB-OG1	-5.21	101.79	109.60
1	C	259	SER	CB-CA-C	5.20	119.31	109.37
1	D	629	PHE	CA-CB-CG	5.20	119.00	113.80
1	C	295	VAL	CA-C-O	5.20	125.52	120.27
1	A	788	PRO	CB-CA-C	-5.20	104.75	111.46
1	B	659	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	985	ASN	CA-C-N	-5.20	115.60	122.98
1	B	985	ASN	C-N-CA	-5.20	115.60	122.98
1	B	611	ARG	N-CA-CB	5.19	119.29	114.10
1	D	357	HIS	ND1-CG-CD2	5.19	111.29	106.10
1	C	233	ASP	CA-C-N	-5.19	114.42	122.67
1	C	233	ASP	C-N-CA	-5.19	114.42	122.67
1	D	19	PRO	N-CA-CB	5.19	108.29	103.41
1	A	159	VAL	CA-C-N	-5.19	113.19	120.56
1	A	159	VAL	C-N-CA	-5.19	113.19	120.56
1	A	747	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	832	ASP	N-CA-CB	-5.18	102.65	111.20
1	A	719	GLN	CB-CA-C	-5.17	98.56	109.38
1	A	913	ALA	CA-C-O	-5.17	115.92	121.56
1	A	382	ASN	CA-C-O	5.17	126.05	119.95
1	D	1022	GLN	N-CA-C	-5.17	100.75	109.07
1	D	742	THR	N-CA-CB	-5.16	102.59	110.85
1	B	1022	GLN	N-CA-CB	5.16	118.59	110.23
1	A	442	ARG	NE-CZ-NH2	-5.16	114.56	119.20
1	A	299	LYS	CA-CB-CG	-5.16	103.79	114.10
1	A	251	ARG	NE-CZ-NH1	5.15	126.65	121.50
1	B	636	ILE	CA-C-N	-5.15	115.84	123.05
1	B	636	ILE	C-N-CA	-5.15	115.84	123.05
1	C	369	GLU	CG-CD-OE2	-5.15	106.56	118.40
1	D	974	HIS	CA-CB-CG	-5.15	108.65	113.80
1	A	747	PHE	N-CA-C	-5.15	100.02	108.41
1	B	988	GLY	N-CA-C	-5.14	106.47	113.37
1	C	294	ASN	CA-CB-CG	-5.14	107.46	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	PRO	O-C-N	5.13	128.39	122.23
1	A	684	GLU	N-CA-C	-5.13	102.32	109.96
1	D	147	ASN	N-CA-CB	-5.12	102.66	110.65
1	A	687	GLN	N-CA-C	-5.12	102.76	110.24
1	B	273	PRO	CB-CA-C	-5.12	103.17	110.75
1	D	769	TRP	CA-C-N	-5.12	116.29	123.10
1	D	769	TRP	C-N-CA	-5.12	116.29	123.10
1	A	233	ASP	CB-CG-OD2	-5.12	106.63	118.40
1	D	297	ASN	CA-CB-CG	-5.12	107.48	112.60
1	D	412	GLU	N-CA-CB	-5.12	102.08	110.68
1	C	803	PRO	N-CA-CB	5.11	108.45	102.88
1	C	855	THR	N-CA-CB	5.11	120.25	111.00
1	C	395	HIS	N-CA-CB	-5.11	101.95	109.98
1	B	795	VAL	CB-CA-C	5.10	117.78	110.33
1	A	795	VAL	CB-CA-C	5.10	118.67	110.82
1	B	829	THR	CA-CB-OG1	-5.10	101.95	109.60
1	C	184	LEU	CB-CA-C	-5.10	100.88	109.50
1	A	250	LEU	CB-CA-C	-5.09	101.94	110.29
1	D	703	PRO	CB-CA-C	-5.09	104.67	112.11
1	A	119	PRO	N-CA-CB	5.09	107.77	103.19
1	D	359	HIS	CA-CB-CG	-5.09	108.71	113.80
1	D	702	GLN	CA-C-O	5.09	123.64	119.36
1	C	274	PHE	CA-CB-CG	-5.09	108.71	113.80
1	C	848	THR	O-C-N	5.09	129.04	122.93
1	C	746	ASP	N-CA-C	5.09	116.54	108.96
1	D	161	TYR	N-CA-CB	-5.09	102.07	111.53
1	B	356	ARG	NE-CZ-NH1	5.08	126.58	121.50
1	B	788	PRO	N-CA-CB	5.08	107.77	103.19
1	C	181	GLU	N-CA-C	5.08	117.80	110.28
1	B	630	ARG	CA-C-N	-5.08	115.32	122.94
1	B	630	ARG	C-N-CA	-5.08	115.32	122.94
1	C	842	TRP	CG-CD2-CE3	-5.08	128.82	133.90
1	D	1022	GLN	CB-CG-CD	5.08	121.23	112.60
1	C	521	LYS	CG-CD-CE	5.08	122.97	111.30
1	A	420	MET	CA-C-N	-5.07	118.44	122.85
1	A	420	MET	C-N-CA	-5.07	118.44	122.85
1	D	116	THR	CA-CB-CG2	-5.07	101.88	110.50
1	A	860	GLY	CA-C-N	-5.07	114.18	122.54
1	A	860	GLY	C-N-CA	-5.07	114.18	122.54
1	B	166	ARG	N-CA-C	5.07	120.09	112.94
1	B	365	GLN	CA-CB-CG	-5.07	103.97	114.10
1	C	480	PRO	N-CA-CB	5.07	108.01	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	680	ILE	CA-C-O	5.06	125.38	120.27
1	C	956	GLN	N-CA-C	-5.06	101.62	109.72
1	C	714	ILE	CB-CG1-CD1	-5.05	103.19	113.80
1	A	721	ARG	O-C-N	-5.05	117.05	123.01
1	A	829	THR	N-CA-CB	-5.05	102.62	110.55
1	B	777	LEU	N-CA-C	-5.05	107.67	113.88
1	A	732	ALA	N-CA-C	5.04	117.61	110.10
1	B	247	CYS	CA-CB-SG	-5.04	102.80	114.40
1	B	403	ASP	CB-CA-C	-5.04	102.42	110.79
1	B	542	MET	CA-C-O	-5.03	114.91	120.60
1	B	855	THR	N-CA-CB	5.03	120.10	111.00
1	B	98	PRO	N-CA-C	-5.03	103.29	111.68
1	C	477	SER	N-CA-CB	-5.02	102.78	110.07
1	C	837	THR	CA-C-O	5.02	125.78	120.36
1	D	882	ILE	CA-CB-CG1	-5.02	101.87	110.40
1	C	469	ASP	O-C-N	5.01	127.44	122.12
1	C	233	ASP	CB-CG-OD2	-5.01	106.87	118.40
1	A	847	LYS	CB-CA-C	5.01	118.39	109.72
1	A	887	GLN	OE1-CD-NE2	5.01	127.61	122.60
1	D	416	GLU	CG-CD-OE1	5.00	129.91	118.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	733	ALA	CA

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	8119	0	7710	175	0
1	B	8114	0	7705	183	0
1	C	8095	0	7681	172	0
1	D	8103	0	7692	168	0
2	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	4	0	0	0	0
2	D	3	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	88	0	132	27	0
4	B	72	0	108	14	0
4	C	84	0	126	26	0
4	D	96	0	144	22	0
5	A	916	0	0	24	0
5	B	985	0	0	16	0
5	C	935	0	0	17	0
5	D	984	0	0	18	0
All	All	36619	0	31298	709	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 (709) 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)
4:B:8601:DMS:C2	4:B:8601:DMS:S	2.03	1.47
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.21	1.18
1:B:376:ILE:HA	1:B:379:MET:HE2	1.23	1.09
1:A:32:PRO:HB2	4:A:8404:DMS:H11	1.33	1.06
1:C:649:ASN:HA	4:C:8425:DMS:H13	1.41	1.03
1:C:367:MET:HB3	1:C:372:MET:HE3	1.50	0.93
1:B:232:ASN:ND2	1:B:237:ARG:HG3	1.84	0.92
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.01	0.91
1:B:745:MET:HE3	1:B:745:MET:H	1.37	0.88
1:B:599:ARG:HG3	1:B:599:ARG:HH11	1.39	0.88
1:A:655:MET:HE1	1:A:662:PRO:HB3	1.54	0.87
1:B:684:GLU:O	1:B:686:PRO:HD3	1.74	0.87
1:A:755:ARG:HD2	5:A:9418:HOH:O	1.75	0.86
1:D:1017:GLN:HG2	1:D:1018:LEU:N	1.90	0.86
1:B:376:ILE:HA	1:B:379:MET:CE	2.07	0.84
1:C:703:PRO:HG2	4:C:8425:DMS:H11	1.59	0.84
1:D:829:THR:O	1:D:830:LEU:HD23	1.78	0.84
1:A:600:GLN:H	1:A:600:GLN:HE21	1.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:HG3	1:C:13:ARG:CZ	2.08	0.83
1:A:107:ILE:HG22	4:A:8410:DMS:H23	1.60	0.83
1:B:13:ARG:HG3	1:C:13:ARG:NH2	1.92	0.83
1:B:600:GLN:H	1:B:600:GLN:HE21	1.24	0.83
1:C:687:GLN:HB3	1:C:688:PRO:HD2	1.60	0.82
1:D:858:ILE:CD1	1:D:864:MET:HG3	2.09	0.82
1:C:745:MET:HE3	1:C:745:MET:HA	1.61	0.81
1:B:847:LYS:HD3	1:B:849:LEU:HD23	1.63	0.81
1:D:807:VAL:O	1:D:811:LYS:HD3	1.79	0.81
1:B:599:ARG:HG3	1:B:599:ARG:NH1	1.89	0.81
1:D:133:TRP:NE1	4:D:8703:DMS:H23	1.95	0.81
1:D:316:HIS:HA	1:D:323:ILE:HD12	1.63	0.80
1:A:233:ASP:HA	4:A:8417:DMS:H13	1.63	0.80
1:A:653:HIS:CD2	1:A:667:GLU:HG3	2.17	0.79
1:B:651:LEU:O	1:B:651:LEU:HD23	1.82	0.79
1:A:843:GLN:HG3	1:A:848:THR:HA	1.63	0.79
1:D:843:GLN:HG2	1:D:848:THR:HA	1.64	0.79
1:C:808:GLU:HA	1:C:811:LYS:NZ	1.96	0.79
1:A:32:PRO:CB	4:A:8404:DMS:H11	2.11	0.79
1:B:679:LEU:C	1:B:680:ILE:HD12	2.07	0.79
1:D:634:GLN:HB2	1:D:682:LEU:HB2	1.64	0.78
1:A:277:GLU:H	1:A:277:GLU:CD	1.90	0.78
1:C:809:ARG:NH1	1:C:877:PRO:HB3	1.99	0.78
1:A:930:VAL:HA	1:A:973:ARG:HD3	1.66	0.78
1:A:703:PRO:HG2	4:A:8425:DMS:H12	1.65	0.77
1:B:1022:GLN:HG3	1:B:1023:LYS:O	1.85	0.77
1:A:863:GLN:CG	1:A:1021:CYS:HB3	2.14	0.77
1:B:678:GLN:NE2	1:B:680:ILE:HD11	1.99	0.77
1:C:745:MET:HG2	5:C:9388:HOH:O	1.83	0.77
1:C:746:ASP:HA	1:C:760:ARG:HG3	1.67	0.77
4:D:8703:DMS:H21	5:D:9600:HOH:O	1.85	0.76
1:C:599:ARG:HG3	1:C:600:GLN:OE1	1.85	0.76
1:C:770:ILE:HD12	1:C:775:GLN:CD	2.10	0.76
1:A:634:GLN:HB3	1:A:682:LEU:HB2	1.66	0.76
1:C:78:LEU:HD22	1:C:80:GLU:OE1	1.86	0.76
1:D:651:LEU:HD13	1:D:651:LEU:C	2.11	0.76
1:D:858:ILE:HD11	1:D:864:MET:HG3	1.65	0.76
5:C:9488:HOH:O	1:D:530:THR:HG22	1.87	0.75
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.69	0.75
1:B:986:ILE:CD1	1:B:1018:LEU:HD21	2.17	0.75
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:8411:DMS:H22	5:B:9552:HOH:O	1.86	0.74
1:C:684:GLU:OE2	1:C:686:PRO:HB3	1.88	0.74
1:C:703:PRO:HD2	4:C:8425:DMS:H12	1.68	0.74
1:C:649:ASN:HA	4:C:8425:DMS:C1	2.17	0.74
1:C:599:ARG:NH2	1:C:795:VAL:HB	2.03	0.73
1:C:835:LEU:HD11	1:C:855:THR:HB	1.70	0.73
1:B:679:LEU:O	1:B:680:ILE:HD12	1.89	0.73
1:D:133:TRP:HE1	4:D:8703:DMS:H23	1.50	0.73
1:B:687:GLN:HE21	1:B:687:GLN:N	1.85	0.73
1:A:243:GLU:OE2	1:A:245:GLN:NE2	2.21	0.73
1:A:241:GLU:OE1	1:A:292:ARG:NE	2.21	0.73
1:D:595:THR:HA	1:D:596:PRO:C	2.13	0.73
4:C:8503:DMS:H13	5:C:9043:HOH:O	1.88	0.73
1:D:360:HIS:CE1	1:D:362:LEU:HB2	2.24	0.73
1:B:658:LEU:O	1:B:661:LYS:HD2	1.88	0.73
1:D:135:GLN:C	1:D:136:GLU:HG2	2.13	0.72
1:C:808:GLU:HA	1:C:811:LYS:HZ3	1.51	0.72
1:A:107:ILE:C	4:A:8419:DMS:H13	2.15	0.72
1:A:583:ASN:OD1	1:A:584:PRO:HD2	1.89	0.72
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.71	0.72
1:B:890:GLN:HG3	1:B:891:VAL:N	2.03	0.71
1:D:664:ALA:HB3	1:D:685:LEU:HD21	1.71	0.71
1:C:745:MET:HA	1:C:745:MET:CE	2.20	0.71
1:C:802:ASP:OD1	1:C:804:ASN:HB2	1.90	0.71
1:B:745:MET:H	1:B:745:MET:CE	2.02	0.71
1:B:133:TRP:CD1	4:B:8504:DMS:H12	2.25	0.71
1:A:746:ASP:HB2	5:A:9486:HOH:O	1.90	0.71
1:D:134:LEU:HA	4:D:8705:DMS:H23	1.73	0.70
1:B:278:ILE:HD12	5:B:9153:HOH:O	1.92	0.70
4:A:8419:DMS:H12	5:A:8931:HOH:O	1.91	0.70
4:D:8421:DMS:H12	5:D:9329:HOH:O	1.91	0.70
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.04	0.70
1:D:379:MET:HE1	1:D:407:LEU:HD13	1.74	0.70
1:D:843:GLN:CG	1:D:848:THR:HA	2.22	0.70
1:B:319:ASP:OD1	1:B:321:THR:N	2.22	0.70
1:A:651:LEU:CD1	1:A:667:GLU:HG2	2.22	0.69
1:B:655:MET:HE1	1:B:662:PRO:HB3	1.73	0.69
1:B:772:ASP:OD1	1:B:773:LYS:HD3	1.92	0.69
1:D:379:MET:HE1	1:D:407:LEU:CD1	2.21	0.69
1:B:655:MET:CE	1:B:662:PRO:HB3	2.22	0.69
1:A:737:ILE:O	1:A:737:ILE:HD13	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:8410:DMS:H11	5:C:8970:HOH:O	1.91	0.69
1:A:80:GLU:OE1	1:A:80:GLU:N	2.23	0.69
1:A:863:GLN:HG3	1:A:1021:CYS:HB3	1.74	0.69
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.13	0.68
4:C:8413:DMS:H13	5:C:9181:HOH:O	1.93	0.68
1:A:655:MET:HE1	1:A:662:PRO:CB	2.24	0.68
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.26	0.68
1:C:593:GLY:O	4:C:8413:DMS:H23	1.94	0.68
1:D:634:GLN:NE2	1:D:682:LEU:O	2.26	0.68
1:D:952:ARG:O	1:D:1018:LEU:HD22	1.93	0.68
1:D:360:HIS:HE1	1:D:362:LEU:HB2	1.58	0.68
1:C:684:GLU:O	1:C:684:GLU:HG3	1.94	0.68
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.29	0.68
1:B:745:MET:HE3	1:B:745:MET:N	2.08	0.67
1:D:859:ASP:CG	1:D:861:SER:H	2.02	0.67
1:C:765:LEU:HD21	1:C:768:MET:CE	2.13	0.67
1:A:749:ILE:HD12	1:A:749:ILE:N	2.09	0.67
1:C:703:PRO:HG2	4:C:8425:DMS:C1	2.24	0.67
1:B:634:GLN:HG2	1:B:682:LEU:O	1.94	0.67
1:B:687:GLN:N	1:B:687:GLN:NE2	2.43	0.67
1:C:730:LEU:N	1:C:730:LEU:HD23	2.09	0.67
1:A:494:THR:HB	1:D:473:ARG:NH2	2.10	0.67
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.11	0.66
1:D:887:GLN:NE2	1:D:980:GLU:O	2.28	0.66
1:A:93:HIS:NE2	4:A:8414:DMS:H21	2.11	0.66
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.60	0.66
4:C:8417:DMS:H22	5:C:9209:HOH:O	1.95	0.66
1:D:230:ARG:HD3	5:D:9609:HOH:O	1.95	0.66
1:D:94:GLY:O	4:D:8421:DMS:H21	1.96	0.66
1:D:595:THR:O	4:D:8413:DMS:H12	1.95	0.66
1:A:887:GLN:NE2	1:A:980:GLU:O	2.26	0.66
1:D:687:GLN:OE1	1:D:688:PRO:HD2	1.95	0.66
1:D:829:THR:C	1:D:830:LEU:HD23	2.20	0.65
1:C:890:GLN:HG3	1:C:891:VAL:N	2.11	0.65
1:D:117:GLU:HB2	5:D:9146:HOH:O	1.96	0.65
1:A:252:ASP:OD1	4:A:8416:DMS:H12	1.96	0.65
1:A:847:LYS:NZ	5:A:9292:HOH:O	2.30	0.65
1:B:678:GLN:HE21	1:B:680:ILE:HD11	1.61	0.65
1:D:237:ARG:NH1	5:D:9254:HOH:O	2.29	0.65
1:D:658:LEU:O	1:D:661:LYS:HG3	1.96	0.64
1:D:579:ASP:HA	5:D:9220:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLN:HG2	1:A:1021:CYS:HB3	1.78	0.64
1:B:379:MET:HE3	1:B:407:LEU:HD11	1.79	0.64
1:B:986:ILE:HD13	1:B:1018:LEU:HD21	1.78	0.64
1:C:599:ARG:NH1	5:C:8969:HOH:O	2.30	0.64
1:A:708:TRP:CZ2	4:A:8403:DMS:H13	2.32	0.64
1:C:599:ARG:HH21	1:C:795:VAL:CG1	2.11	0.64
1:A:630:ARG:HA	4:A:8503:DMS:O	1.98	0.63
1:B:847:LYS:HD3	1:B:849:LEU:CD2	2.27	0.63
1:D:770:ILE:HD12	1:D:775:GLN:CD	2.23	0.63
1:D:858:ILE:HD12	1:D:864:MET:HG3	1.79	0.63
1:A:579:ASP:O	1:A:582:GLY:N	2.26	0.63
1:D:292:ARG:HH12	4:D:8412:DMS:H23	1.63	0.63
1:D:708:TRP:CZ2	4:D:8403:DMS:H13	2.34	0.63
1:C:878:HIS:HD2	5:C:8701:HOH:O	1.79	0.63
1:A:832:ASP:OD1	1:A:832:ASP:N	2.28	0.63
1:C:595:THR:HA	1:C:596:PRO:C	2.24	0.63
1:D:787:ALA:HA	1:D:968:MET:HE2	1.79	0.63
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.29	0.63
1:B:730:LEU:CB	1:B:731:PRO:HD2	2.29	0.62
1:D:859:ASP:OD2	1:D:861:SER:N	2.29	0.62
1:A:595:THR:HA	1:A:596:PRO:C	2.24	0.62
1:C:240:LEU:C	1:C:240:LEU:HD23	2.25	0.62
1:D:878:HIS:HD2	5:D:8818:HOH:O	1.83	0.62
1:A:112:PRO:HD2	1:A:113:PHE:CE1	2.33	0.62
1:C:360:HIS:CE1	1:C:362:LEU:HB2	2.35	0.62
1:C:830:LEU:N	1:C:830:LEU:HD23	2.14	0.61
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.30	0.61
1:B:236:SER:C	1:B:237:ARG:HG2	2.25	0.61
1:B:746:ASP:OD1	1:B:757:GLN:NE2	2.34	0.61
1:A:800:ARG:HD3	1:A:801:ILE:N	2.15	0.61
1:B:730:LEU:HB2	1:B:731:PRO:HD2	1.83	0.61
1:C:367:MET:HB3	1:C:372:MET:CE	2.28	0.61
1:D:577:LYS:O	1:D:584:PRO:HA	2.01	0.61
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.82	0.61
1:B:890:GLN:CG	1:B:891:VAL:N	2.63	0.61
1:A:768:MET:HE1	1:A:1020:TRP:CE2	2.35	0.60
1:D:46:ARG:HB3	1:D:47:PRO:HD2	1.82	0.60
1:B:986:ILE:HD11	1:B:1018:LEU:HD21	1.82	0.60
1:D:681:GLU:HG2	5:D:9421:HOH:O	1.99	0.60
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.36	0.60
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:GLY:O	1:A:662:PRO:HD3	2.02	0.60
1:B:277:GLU:HG2	5:B:9401:HOH:O	2.01	0.60
1:B:637:GLU:CD	1:B:677:LYS:HE2	2.25	0.60
1:D:438:GLU:HG2	1:D:442:ARG:HD2	1.83	0.60
1:C:651:LEU:HD12	1:C:701:VAL:O	2.01	0.60
1:B:685:LEU:O	1:B:687:GLN:NE2	2.35	0.60
1:C:684:GLU:O	1:C:686:PRO:HD3	2.01	0.60
1:C:743:SER:O	1:C:760:ARG:NH1	2.27	0.60
1:B:379:MET:CE	1:B:407:LEU:HD11	2.32	0.60
1:A:135:GLN:NE2	5:A:9437:HOH:O	2.35	0.59
1:D:126:THR:CG2	1:D:181:GLU:HG2	2.32	0.59
1:D:133:TRP:HE1	4:D:8703:DMS:C2	2.15	0.59
1:D:231:PHE:O	4:D:8417:DMS:H23	2.02	0.59
1:B:878:HIS:HD2	5:B:8690:HOH:O	1.85	0.59
4:A:8419:DMS:H22	5:A:8957:HOH:O	2.01	0.59
1:D:73:TRP:CE2	1:D:122:CYS:HB3	2.37	0.59
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.38	0.59
1:A:890:GLN:HG3	1:A:891:VAL:N	2.18	0.59
1:B:387:VAL:HG22	5:B:9493:HOH:O	2.02	0.59
1:D:373:VAL:O	1:D:377:LEU:HG	2.03	0.59
1:B:795:VAL:HG12	5:B:9500:HOH:O	2.03	0.58
1:C:296:GLU:HG2	4:C:8601:DMS:H12	1.83	0.58
1:A:655:MET:HG2	5:A:8968:HOH:O	2.01	0.58
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.16	0.58
1:C:278:ILE:HD13	1:C:278:ILE:N	2.16	0.58
1:A:267:VAL:O	4:A:8602:DMS:H23	2.04	0.58
1:C:296:GLU:HA	1:C:296:GLU:OE1	2.02	0.58
1:D:768:MET:HE1	1:D:1020:TRP:CE2	2.39	0.58
1:B:597:ASN:OD1	1:B:599:ARG:HD3	2.04	0.58
1:D:68:ALA:O	1:D:70:PRO:HD3	2.03	0.58
1:C:599:ARG:HH21	1:C:795:VAL:HB	1.68	0.58
1:D:859:ASP:OD2	1:D:861:SER:HB3	2.03	0.58
1:C:599:ARG:HG3	1:C:600:GLN:H	1.69	0.57
1:C:734:SER:CB	1:C:860:GLY:HA3	2.34	0.57
1:D:126:THR:HG23	1:D:181:GLU:HG2	1.86	0.57
1:A:347:LYS:HE3	5:A:9435:HOH:O	2.04	0.57
1:A:683:PRO:O	1:A:685:LEU:HG	2.04	0.57
1:C:824:GLN:O	1:C:838:THR:HA	2.04	0.57
1:C:688:PRO:HG3	1:C:694:LEU:HD11	1.86	0.57
1:A:473:ARG:HH11	1:A:476:LYS:HB2	1.69	0.57
1:A:494:THR:CB	1:D:473:ARG:HH22	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:MET:HE2	1:A:790:ASP:CG	2.30	0.57
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.86	0.57
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.85	0.57
1:D:805:ALA:O	1:D:809:ARG:HG3	2.05	0.57
1:B:376:ILE:CA	1:B:379:MET:HE2	2.16	0.57
1:D:687:GLN:CD	1:D:688:PRO:HD2	2.30	0.57
1:D:710:GLU:HG2	5:D:9085:HOH:O	2.05	0.56
1:A:730:LEU:HD21	1:B:823:LEU:HB3	1.87	0.56
1:B:431:ARG:HG2	5:C:9420:HOH:O	2.05	0.56
1:B:678:GLN:HG2	1:B:680:ILE:CD1	2.34	0.56
1:A:533:LEU:C	1:A:533:LEU:HD23	2.30	0.56
1:B:748:CYS:C	1:B:749:ILE:HD12	2.31	0.56
1:C:615:PRO:O	1:C:618:THR:HG22	2.05	0.56
1:B:595:THR:HA	1:B:596:PRO:C	2.31	0.56
1:C:730:LEU:CB	1:C:731:PRO:HD2	2.35	0.56
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.88	0.56
1:B:876:THR:OG1	1:B:877:PRO:HD2	2.06	0.56
1:C:757:GLN:OE1	1:C:769:TRP:HH2	1.87	0.56
1:C:317:THR:OG1	1:C:319:ASP:OD1	2.24	0.55
1:B:240:LEU:C	1:B:240:LEU:HD23	2.30	0.55
1:D:890:GLN:HG3	1:D:891:VAL:N	2.21	0.55
1:D:1022:GLN:HG3	1:D:1023:LYS:N	2.01	0.55
1:B:78:LEU:HB3	1:B:80:GLU:CG	2.36	0.55
1:C:805:ALA:HB3	1:C:808:GLU:HG2	1.89	0.55
1:B:890:GLN:HG2	5:B:9553:HOH:O	2.06	0.55
1:B:363:HIS:HD2	5:B:9171:HOH:O	1.89	0.55
1:C:133:TRP:NE1	4:C:8504:DMS:H21	2.22	0.54
1:C:809:ARG:CZ	1:C:877:PRO:HB3	2.36	0.54
1:D:299:LYS:NZ	5:D:9387:HOH:O	2.23	0.54
4:D:8406:DMS:O	5:D:9596:HOH:O	2.18	0.54
1:A:655:MET:CE	1:A:662:PRO:HA	2.37	0.54
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.89	0.54
1:A:494:THR:HB	1:D:473:ARG:HH22	1.72	0.54
1:A:737:ILE:HD13	1:A:737:ILE:C	2.31	0.54
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.42	0.54
1:D:292:ARG:HH12	4:D:8412:DMS:C2	2.19	0.54
1:B:655:MET:SD	1:B:656:VAL:N	2.80	0.54
1:C:360:HIS:HE1	1:C:362:LEU:HB2	1.71	0.54
1:D:240:LEU:HD23	1:D:240:LEU:C	2.33	0.54
1:A:878:HIS:HD2	5:A:8676:HOH:O	1.90	0.54
1:D:114:VAL:HB	1:D:115:PRO:HD2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ASP:OD2	5:A:9405:HOH:O	2.19	0.54
1:A:817:GLN:HG2	5:A:8938:HOH:O	2.08	0.54
1:D:951:TRP:HB3	1:D:1018:LEU:HD11	1.89	0.54
1:B:859:ASP:OD1	1:B:861:SER:OG	2.23	0.54
1:A:108:THR:N	4:A:8419:DMS:H13	2.23	0.53
1:D:843:GLN:HG2	1:D:848:THR:CA	2.36	0.53
1:A:237:ARG:HG2	1:A:296:GLU:OE1	2.08	0.53
1:A:863:GLN:HG3	1:A:1021:CYS:CB	2.38	0.53
1:B:945:ASN:HB3	1:B:1023:LYS:HE2	1.89	0.53
1:B:687:GLN:HE21	1:B:687:GLN:H	1.53	0.53
1:C:778:THR:HG23	1:C:887:GLN:HB3	1.90	0.53
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.23	0.53
1:B:615:PRO:O	1:B:618:THR:HG22	2.08	0.53
1:B:70:PRO:HG2	1:B:78:LEU:HD21	1.91	0.53
1:B:673:ALA:HB1	1:B:674:PRO:HD2	1.90	0.53
4:C:8602:DMS:H12	5:C:9271:HOH:O	2.08	0.53
1:D:682:LEU:C	1:D:683:PRO:O	2.49	0.53
1:C:513:PRO:HG2	5:C:8615:HOH:O	2.08	0.53
1:D:46:ARG:HB3	1:D:47:PRO:CD	2.38	0.53
1:D:615:PRO:O	1:D:618:THR:HG22	2.08	0.53
1:A:252:ASP:CG	4:A:8416:DMS:H12	2.34	0.52
1:B:733:ALA:O	1:B:734:SER:O	2.28	0.52
1:D:580:GLU:O	1:D:580:GLU:OE1	2.27	0.52
1:A:783:GLN:HG2	1:A:881:ARG:HD2	1.90	0.52
1:A:809:ARG:HH21	1:A:877:PRO:HB3	1.74	0.52
1:B:78:LEU:HB3	1:B:80:GLU:HG3	1.92	0.52
1:D:237:ARG:NH1	1:D:296:GLU:OE1	2.43	0.52
1:B:663:LEU:C	1:B:663:LEU:HD22	2.35	0.52
1:B:317:THR:OG1	1:B:319:ASP:OD1	2.27	0.52
1:B:658:LEU:HD21	1:B:690:SER:HB3	1.92	0.52
1:C:599:ARG:NH2	1:C:795:VAL:CB	2.72	0.52
1:C:730:LEU:HB3	1:C:731:PRO:HD2	1.91	0.52
1:C:930:VAL:HA	1:C:973:ARG:HD3	1.91	0.52
1:B:749:ILE:HD12	1:B:749:ILE:N	2.25	0.51
1:A:637:GLU:OE2	1:A:677:LYS:HE3	2.10	0.51
1:A:316:HIS:CB	4:A:8406:DMS:H23	2.41	0.51
1:B:59:ARG:NH2	1:B:81:ALA:HB3	2.25	0.51
1:C:78:LEU:HB3	1:C:80:GLU:CD	2.35	0.51
1:C:634:GLN:CD	1:C:634:GLN:H	2.13	0.51
1:C:829:THR:C	1:C:830:LEU:HD23	2.35	0.51
1:A:742:THR:HG22	1:A:743:SER:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:632:SER:O	1:B:635:THR:N	2.37	0.51
1:D:292:ARG:NH1	4:D:8412:DMS:H23	2.25	0.51
1:D:729:THR:HG23	5:D:9324:HOH:O	2.11	0.51
1:B:296:GLU:OE1	1:B:296:GLU:HA	2.11	0.51
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.26	0.51
1:B:631:LEU:HD12	1:B:635:THR:O	2.11	0.50
1:D:653:HIS:ND1	1:D:701:VAL:HG21	2.26	0.50
1:B:542:MET:HA	1:B:604:ASN:HA	1.93	0.50
1:D:1022:GLN:HG3	1:D:1023:LYS:HG2	1.91	0.50
1:A:378:LEU:HD11	5:A:8867:HOH:O	2.11	0.50
4:A:8416:DMS:H12	5:A:9210:HOH:O	2.10	0.50
1:C:764:PHE:CE1	1:C:781:ARG:NH1	2.80	0.50
1:D:962:TYR:OH	4:D:8508:DMS:H11	2.10	0.50
1:A:673:ALA:HB1	1:A:674:PRO:HD2	1.92	0.50
1:B:651:LEU:HD23	1:B:651:LEU:C	2.36	0.50
1:C:718:GLN:HG2	4:C:8503:DMS:H12	1.92	0.50
1:C:833:ALA:HB1	1:C:858:ILE:O	2.11	0.50
1:D:114:VAL:HB	1:D:115:PRO:CD	2.42	0.50
1:A:890:GLN:CG	1:A:891:VAL:N	2.75	0.50
1:B:375:ASP:O	1:B:379:MET:HG3	2.12	0.50
1:C:275:GLY:O	4:C:8412:DMS:H12	2.12	0.50
1:C:127:PHE:CE2	1:C:184:LEU:HG	2.47	0.50
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.93	0.50
1:A:88:SER:HA	1:A:366:VAL:HG21	1.94	0.50
1:B:763:GLY:HA3	1:B:822:LEU:HD13	1.94	0.50
1:C:88:SER:HA	1:C:366:VAL:HG21	1.92	0.50
1:A:45:ASP:OD2	5:A:9168:HOH:O	2.20	0.50
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.94	0.50
1:C:699:ARG:NH2	5:C:9404:HOH:O	2.45	0.50
1:A:662:PRO:O	1:A:663:LEU:HD23	2.12	0.50
1:B:16:TRP:CG	1:B:189:LEU:CD1	2.94	0.50
1:A:559:TYR:CE2	1:B:522:LYS:HA	2.47	0.49
1:A:764:PHE:CE1	1:A:781:ARG:NH1	2.80	0.49
1:B:777:LEU:HG	1:B:889:ALA:HA	1.94	0.49
1:C:811:LYS:HZ3	1:C:811:LYS:HB2	1.78	0.49
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.24	0.49
4:D:8409:DMS:H23	5:D:9076:HOH:O	2.11	0.49
1:D:318:ALA:HB3	5:D:9568:HOH:O	2.12	0.49
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.30	0.49
1:A:851:ILE:O	1:A:870:VAL:HA	2.13	0.49
1:C:777:LEU:HG	1:C:889:ALA:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:LYS:HE2	5:C:9333:HOH:O	2.12	0.49
1:D:651:LEU:HD12	1:D:653:HIS:CE1	2.47	0.49
1:A:316:HIS:HB2	4:A:8406:DMS:H23	1.95	0.49
1:A:633:GLY:O	1:A:634:GLN:OE1	2.30	0.49
1:A:250:LEU:C	1:A:251:ARG:HG2	2.38	0.48
4:A:8502:DMS:H13	5:A:9284:HOH:O	2.12	0.48
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.95	0.48
1:D:73:TRP:CZ2	1:D:122:CYS:HB3	2.47	0.48
1:D:542:MET:HE2	1:D:790:ASP:CG	2.38	0.48
1:D:651:LEU:CD1	1:D:653:HIS:CE1	2.97	0.48
1:A:655:MET:HE2	1:A:656:VAL:O	2.12	0.48
1:B:807:VAL:CG1	1:B:808:GLU:N	2.75	0.48
1:C:734:SER:HB3	1:C:860:GLY:HA3	1.96	0.48
1:C:599:ARG:HH21	1:C:795:VAL:CB	2.25	0.48
1:C:819:GLU:H	1:C:819:GLU:HG2	1.45	0.48
1:D:687:GLN:CG	1:D:688:PRO:HD2	2.43	0.48
1:A:59:ARG:HG2	4:A:8502:DMS:C1	2.43	0.48
1:D:60:PHE:HA	1:D:122:CYS:O	2.14	0.48
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.49	0.48
1:C:79:PRO:HD2	1:C:80:GLU:OE2	2.14	0.48
1:C:811:LYS:NZ	1:C:811:LYS:HB2	2.29	0.48
1:D:340:GLY:O	1:D:561:ARG:HG2	2.14	0.48
1:D:379:MET:HB2	1:D:379:MET:HE2	1.40	0.48
1:B:730:LEU:H	1:B:730:LEU:HG	1.50	0.48
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.49	0.48
1:C:887:GLN:NE2	1:C:980:GLU:O	2.46	0.48
1:C:919:ASP:O	1:C:920:LEU:HD23	2.14	0.48
1:D:660:GLY:O	1:D:662:PRO:HD3	2.14	0.48
1:A:600:GLN:HE21	1:A:600:GLN:N	2.03	0.48
1:A:735:HIS:CD2	1:A:735:HIS:N	2.81	0.48
1:C:651:LEU:HD12	1:C:651:LEU:N	2.28	0.48
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.49	0.47
1:D:806:TRP:CD2	1:D:991:MET:HE1	2.49	0.47
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.95	0.47
1:C:387:VAL:HG22	5:C:9470:HOH:O	2.13	0.47
1:C:651:LEU:HD13	1:C:653:HIS:CE1	2.50	0.47
1:D:379:MET:HE1	1:D:407:LEU:HD11	1.93	0.47
1:D:893:GLU:O	1:D:893:GLU:HG2	2.13	0.47
1:C:133:TRP:CD1	4:C:8504:DMS:H21	2.49	0.47
1:C:687:GLN:CB	1:C:688:PRO:HD2	2.32	0.47
1:A:754:LYS:NZ	5:A:9390:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:LEU:HD11	1:A:855:THR:HB	1.95	0.47
1:B:645:ARG:NH2	1:B:648:ASP:OD1	2.47	0.47
1:D:379:MET:CE	1:D:407:LEU:HD11	2.45	0.47
1:A:290:THR:O	4:A:8412:DMS:H23	2.14	0.47
1:C:147:ASN:HA	1:C:148:SER:HA	1.64	0.47
1:C:356:ARG:HD2	1:C:379:MET:HE1	1.96	0.47
1:D:63:PHE:HB3	1:D:64:PRO:HD2	1.96	0.47
1:D:134:LEU:CA	4:D:8705:DMS:H23	2.41	0.47
1:A:433:LEU:N	1:A:434:PRO:CD	2.77	0.47
1:A:844:HIS:HD2	5:A:9350:HOH:O	1.98	0.47
1:B:568:TRP:CD2	1:B:569:ASP:HB3	2.49	0.47
1:C:989:PHE:CD1	1:C:989:PHE:N	2.83	0.47
1:A:241:GLU:OE2	1:A:292:ARG:NH2	2.48	0.47
1:A:506:VAL:CG1	1:A:521:LYS:HE3	2.45	0.47
1:A:521:LYS:HE2	5:A:9021:HOH:O	2.13	0.47
1:A:826:THR:OG1	1:A:837:THR:HB	2.15	0.47
1:C:292:ARG:HH12	4:C:8412:DMS:C2	2.27	0.47
1:C:356:ARG:HD2	1:C:379:MET:CE	2.45	0.47
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.50	0.47
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.15	0.47
1:D:664:ALA:HB3	1:D:685:LEU:CD2	2.40	0.47
1:A:32:PRO:CB	4:A:8404:DMS:C1	2.88	0.47
1:B:241:GLU:OE1	1:B:292:ARG:HG2	2.15	0.47
1:B:708:TRP:CZ2	4:B:8403:DMS:H13	2.50	0.47
1:C:70:PRO:HG2	1:C:78:LEU:HD21	1.96	0.47
1:C:658:LEU:O	1:C:659:ASP:C	2.55	0.47
1:D:36:TRP:HH2	4:D:8404:DMS:H21	1.80	0.47
1:B:962:TYR:OH	4:B:8508:DMS:H23	2.15	0.47
1:C:708:TRP:CZ2	4:C:8403:DMS:H13	2.50	0.47
1:D:667:GLU:C	1:D:668:VAL:HG23	2.39	0.47
1:A:369:GLU:O	1:A:373:VAL:HG23	2.15	0.46
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.15	0.46
1:B:319:ASP:OD1	1:B:320:GLY:N	2.47	0.46
1:D:513:PRO:O	1:D:514:ALA:HB3	2.14	0.46
1:B:127:PHE:CE2	1:B:184:LEU:HG	2.50	0.46
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.97	0.46
1:B:796:SER:HB3	1:B:999:TRP:HB3	1.97	0.46
1:D:521:LYS:HE2	5:D:9164:HOH:O	2.15	0.46
1:D:806:TRP:CE2	1:D:991:MET:HE1	2.50	0.46
1:A:126:THR:HA	1:A:182:ASN:O	2.15	0.46
1:A:434:PRO:HB3	1:D:434:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:8409:DMS:O	5:B:9107:HOH:O	2.21	0.46
1:C:599:ARG:NH2	1:C:795:VAL:CG1	2.78	0.46
1:C:745:MET:HE3	1:C:745:MET:CA	2.39	0.46
1:A:73:TRP:CE2	1:A:122:CYS:HB3	2.50	0.46
1:A:387:VAL:HG22	5:A:9450:HOH:O	2.15	0.46
1:A:809:ARG:NH2	1:A:877:PRO:HB3	2.30	0.46
1:C:296:GLU:HG2	4:C:8601:DMS:C1	2.46	0.46
1:C:610:ASP:O	1:C:611:ARG:HB2	2.16	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.15	0.46
1:A:843:GLN:HG2	1:A:847:LYS:C	2.41	0.46
1:B:216:HIS:CE1	4:B:8504:DMS:H21	2.50	0.46
1:D:858:ILE:CD1	1:D:858:ILE:N	2.79	0.46
1:D:961:ARG:NE	1:D:981:GLY:O	2.49	0.46
1:A:655:MET:HE1	1:A:662:PRO:CA	2.46	0.46
1:A:774:LYS:HB2	1:A:774:LYS:HE2	1.61	0.46
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.51	0.46
1:A:127:PHE:N	1:A:127:PHE:CD2	2.81	0.46
1:A:593:GLY:O	1:A:595:THR:HG22	2.14	0.46
1:C:619:GLU:HG2	1:C:909:ARG:HG3	1.98	0.46
1:C:651:LEU:HD12	1:C:651:LEU:H	1.80	0.46
1:C:843:GLN:HA	1:C:847:LYS:O	2.16	0.46
1:D:986:ILE:HD12	1:D:986:ILE:HG21	1.49	0.46
1:A:890:GLN:OE1	1:A:948:PRO:HD3	2.16	0.46
4:A:8410:DMS:H13	5:A:8859:HOH:O	2.14	0.46
1:B:637:GLU:OE2	1:B:677:LYS:HE2	2.15	0.46
1:C:843:GLN:HG2	1:C:848:THR:HA	1.97	0.46
1:D:682:LEU:O	1:D:683:PRO:O	2.34	0.46
1:D:736:ALA:HB3	1:D:751:LEU:HD11	1.98	0.46
4:B:8508:DMS:H13	5:B:8727:HOH:O	2.15	0.46
1:C:667:GLU:C	1:C:668:VAL:HG23	2.41	0.46
1:C:730:LEU:HD23	1:C:730:LEU:H	1.78	0.46
1:A:634:GLN:HE21	1:A:685:LEU:HD11	1.80	0.45
1:A:890:GLN:HG3	1:A:891:VAL:H	1.78	0.45
1:B:655:MET:HE3	1:B:662:PRO:HB3	1.95	0.45
1:C:266:GLN:NE2	4:C:8602:DMS:S	2.90	0.45
1:D:88:SER:HA	1:D:366:VAL:HG21	1.98	0.45
1:A:362:LEU:HA	1:A:362:LEU:HD22	1.68	0.45
1:C:16:TRP:CG	1:C:189:LEU:CD1	2.99	0.45
1:C:703:PRO:HD2	4:C:8425:DMS:C1	2.42	0.45
1:D:80:GLU:H	1:D:80:GLU:HG3	1.58	0.45
1:A:651:LEU:HD13	1:A:667:GLU:HG2	1.96	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:MET:HE2	1:A:662:PRO:HA	1.97	0.45
1:A:843:GLN:HG3	1:A:848:THR:CA	2.38	0.45
1:A:580:GLU:O	1:A:580:GLU:OE1	2.35	0.45
1:A:730:LEU:HD12	1:A:730:LEU:N	2.32	0.45
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.98	0.45
1:B:100:TYR:CE1	1:B:602:CYS:HB3	2.51	0.45
1:B:655:MET:SD	1:B:664:ALA:O	2.74	0.45
1:C:292:ARG:HH12	4:C:8412:DMS:H23	1.81	0.45
1:C:655:MET:O	1:C:655:MET:HG3	2.14	0.45
1:C:687:GLN:CB	1:C:688:PRO:CD	2.94	0.45
1:D:770:ILE:HD12	1:D:775:GLN:NE2	2.31	0.45
1:A:411:ASP:OD2	1:A:447:ASP:OD2	2.33	0.45
1:A:646:HIS:NE2	1:A:671:ASP:OD2	2.44	0.45
1:B:292:ARG:NH1	4:B:8412:DMS:C2	2.79	0.45
1:B:701:VAL:HG22	1:B:714:ILE:HG12	1.98	0.45
1:B:731:PRO:HB2	1:B:732:ALA:H	1.64	0.45
1:B:796:SER:OG	1:B:800:ARG:NH2	2.49	0.45
1:C:749:ILE:N	1:C:749:ILE:HD12	2.31	0.45
1:D:105:TYR:O	4:D:8419:DMS:O	2.34	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.51	0.45
1:A:241:GLU:CD	1:A:292:ARG:NH2	2.74	0.45
1:B:85:VAL:HG12	1:B:86:VAL:N	2.28	0.45
1:C:377:LEU:CD2	1:C:708:TRP:HA	2.47	0.45
1:D:441:THR:O	1:D:445:GLN:HG3	2.17	0.45
1:D:833:ALA:HB1	1:D:858:ILE:O	2.16	0.45
1:D:824:GLN:HB3	1:D:839:ALA:HB3	1.98	0.45
1:A:843:GLN:HA	1:A:847:LYS:O	2.17	0.45
1:C:100:TYR:CZ	1:C:602:CYS:HB3	2.51	0.45
1:A:241:GLU:CD	1:A:292:ARG:HH21	2.25	0.45
1:B:678:GLN:HG2	1:B:680:ILE:HD11	1.99	0.45
1:B:745:MET:N	1:B:745:MET:SD	2.88	0.45
1:C:250:LEU:O	1:C:251:ARG:HD3	2.16	0.45
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.98	0.45
1:D:420:MET:HB3	1:D:420:MET:HE3	1.75	0.45
1:B:731:PRO:O	1:B:732:ALA:HB2	2.16	0.45
1:C:569:ASP:O	1:C:605:GLY:HA2	2.17	0.45
1:D:549:PHE:CE2	1:D:620:ALA:HA	2.52	0.45
1:A:338:GLU:OE1	5:A:9270:HOH:O	2.21	0.44
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.52	0.44
1:B:668:VAL:HG12	1:B:669:PRO:O	2.17	0.44
1:C:656:VAL:O	1:C:663:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASN:HA	1:D:148:SER:HA	1.68	0.44
1:A:594:ASP:C	1:A:595:THR:HG22	2.41	0.44
1:C:601:PHE:CD1	1:C:796:SER:HA	2.51	0.44
1:C:785:THR:O	1:C:881:ARG:HD2	2.16	0.44
1:D:859:ASP:OD1	1:D:861:SER:OG	2.26	0.44
1:C:651:LEU:HD13	1:C:653:HIS:HE1	1.82	0.44
1:D:932:PRO:HD2	1:D:970:THR:O	2.17	0.44
1:B:142:ILE:HG12	1:B:170:GLU:HG2	2.00	0.44
1:C:78:LEU:HB3	1:C:80:GLU:OE2	2.18	0.44
1:C:712:GLY:O	1:C:713:HIS:C	2.57	0.44
1:B:80:GLU:H	1:B:80:GLU:HG2	1.18	0.44
1:B:233:ASP:HA	4:B:8417:DMS:H22	2.00	0.44
1:B:680:ILE:HD12	1:B:680:ILE:N	2.31	0.44
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	2.00	0.44
1:C:703:PRO:CD	4:C:8425:DMS:H12	2.43	0.44
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.53	0.44
1:B:835:LEU:HD11	1:B:855:THR:HB	1.98	0.44
1:A:655:MET:HE1	1:A:662:PRO:HA	1.99	0.44
1:B:88:SER:HA	1:B:366:VAL:HG21	2.00	0.44
1:B:360:HIS:ND1	1:B:361:PRO:HD2	2.33	0.44
1:D:933:SER:O	1:D:934:GLU:C	2.61	0.44
1:A:98:PRO:HB2	1:A:203:TRP:CE3	2.53	0.44
1:A:577:LYS:O	1:A:584:PRO:HA	2.18	0.44
1:A:658:LEU:O	1:A:659:ASP:C	2.61	0.44
1:B:920:LEU:HB3	1:B:921:PRO:HD2	2.00	0.44
1:A:850:PHE:HA	1:A:871:GLU:O	2.18	0.44
1:C:744:GLU:O	1:C:760:ARG:HD3	2.18	0.44
1:C:951:TRP:HA	1:C:1019:VAL:O	2.18	0.44
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.98	0.43
1:C:988:GLY:C	1:C:989:PHE:CD1	2.96	0.43
1:B:600:GLN:HE21	1:B:600:GLN:N	2.03	0.43
1:C:835:LEU:CD1	1:C:855:THR:HB	2.44	0.43
1:B:654:TRP:CE3	1:B:665:SER:HA	2.54	0.43
1:C:748:CYS:C	1:C:749:ILE:HD12	2.44	0.43
1:D:844:HIS:O	1:D:845:GLN:HB2	2.17	0.43
4:D:8503:DMS:O	5:D:8975:HOH:O	2.20	0.43
4:A:8404:DMS:H13	5:A:9018:HOH:O	2.18	0.43
1:B:687:GLN:HA	1:B:688:PRO:HD3	1.69	0.43
1:C:628:GLN:NE2	4:C:8402:DMS:O	2.45	0.43
1:A:362:LEU:O	1:A:362:LEU:HD13	2.18	0.43
1:A:735:HIS:O	1:A:736:ALA:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PHE:O	4:B:8417:DMS:H23	2.18	0.43
1:C:808:GLU:HA	1:C:811:LYS:HZ1	1.80	0.43
1:D:100:TYR:OH	1:D:601:PHE:HB3	2.19	0.43
1:D:133:TRP:CD1	4:D:8703:DMS:H23	2.52	0.43
1:D:845:GLN:OE1	1:D:845:GLN:HA	2.18	0.43
1:A:105:TYR:CE2	1:A:199:ASP:HB2	2.54	0.43
1:A:231:PHE:O	4:A:8417:DMS:H23	2.18	0.43
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.01	0.43
1:B:73:TRP:CZ2	1:B:185:ALA:HB1	2.54	0.43
1:B:961:ARG:NH1	5:B:9162:HOH:O	2.33	0.43
1:D:433:LEU:N	1:D:434:PRO:CD	2.82	0.43
1:A:107:ILE:CG2	4:A:8410:DMS:H23	2.41	0.43
1:A:977:HIS:O	1:A:978:ALA:C	2.56	0.43
1:B:147:ASN:HA	1:B:148:SER:HA	1.54	0.43
1:B:601:PHE:CD1	1:B:796:SER:HA	2.54	0.43
1:B:670:LEU:HA	1:B:670:LEU:HD23	1.35	0.43
1:B:773:LYS:N	1:B:773:LYS:CD	2.79	0.43
1:C:651:LEU:HD13	1:C:701:VAL:HB	2.01	0.43
1:A:587:ALA:HB1	1:A:591:ASP:HB2	2.01	0.43
1:A:682:LEU:HD23	1:A:682:LEU:HA	1.83	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:B:730:LEU:CB	1:B:731:PRO:CD	2.97	0.43
1:C:372:MET:HE1	1:C:395:HIS:HB3	1.99	0.43
1:D:708:TRP:CH2	4:D:8403:DMS:H13	2.53	0.43
1:A:427:THR:HG22	1:A:436:MET:SD	2.59	0.43
1:B:216:HIS:ND1	4:B:8504:DMS:H21	2.34	0.43
1:B:647:SER:OG	1:B:672:VAL:HG23	2.18	0.43
1:B:669:PRO:CB	5:B:9418:HOH:O	2.66	0.43
1:D:237:ARG:NH1	1:D:237:ARG:CG	2.79	0.43
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.83	0.43
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.47	0.43
1:D:305:ILE:HD11	1:D:645:ARG:HB3	2.01	0.42
1:D:581:ASN:N	1:D:581:ASN:OD1	2.51	0.42
1:A:240:LEU:C	1:A:240:LEU:HD23	2.44	0.42
1:A:949:HIS:O	1:A:1023:LYS:NZ	2.53	0.42
1:C:246:MET:SD	1:C:246:MET:C	3.02	0.42
1:C:730:LEU:N	1:C:730:LEU:CD2	2.81	0.42
1:C:820:ALA:HB2	1:C:842:TRP:CE2	2.54	0.42
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.42
1:A:436:MET:O	1:A:437:SER:C	2.62	0.42
1:B:872:VAL:O	1:B:873:ALA:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:753:ASN:CG	1:C:754:LYS:HZ3	2.28	0.42
1:D:427:THR:HG22	1:D:436:MET:SD	2.59	0.42
1:A:494:THR:CB	1:D:473:ARG:NH2	2.75	0.42
1:A:749:ILE:N	1:A:749:ILE:CD1	2.79	0.42
1:B:336:ARG:HD3	5:B:9199:HOH:O	2.19	0.42
1:C:545:SER:O	1:C:909:ARG:HD3	2.19	0.42
1:B:577:LYS:O	1:B:584:PRO:HA	2.18	0.42
1:B:815:HIS:CD2	1:B:849:LEU:HD13	2.55	0.42
1:A:854:LYS:HA	1:A:867:THR:O	2.19	0.42
1:B:262:GLN:NE2	1:B:262:GLN:C	2.78	0.42
1:B:661:LYS:HA	1:B:662:PRO:HD3	1.52	0.42
1:C:655:MET:SD	1:C:657:ALA:HB2	2.60	0.42
1:A:781:ARG:NH1	5:A:9274:HOH:O	2.53	0.42
1:B:104:THR:HB	5:B:9533:HOH:O	2.19	0.42
1:B:708:TRP:CH2	4:B:8403:DMS:H13	2.54	0.42
1:B:773:LYS:HD3	1:B:773:LYS:N	2.35	0.42
1:C:49:GLN:HG2	5:C:9432:HOH:O	2.19	0.42
1:D:682:LEU:O	1:D:683:PRO:C	2.60	0.42
1:D:780:LEU:HA	1:D:886:CYS:HB3	2.02	0.42
1:A:57:GLU:HB3	1:A:83:THR:CG2	2.50	0.42
1:A:357:HIS:CD2	5:A:9479:HOH:O	2.72	0.42
1:A:632:SER:O	1:A:633:GLY:C	2.62	0.42
1:B:127:PHE:CD2	1:B:127:PHE:N	2.88	0.42
1:B:569:ASP:O	1:B:605:GLY:HA2	2.19	0.42
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.51	0.42
1:D:814:GLY:HA3	1:D:844:HIS:CG	2.55	0.42
1:A:390:SER:HA	1:A:391:HIS:HA	1.85	0.42
1:A:473:ARG:HD3	5:D:8713:HOH:O	2.18	0.42
1:A:950:GLN:OE1	1:A:952:ARG:NE	2.37	0.42
1:D:78:LEU:HD23	1:D:78:LEU:HA	1.75	0.42
1:D:664:ALA:CB	1:D:685:LEU:HD21	2.44	0.42
1:A:35:SER:HB2	1:A:217:LYS:HD3	2.02	0.42
4:B:8403:DMS:H21	5:B:8899:HOH:O	2.19	0.42
1:C:387:VAL:HG13	5:C:9470:HOH:O	2.19	0.42
1:C:533:LEU:C	1:C:533:LEU:HD23	2.45	0.42
1:C:718:GLN:HG2	4:C:8503:DMS:C1	2.50	0.42
1:D:739:HIS:O	1:D:749:ILE:HA	2.19	0.42
1:C:50:GLN:CD	1:C:50:GLN:N	2.78	0.41
1:B:937:LEU:HA	1:B:957:PHE:O	2.20	0.41
1:A:637:GLU:CD	1:A:677:LYS:HE3	2.45	0.41
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:VAL:HG12	1:B:613:PRO:HA	2.02	0.41
1:B:908:ASP:HB3	1:B:1007:PHE:CD1	2.55	0.41
1:C:59:ARG:NH2	1:C:81:ALA:HB3	2.34	0.41
1:C:770:ILE:HD12	1:C:775:GLN:CG	2.50	0.41
1:D:390:SER:HA	1:D:391:HIS:HA	1.94	0.41
1:A:753:ASN:OD1	1:A:753:ASN:N	2.51	0.41
1:C:363:HIS:HD2	5:C:9179:HOH:O	2.02	0.41
1:B:181:GLU:OE2	5:B:9427:HOH:O	2.22	0.41
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.39	0.41
1:B:568:TRP:CD1	1:B:568:TRP:C	2.98	0.41
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.02	0.41
1:C:685:LEU:HA	1:C:686:PRO:HD3	1.52	0.41
1:C:745:MET:CE	1:C:745:MET:CA	2.96	0.41
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.02	0.41
1:D:599:ARG:HH11	1:D:599:ARG:HD2	1.66	0.41
1:D:663:LEU:HD22	1:D:694:LEU:HD21	2.02	0.41
1:B:531:ARG:HB3	1:B:532:PRO:HD2	2.01	0.41
1:B:733:ALA:O	1:B:734:SER:C	2.63	0.41
1:C:472:TYR:OH	1:C:476:LYS:HE2	2.21	0.41
1:C:515:VAL:N	1:C:516:PRO:CD	2.83	0.41
1:D:878:HIS:HE1	5:D:9360:HOH:O	2.02	0.41
1:B:687:GLN:NE2	1:B:687:GLN:CA	2.83	0.41
1:B:777:LEU:HD23	1:B:777:LEU:HA	1.90	0.41
1:D:506:VAL:CG1	1:D:521:LYS:HE3	2.51	0.41
1:D:997:ASP:HB2	1:D:999:TRP:CZ2	2.56	0.41
1:A:964:GLN:O	1:A:968:MET:HB2	2.21	0.41
1:B:85:VAL:CG1	1:B:86:VAL:N	2.82	0.41
1:B:773:LYS:HA	1:B:773:LYS:HD2	1.68	0.41
1:B:977:HIS:CD2	1:B:977:HIS:C	2.98	0.41
1:C:577:LYS:HB3	1:C:577:LYS:HE3	1.91	0.41
1:C:753:ASN:N	1:C:753:ASN:OD1	2.52	0.41
1:C:806:TRP:CD2	1:C:991:MET:HE1	2.56	0.41
1:C:910:LEU:HD12	1:C:910:LEU:C	2.46	0.41
1:A:699:ARG:HH11	1:A:699:ARG:HD2	1.74	0.41
1:A:764:PHE:CD1	1:A:781:ARG:NH1	2.89	0.41
1:B:13:ARG:HD3	1:B:13:ARG:HA	1.78	0.41
1:B:681:GLU:H	1:B:681:GLU:HG2	1.67	0.41
1:B:782:ASP:OD1	1:B:854:LYS:NZ	2.52	0.41
1:C:584:PRO:O	4:C:8411:DMS:H23	2.20	0.41
1:D:225:PHE:HA	1:D:243:GLU:O	2.21	0.41
1:D:367:MET:HE2	1:D:372:MET:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:533:LEU:C	1:D:533:LEU:HD23	2.45	0.41
1:C:1022:GLN:HE21	1:C:1022:GLN:HB3	1.57	0.41
1:A:988:GLY:C	1:A:989:PHE:CD1	2.99	0.40
1:B:654:TRP:O	1:B:665:SER:HB2	2.20	0.40
1:B:807:VAL:HG13	1:B:808:GLU:N	2.35	0.40
1:B:1022:GLN:NE2	1:B:1023:LYS:O	2.52	0.40
1:C:872:VAL:O	1:C:873:ALA:C	2.63	0.40
1:D:843:GLN:HG3	1:D:848:THR:HA	2.02	0.40
1:C:878:HIS:CE1	1:C:1010:SER:HB3	2.56	0.40
1:D:733:ALA:O	1:D:735:HIS:ND1	2.53	0.40
1:A:200:GLN:HG2	1:A:391:HIS:HB2	2.02	0.40
1:A:615:PRO:O	1:A:618:THR:HG22	2.22	0.40
1:A:634:GLN:NE2	1:A:682:LEU:HD12	2.36	0.40
1:A:703:PRO:HG2	4:A:8425:DMS:C1	2.43	0.40
1:A:952:ARG:NH2	1:A:1021:CYS:SG	2.94	0.40
1:B:46:ARG:HH11	1:B:46:ARG:HD2	1.78	0.40
1:C:16:TRP:CD2	1:C:189:LEU:CD1	3.04	0.40
1:C:634:GLN:OE1	1:C:681:GLU:HG2	2.21	0.40
1:C:781:ARG:HG2	1:C:781:ARG:HH11	1.85	0.40
1:D:651:LEU:C	1:D:651:LEU:CD1	2.86	0.40
1:D:687:GLN:HA	1:D:688:PRO:HD3	1.61	0.40
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.69	0.40
1:A:995:GLY:C	1:A:997:ASP:N	2.78	0.40
1:B:114:VAL:HB	1:B:115:PRO:CD	2.51	0.40
1:C:100:TYR:CE2	1:C:602:CYS:HB3	2.56	0.40
1:C:654:TRP:NE1	1:C:666:GLY:HA3	2.35	0.40
1:D:844:HIS:O	1:D:845:GLN:C	2.61	0.40
1:A:246:MET:C	1:A:246:MET:SD	3.05	0.40
1:A:891:VAL:HG23	1:A:981:GLY:HA2	2.02	0.40
1:B:16:TRP:CD2	1:B:189:LEU:CD1	3.04	0.40
1:B:378:LEU:HD23	1:B:378:LEU:HA	1.96	0.40
1:B:379:MET:CE	1:B:407:LEU:CD1	2.99	0.40
1:B:634:GLN:CG	1:B:682:LEU:HB2	2.47	0.40
1:C:670:LEU:HA	1:C:670:LEU:HD23	1.85	0.40
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1006/1023 (98%)	972 (97%)	33 (3%)	1 (0%)	48	27
1	B	1005/1023 (98%)	962 (96%)	36 (4%)	7 (1%)	18	6
1	C	1003/1023 (98%)	968 (96%)	32 (3%)	3 (0%)	36	20
1	D	1004/1023 (98%)	961 (96%)	39 (4%)	4 (0%)	30	14
All	All	4018/4092 (98%)	3863 (96%)	140 (4%)	15 (0%)	30	14

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	690	SER
1	B	731	PRO
1	B	732	ALA
1	B	734	SER
1	D	688	PRO
1	C	734	SER
1	D	734	SER
1	A	688	PRO
1	B	688	PRO
1	B	733	ALA
1	D	164	ASP
1	B	164	ASP
1	C	687	GLN
1	C	732	ALA
1	D	683	PRO

5.3.2 Protein sidechains

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	863/875 (99%)	831 (96%)	32 (4%)	30	10
1	B	863/875 (99%)	822 (95%)	41 (5%)	23	6
1	C	861/875 (98%)	825 (96%)	36 (4%)	26	7
1	D	862/875 (98%)	817 (95%)	45 (5%)	21	5
All	All	3449/3500 (98%)	3295 (96%)	154 (4%)	24	7

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	71	GLU
1	A	117	GLU
1	A	130	ASP
1	A	250	LEU
1	A	277	GLU
1	A	362	LEU
1	A	370	GLN
1	A	377	LEU
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	595	THR
1	A	600	GLN
1	A	655	MET
1	A	684	GLU
1	A	685	LEU
1	A	735	HIS
1	A	737	ILE
1	A	749	ILE
1	A	755	ARG
1	A	773	LYS
1	A	800	ARG
1	A	817	GLN
1	A	829	THR
1	A	843	GLN
1	A	847	LYS
1	A	885	ASN
1	A	956	GLN
1	A	986	ILE
1	A	1017	GLN

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Mol	Chain	Res	Type
1	A	1023	LYS
1	B	13	ARG
1	B	49	GLN
1	B	71	GLU
1	B	80	GLU
1	B	211	ASP
1	B	230	ARG
1	B	237	ARG
1	B	251	ARG
1	B	262	GLN
1	B	344	LEU
1	B	367	MET
1	B	370	GLN
1	B	546	LEU
1	B	595	THR
1	B	599	ARG
1	B	600	GLN
1	B	630	ARG
1	B	646	HIS
1	B	651	LEU
1	B	661	LYS
1	B	663	LEU
1	B	670	LEU
1	B	672	VAL
1	B	681	GLU
1	B	687	GLN
1	B	689	GLU
1	B	690	SER
1	B	730	LEU
1	B	734	SER
1	B	737	ILE
1	B	745	MET
1	B	766	SER
1	B	773	LYS
1	B	795	VAL
1	B	800	ARG
1	B	804	ASN
1	B	847	LYS
1	B	890	GLN
1	B	1017	GLN
1	B	1022	GLN
1	B	1023	LYS

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Mol	Chain	Res	Type
1	C	75	GLU
1	C	80	GLU
1	C	117	GLU
1	C	136	GLU
1	C	178	ARG
1	C	262	GLN
1	C	264	GLU
1	C	278	ILE
1	C	344	LEU
1	C	362	LEU
1	C	519	SER
1	C	546	LEU
1	C	595	THR
1	C	630	ARG
1	C	634	GLN
1	C	651	LEU
1	C	653	HIS
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	684	GLU
1	C	685	LEU
1	C	687	GLN
1	C	690	SER
1	C	699	ARG
1	C	730	LEU
1	C	737	ILE
1	C	745	MET
1	C	750	GLU
1	C	804	ASN
1	C	819	GLU
1	C	847	LYS
1	C	956	GLN
1	C	986	ILE
1	C	1022	GLN
1	C	1023	LYS
1	D	71	GLU
1	D	80	GLU
1	D	128	ASN
1	D	230	ARG
1	D	237	ARG
1	D	249	GLU

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Mol	Chain	Res	Type
1	D	277	GLU
1	D	319	ASP
1	D	362	LEU
1	D	370	GLN
1	D	511	PRO
1	D	519	SER
1	D	546	LEU
1	D	580	GLU
1	D	630	ARG
1	D	632	SER
1	D	651	LEU
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	672	VAL
1	D	681	GLU
1	D	684	GLU
1	D	685	LEU
1	D	687	GLN
1	D	689	GLU
1	D	730	LEU
1	D	734	SER
1	D	737	ILE
1	D	754	LYS
1	D	755	ARG
1	D	761	GLN
1	D	772	ASP
1	D	773	LYS
1	D	817	GLN
1	D	829	THR
1	D	849	LEU
1	D	858	ILE
1	D	859	ASP
1	D	910	LEU
1	D	956	GLN
1	D	986	ILE
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	262	GLN
1	A	266	GLN
1	A	363	HIS
1	A	445	GLN
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	653	HIS
1	A	735	HIS
1	A	817	GLN
1	A	844	HIS
1	A	878	HIS
1	B	262	GLN
1	B	363	HIS
1	B	370	GLN
1	B	485	GLN
1	B	554	GLN
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	675	GLN
1	B	687	GLN
1	B	757	GLN
1	B	844	HIS
1	B	878	HIS
1	B	903	GLN
1	B	977	HIS
1	C	163	GLN
1	C	363	HIS
1	C	394	ASN
1	C	445	GLN
1	C	485	GLN
1	C	624	GLN
1	C	646	HIS
1	C	653	HIS
1	C	687	GLN
1	C	783	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	C	1022	GLN
1	D	163	GLN

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Mol	Chain	Res	Type
1	D	624	GLN
1	D	634	GLN
1	D	757	GLN
1	D	761	GLN
1	D	775	GLN
1	D	878	HIS
1	D	950	GLN
1	D	977	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 113 ligands modelled in this entry, 28 are monoatomic - leaving 85 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	$\# Z > 2$
4	DMS	B	8409	-	3,3,3	2.74	1 (33%)	3,3,3	0.58	0
4	DMS	D	8410	-	3,3,3	1.98	1 (33%)	3,3,3	0.25	0
4	DMS	B	8408	-	3,3,3	1.29	0	3,3,3	0.09	0
4	DMS	C	8403	-	3,3,3	1.45	1 (33%)	3,3,3	0.32	0
4	DMS	C	8409	-	3,3,3	2.20	1 (33%)	3,3,3	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	B	8601	-	3,3,3	2.57	1 (33%)	3,3,3	0.80	0
4	DMS	A	8402	-	3,3,3	1.23	0	3,3,3	0.76	0
4	DMS	D	8416	-	3,3,3	0.28	0	3,3,3	0.54	0
4	DMS	C	8404	-	3,3,3	1.32	0	3,3,3	1.11	0
4	DMS	A	8412	-	3,3,3	2.14	1 (33%)	3,3,3	0.48	0
4	DMS	D	8413	-	3,3,3	0.84	0	3,3,3	0.03	0
4	DMS	C	8601	-	3,3,3	0.66	0	3,3,3	0.52	0
4	DMS	A	8419	-	3,3,3	1.13	0	3,3,3	0.40	0
4	DMS	A	8410	-	3,3,3	0.58	0	3,3,3	0.55	0
4	DMS	A	8421	-	3,3,3	1.00	0	3,3,3	0.77	0
4	DMS	B	8425	3	3,3,3	1.14	0	3,3,3	0.41	0
4	DMS	D	8411	-	3,3,3	1.39	0	3,3,3	0.22	0
4	DMS	A	8404	-	3,3,3	1.53	1 (33%)	3,3,3	0.58	0
4	DMS	B	8401	-	3,3,3	0.98	0	3,3,3	0.43	0
4	DMS	A	8602	-	3,3,3	0.73	0	3,3,3	0.22	0
4	DMS	A	8501	-	3,3,3	0.78	0	3,3,3	0.43	0
4	DMS	B	8502	-	3,3,3	1.53	0	3,3,3	1.23	1 (33%)
4	DMS	C	8401	-	3,3,3	1.79	1 (33%)	3,3,3	0.39	0
4	DMS	D	8419	-	3,3,3	0.59	0	3,3,3	0.49	0
4	DMS	A	8414	-	3,3,3	0.42	0	3,3,3	0.20	0
4	DMS	B	8504	-	3,3,3	0.39	0	3,3,3	0.11	0
4	DMS	A	8401	-	3,3,3	1.23	0	3,3,3	0.53	0
4	DMS	A	8403	-	3,3,3	1.82	1 (33%)	3,3,3	0.65	0
4	DMS	A	8409	-	3,3,3	2.40	2 (66%)	3,3,3	0.52	0
4	DMS	C	8411	-	3,3,3	1.16	0	3,3,3	0.30	0
4	DMS	A	8417	-	3,3,3	1.02	0	3,3,3	0.80	0
4	DMS	D	8402	-	3,3,3	1.39	0	3,3,3	0.23	0
4	DMS	C	8602	-	3,3,3	0.58	0	3,3,3	0.22	0
4	DMS	D	8412	-	3,3,3	1.67	1 (33%)	3,3,3	0.54	0
4	DMS	C	8501	-	3,3,3	1.58	1 (33%)	3,3,3	0.77	0
4	DMS	D	8406	-	3,3,3	0.88	0	3,3,3	0.53	0
4	DMS	B	8414	-	3,3,3	1.06	0	3,3,3	0.39	0
4	DMS	A	8504	-	3,3,3	0.97	0	3,3,3	0.42	0
4	DMS	C	8402	-	3,3,3	2.28	1 (33%)	3,3,3	0.16	0
4	DMS	D	8403	-	3,3,3	1.30	0	3,3,3	0.34	0
4	DMS	D	8409	-	3,3,3	2.00	1 (33%)	3,3,3	1.40	1 (33%)
4	DMS	D	8705	-	3,3,3	2.01	1 (33%)	3,3,3	0.31	0
4	DMS	B	8412	-	3,3,3	0.90	0	3,3,3	0.25	0
4	DMS	A	8408	-	3,3,3	0.58	0	3,3,3	0.34	0
4	DMS	B	8417	-	3,3,3	0.85	0	3,3,3	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	D	8404	-	3,3,3	1.21	0	3,3,3	0.51	0
4	DMS	A	8503	-	3,3,3	1.08	0	3,3,3	0.75	0
4	DMS	C	8425	3	3,3,3	1.07	0	3,3,3	0.12	0
4	DMS	B	8403	-	3,3,3	1.13	0	3,3,3	0.14	0
4	DMS	B	8402	-	3,3,3	1.85	1 (33%)	3,3,3	1.28	1 (33%)
4	DMS	D	8417	-	3,3,3	0.47	0	3,3,3	0.22	0
4	DMS	D	8405	-	3,3,3	0.81	0	3,3,3	0.50	0
4	DMS	D	8701	-	3,3,3	1.55	1 (33%)	3,3,3	0.46	0
4	DMS	D	8501	-	3,3,3	0.85	0	3,3,3	0.37	0
4	DMS	B	8404	-	3,3,3	1.02	0	3,3,3	0.51	0
4	DMS	D	8508	-	3,3,3	1.42	0	3,3,3	0.90	0
4	DMS	C	8413	-	3,3,3	0.72	0	3,3,3	0.29	0
4	DMS	D	8408	-	3,3,3	1.35	1 (33%)	3,3,3	0.26	0
4	DMS	D	8503	-	3,3,3	0.69	0	3,3,3	0.79	0
4	DMS	A	8502	-	3,3,3	2.15	1 (33%)	3,3,3	1.01	0
4	DMS	C	8503	-	3,3,3	0.87	0	3,3,3	1.44	1 (33%)
4	DMS	B	8421	-	3,3,3	0.59	0	3,3,3	0.38	0
4	DMS	C	8421	-	3,3,3	1.25	0	3,3,3	0.57	0
4	DMS	D	8421	-	3,3,3	0.33	0	3,3,3	0.49	0
4	DMS	B	8416	-	3,3,3	1.02	0	3,3,3	0.25	0
4	DMS	C	8408	-	3,3,3	0.77	0	3,3,3	1.10	0
4	DMS	A	8405	-	3,3,3	1.32	1 (33%)	3,3,3	0.45	0
4	DMS	C	8417	-	3,3,3	0.28	0	3,3,3	0.42	0
4	DMS	C	8416	-	3,3,3	0.69	0	3,3,3	0.31	0
4	DMS	D	8414	-	3,3,3	0.40	0	3,3,3	0.55	0
4	DMS	C	8405	-	3,3,3	2.67	2 (66%)	3,3,3	0.26	0
4	DMS	C	8414	-	3,3,3	1.81	1 (33%)	3,3,3	1.20	0
4	DMS	A	8411	-	3,3,3	1.54	1 (33%)	3,3,3	0.49	0
4	DMS	C	8504	-	3,3,3	1.26	0	3,3,3	1.09	0
4	DMS	A	8425	3	3,3,3	1.24	0	3,3,3	0.71	0
4	DMS	B	8508	-	3,3,3	2.11	1 (33%)	3,3,3	0.81	0
4	DMS	C	8410	-	3,3,3	0.70	0	3,3,3	0.16	0
4	DMS	D	8703	-	3,3,3	0.84	0	3,3,3	0.27	0
4	DMS	A	8416	-	3,3,3	2.10	2 (66%)	3,3,3	0.62	0
4	DMS	A	8406	-	3,3,3	1.85	1 (33%)	3,3,3	0.42	0
4	DMS	B	8411	-	3,3,3	0.55	0	3,3,3	0.82	0
4	DMS	D	8401	-	3,3,3	1.69	1 (33%)	3,3,3	0.12	0
4	DMS	C	8412	-	3,3,3	1.22	0	3,3,3	1.38	1 (33%)
4	DMS	B	8405	-	3,3,3	2.28	1 (33%)	3,3,3	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	DMS	D	8425	3	3,3,3	0.97	0	3,3,3	0.37	0

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	8409	DMS	O-S	4.71	1.81	1.50
4	C	8405	DMS	O-S	4.02	1.76	1.50
4	B	8601	DMS	C2-S	3.89	2.03	1.76
4	C	8409	DMS	O-S	3.75	1.75	1.50
4	B	8405	DMS	O-S	3.61	1.74	1.50
4	A	8409	DMS	O-S	3.43	1.72	1.50
4	A	8502	DMS	C1-S	3.43	2.00	1.76
4	C	8402	DMS	C2-S	3.27	1.99	1.76
4	A	8406	DMS	C2-S	-3.13	1.53	1.76
4	A	8412	DMS	C1-S	3.12	1.98	1.76
4	B	8508	DMS	C1-S	2.97	1.97	1.76
4	D	8409	DMS	O-S	2.95	1.69	1.50
4	A	8416	DMS	O-S	-2.90	1.31	1.50
4	D	8705	DMS	C1-S	-2.81	1.55	1.76
4	A	8403	DMS	C2-S	2.80	1.96	1.76
4	B	8402	DMS	C2-S	2.75	1.95	1.76
4	C	8401	DMS	C2-S	2.43	1.93	1.76
4	D	8410	DMS	C2-S	2.40	1.93	1.76
4	C	8403	DMS	O-S	2.36	1.65	1.50
4	C	8414	DMS	O-S	-2.35	1.34	1.50
4	C	8501	DMS	C1-S	-2.34	1.59	1.76
4	A	8405	DMS	O-S	2.26	1.65	1.50
4	C	8405	DMS	C1-S	2.26	1.92	1.76
4	D	8701	DMS	C1-S	2.24	1.92	1.76
4	A	8416	DMS	C1-S	-2.20	1.60	1.76
4	A	8404	DMS	O-S	-2.19	1.35	1.50
4	D	8401	DMS	O-S	2.15	1.64	1.50
4	D	8412	DMS	O-S	2.12	1.64	1.50
4	D	8408	DMS	C1-S	2.06	1.90	1.76
4	A	8409	DMS	C1-S	2.06	1.90	1.76
4	A	8411	DMS	C1-S	2.02	1.90	1.76

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8503	DMS	C2-S-C1	2.40	110.74	98.42
4	D	8409	DMS	C2-S-C1	2.37	110.58	98.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	8412	DMS	C2-S-C1	2.36	110.50	98.42
4	B	8402	DMS	C2-S-C1	2.17	109.55	98.42
4	B	8502	DMS	C2-S-C1	2.13	109.32	98.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

46 monomers are involved in 89 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	8409	DMS	1	0
4	C	8403	DMS	1	0
4	B	8601	DMS	1	0
4	A	8412	DMS	1	0
4	D	8413	DMS	1	0
4	C	8601	DMS	2	0
4	A	8419	DMS	4	0
4	A	8410	DMS	3	0
4	A	8404	DMS	4	0
4	A	8602	DMS	1	0
4	D	8419	DMS	1	0
4	A	8414	DMS	1	0
4	B	8504	DMS	3	0
4	A	8403	DMS	1	0
4	C	8411	DMS	1	0
4	A	8417	DMS	2	0
4	C	8602	DMS	2	0
4	D	8412	DMS	3	0
4	D	8406	DMS	1	0
4	C	8402	DMS	1	0
4	D	8403	DMS	2	0
4	D	8409	DMS	1	0
4	D	8705	DMS	2	0
4	B	8412	DMS	1	0
4	B	8417	DMS	2	0
4	D	8404	DMS	1	0
4	A	8503	DMS	1	0
4	C	8425	DMS	7	0
4	B	8403	DMS	3	0
4	D	8417	DMS	1	0
4	D	8508	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	8413	DMS	2	0
4	D	8503	DMS	1	0
4	A	8502	DMS	2	0
4	C	8503	DMS	3	0
4	D	8421	DMS	2	0
4	C	8417	DMS	1	0
4	C	8504	DMS	2	0
4	A	8425	DMS	2	0
4	B	8508	DMS	2	0
4	C	8410	DMS	1	0
4	D	8703	DMS	5	0
4	A	8416	DMS	3	0
4	A	8406	DMS	2	0
4	B	8411	DMS	1	0
4	C	8412	DMS	3	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	1010/1023 (98%)	-0.15	36 (3%)	46	48	9, 18, 47, 97	0
1	B	1009/1023 (98%)	-0.19	34 (3%)	48	50	9, 17, 44, 94	0
1	C	1007/1023 (98%)	-0.25	25 (2%)	58	61	8, 17, 45, 99	0
1	D	1008/1023 (98%)	-0.19	41 (4%)	41	43	9, 17, 46, 94	0
All	All	4034/4092 (98%)	-0.19	136 (3%)	48	50	8, 17, 45, 99	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	VAL	6.7
1	A	798	ALA	6.2
1	B	730	LEU	5.9
1	B	685	LEU	4.8
1	D	736	ALA	4.7
1	C	732	ALA	4.4
1	D	733	ALA	4.3
1	A	686	PRO	4.3
1	C	685	LEU	4.2
1	A	730	LEU	4.2
1	B	745	MET	4.2
1	A	829	THR	4.1
1	C	730	LEU	4.1
1	A	688	PRO	4.0
1	D	686	PRO	4.0
1	C	687	GLN	4.0
1	C	733	ALA	4.0
1	B	686	PRO	3.9
1	A	801	ILE	3.9
1	C	736	ALA	3.9
1	B	731	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	686	PRO	3.8
1	D	685	LEU	3.8
1	B	732	ALA	3.7
1	B	1022	GLN	3.7
1	B	1023	LYS	3.6
1	C	735	HIS	3.6
1	A	732	ALA	3.6
1	A	634	GLN	3.6
1	A	1023	LYS	3.5
1	D	730	LEU	3.5
1	A	685	LEU	3.5
1	D	735	HIS	3.5
1	C	820	ALA	3.4
1	D	801	ILE	3.4
1	A	735	HIS	3.4
1	A	731	PRO	3.4
1	A	729	THR	3.3
1	D	732	ALA	3.3
1	A	771	GLY	3.2
1	B	801	ILE	3.2
1	C	1022	GLN	3.2
1	D	634	GLN	3.2
1	C	761	GLN	3.2
1	B	737	ILE	3.1
1	B	663	LEU	3.1
1	A	737	ILE	3.0
1	C	731	PRO	3.0
1	C	689	GLU	3.0
1	A	733	ALA	3.0
1	B	733	ALA	3.0
1	C	795	VAL	3.0
1	B	862	GLY	3.0
1	D	1023	LYS	2.9
1	C	797	GLU	2.9
1	D	690	SER	2.9
1	D	71	GLU	2.9
1	B	734	SER	2.9
1	B	735	HIS	2.9
1	A	846	GLY	2.8
1	B	819	GLU	2.8
1	C	1023	LYS	2.8
1	D	1018	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	737	ILE	2.8
1	B	800	ARG	2.8
1	D	684	GLU	2.8
1	A	689	GLU	2.7
1	B	687	GLN	2.7
1	C	663	LEU	2.7
1	B	729	THR	2.7
1	D	687	GLN	2.7
1	D	731	PRO	2.6
1	D	737	ILE	2.6
1	D	734	SER	2.6
1	A	79	PRO	2.6
1	B	817	GLN	2.6
1	D	683	PRO	2.6
1	D	688	PRO	2.6
1	A	687	GLN	2.5
1	D	666	GLY	2.5
1	B	653	HIS	2.5
1	B	47	PRO	2.5
1	B	795	VAL	2.5
1	D	80	GLU	2.5
1	D	771	GLY	2.4
1	D	820	ALA	2.4
1	A	583	ASN	2.4
1	B	684	GLU	2.4
1	D	773	LYS	2.4
1	D	846	GLY	2.4
1	D	845	GLN	2.4
1	C	601	PHE	2.4
1	D	797	GLU	2.4
1	A	845	GLN	2.3
1	A	684	GLU	2.3
1	B	578	TYR	2.3
1	B	804	ASN	2.3
1	A	580	GLU	2.3
1	A	772	ASP	2.3
1	D	831	ALA	2.3
1	B	80	GLU	2.3
1	D	681	GLU	2.3
1	D	755	ARG	2.3
1	A	847	LYS	2.3
1	A	683	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	632	SER	2.3
1	C	821	ALA	2.2
1	A	831	ALA	2.2
1	B	818	ALA	2.2
1	B	659	ASP	2.2
1	D	829	THR	2.2
1	A	664	ALA	2.2
1	B	654	TRP	2.2
1	D	651	LEU	2.2
1	B	728	VAL	2.1
1	A	794	ALA	2.1
1	A	655	MET	2.1
1	C	729	THR	2.1
1	B	634	GLN	2.1
1	B	845	GLN	2.1
1	D	599	ARG	2.1
1	B	771	GLY	2.1
1	A	682	LEU	2.1
1	C	842	TRP	2.1
1	D	75	GLU	2.1
1	D	729	THR	2.1
1	A	669	PRO	2.1
1	A	601	PHE	2.1
1	D	770	ILE	2.1
1	D	76	CYS	2.1
1	D	362	LEU	2.1
1	C	770	ILE	2.1
1	C	684	GLU	2.0
1	A	977	HIS	2.0
1	C	1017	GLN	2.0
1	D	847	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	DMS	A	8421	4/4	0.75	0.21	35,58,84,100	0
4	DMS	C	8504	4/4	0.75	0.23	36,68,72,73	0
4	DMS	C	8413	4/4	0.76	0.21	42,69,100,100	0
4	DMS	C	8503	4/4	0.79	0.17	30,35,46,59	0
4	DMS	D	8419	4/4	0.80	0.22	54,72,74,95	0
4	DMS	D	8425	4/4	0.82	0.20	16,27,33,36	4
4	DMS	D	8421	4/4	0.83	0.20	42,61,71,100	0
4	DMS	A	8503	4/4	0.84	0.25	41,50,94,100	0
2	MG	C	3004	1/1	0.84	0.16	52,52,52,52	0
4	DMS	C	8601	4/4	0.84	0.21	49,50,73,100	0
4	DMS	D	8417	4/4	0.85	0.17	26,32,41,100	0
4	DMS	D	8503	4/4	0.85	0.21	43,44,59,100	0
4	DMS	D	8703	4/4	0.85	0.22	37,58,59,100	0
2	MG	A	3005	1/1	0.86	0.10	42,42,42,42	0
4	DMS	D	8416	4/4	0.86	0.15	25,43,52,77	0
4	DMS	A	8417	4/4	0.86	0.20	26,26,68,100	0
4	DMS	B	8508	4/4	0.86	0.14	36,41,50,64	0
4	DMS	B	8421	4/4	0.87	0.16	32,60,64,68	0
4	DMS	A	8502	4/4	0.87	0.18	23,38,48,83	0
4	DMS	C	8602	4/4	0.87	0.18	25,45,68,100	0
4	DMS	A	8419	4/4	0.87	0.22	65,67,69,100	0
4	DMS	D	8508	4/4	0.87	0.16	39,47,52,59	0
4	DMS	B	8417	4/4	0.87	0.15	31,39,48,62	0
4	DMS	A	8425	4/4	0.88	0.15	29,37,46,51	0
4	DMS	D	8413	4/4	0.88	0.17	28,56,73,100	0
4	DMS	A	8416	4/4	0.88	0.15	20,39,63,71	0
4	DMS	B	8425	4/4	0.88	0.13	32,33,41,56	0
4	DMS	A	8404	4/4	0.88	0.13	19,26,41,49	0
4	DMS	D	8705	4/4	0.88	0.16	18,50,52,67	0
4	DMS	D	8501	4/4	0.89	0.11	25,33,43,59	0
4	DMS	C	8421	4/4	0.90	0.15	41,44,60,65	0
4	DMS	D	8414	4/4	0.90	0.20	33,50,100,100	0
4	DMS	D	8410	4/4	0.90	0.14	40,52,57,60	0
4	DMS	C	8417	4/4	0.91	0.12	33,36,45,63	0
4	DMS	A	8602	4/4	0.91	0.19	35,49,98,100	0
4	DMS	C	8425	4/4	0.91	0.19	44,50,66,88	0
4	DMS	C	8501	4/4	0.91	0.14	27,31,39,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	A	8414	4/4	0.91	0.19	22,43,69,100	0
4	DMS	A	8406	4/4	0.91	0.15	12,45,59,77	0
4	DMS	C	8414	4/4	0.91	0.10	23,25,34,42	0
4	DMS	C	8416	4/4	0.92	0.15	44,51,52,100	0
4	DMS	D	8409	4/4	0.92	0.11	24,33,33,40	0
3	NA	D	3104	1/1	0.92	0.12	35,35,35,35	0
4	DMS	B	8404	4/4	0.93	0.15	24,29,41,100	0
3	NA	A	3104	1/1	0.93	0.12	29,29,29,29	0
4	DMS	A	8501	4/4	0.93	0.10	20,25,41,42	0
4	DMS	A	8410	4/4	0.93	0.17	41,49,78,100	0
4	DMS	B	8504	4/4	0.93	0.15	30,33,44,82	0
4	DMS	A	8412	4/4	0.93	0.16	28,33,41,100	0
4	DMS	B	8601	4/4	0.93	0.13	33,36,39,39	0
3	NA	D	3103	1/1	0.93	0.14	36,36,36,36	0
3	NA	C	3104	1/1	0.94	0.09	28,28,28,28	0
3	NA	A	3103	1/1	0.94	0.11	38,38,38,38	0
4	DMS	A	8408	4/4	0.94	0.13	21,34,39,80	0
3	NA	B	3104	1/1	0.94	0.12	33,33,33,33	0
4	DMS	B	8408	4/4	0.94	0.15	33,34,35,100	0
4	DMS	B	8409	4/4	0.94	0.09	21,26,39,44	0
4	DMS	C	8410	4/4	0.94	0.12	26,40,42,49	0
4	DMS	B	8416	4/4	0.94	0.10	32,33,42,49	0
4	DMS	D	8406	4/4	0.95	0.11	21,25,26,42	0
4	DMS	A	8411	4/4	0.95	0.11	25,34,36,44	0
4	DMS	B	8414	4/4	0.95	0.10	25,36,42,46	0
4	DMS	B	8502	4/4	0.95	0.09	22,27,37,41	0
4	DMS	D	8404	4/4	0.95	0.10	22,27,43,76	0
4	DMS	A	8409	4/4	0.96	0.07	23,25,28,41	0
4	DMS	C	8405	4/4	0.96	0.10	28,31,31,36	0
4	DMS	C	8408	4/4	0.96	0.09	26,28,34,40	0
4	DMS	C	8409	4/4	0.96	0.08	29,30,33,36	0
4	DMS	A	8504	4/4	0.96	0.12	23,40,44,77	0
2	MG	D	3005	1/1	0.96	0.06	26,26,26,26	0
2	MG	C	3006	1/1	0.96	0.07	31,31,31,31	0
4	DMS	B	8405	4/4	0.96	0.11	31,36,37,40	0
4	DMS	B	8412	4/4	0.97	0.07	26,29,33,36	0
4	DMS	B	8402	4/4	0.97	0.07	16,16,21,22	0
4	DMS	C	8411	4/4	0.97	0.13	25,31,31,100	0
4	DMS	D	8408	4/4	0.97	0.08	18,30,35,45	0
4	DMS	C	8412	4/4	0.97	0.10	30,37,38,41	0
4	DMS	C	8404	4/4	0.97	0.08	17,23,30,37	0
4	DMS	D	8411	4/4	0.97	0.12	31,33,34,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	DMS	D	8412	4/4	0.97	0.11	27,27,35,100	0
4	DMS	D	8701	4/4	0.97	0.13	15,18,24,53	0
4	DMS	B	8403	4/4	0.97	0.07	22,23,28,30	0
4	DMS	B	8411	4/4	0.97	0.10	33,34,34,46	0
3	NA	B	3103	1/1	0.98	0.07	26,26,26,26	0
4	DMS	A	8402	4/4	0.98	0.07	15,17,23,36	0
4	DMS	A	8403	4/4	0.98	0.07	21,23,28,29	0
2	MG	A	3002	1/1	0.98	0.04	17,17,17,17	0
4	DMS	D	8401	4/4	0.98	0.06	14,17,19,20	0
4	DMS	D	8402	4/4	0.98	0.06	12,20,21,23	0
4	DMS	D	8403	4/4	0.98	0.06	21,26,28,31	0
3	NA	C	3103	1/1	0.98	0.09	27,27,27,27	0
4	DMS	D	8405	4/4	0.98	0.09	24,25,39,45	0
4	DMS	C	8402	4/4	0.98	0.07	16,16,23,25	0
4	DMS	B	8401	4/4	0.98	0.07	16,19,21,23	0
3	NA	A	3101	1/1	0.98	0.09	23,23,23,23	0
3	NA	D	3101	1/1	0.98	0.09	24,24,24,24	0
3	NA	B	3101	1/1	0.98	0.08	17,17,17,17	0
4	DMS	C	8401	4/4	0.99	0.06	14,15,19,20	0
3	NA	B	3102	1/1	0.99	0.06	13,13,13,13	0
4	DMS	C	8403	4/4	0.99	0.06	16,21,24,30	0
2	MG	D	3002	1/1	0.99	0.04	16,16,16,16	0
2	MG	B	3002	1/1	0.99	0.03	15,15,15,15	0
4	DMS	A	8405	4/4	0.99	0.05	25,25,26,29	0
3	NA	C	3101	1/1	0.99	0.04	18,18,18,18	0
3	NA	C	3102	1/1	0.99	0.05	14,14,14,14	0
2	MG	C	3002	1/1	0.99	0.02	13,13,13,13	0
3	NA	A	3102	1/1	0.99	0.03	12,12,12,12	0
2	MG	A	3001	1/1	0.99	0.03	17,17,17,17	0
3	NA	D	3102	1/1	0.99	0.03	12,12,12,12	0
2	MG	B	3001	1/1	0.99	0.07	14,14,14,14	0
2	MG	D	3001	1/1	0.99	0.04	14,14,14,14	0
4	DMS	A	8401	4/4	0.99	0.04	12,15,15,17	0
2	MG	C	3001	1/1	1.00	0.09	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.