



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:46 AM UTC

PDB ID : 3I3B / pdb_00003i3b
Title : E.coli (lacZ) Beta-Galactosidase (M542A) in Complex with D-Galactopyranosyl-1-on
Authors : Dugdale, M.L.; Dymianiw, D.; Minhas, B.; Huber, R.E.
Deposited on : 2009-06-30
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

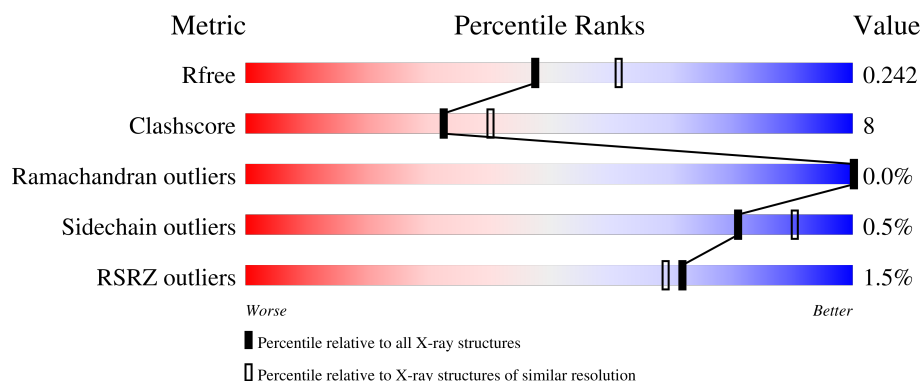
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	1023	2% 77% 22% .
1	B	1023	% 75% 23% ..
1	C	1023	2% 80% 18% ..
1	D	1023	% 79% 19% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36275 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
			8122	5136	1440	1509	37			
1	B	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	C	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			
1	D	1011	Total	C	N	O	S	0	0	0
			8122	5136	1440	1509	37			

There are 36 discrepancies between the modelled and reference sequences:

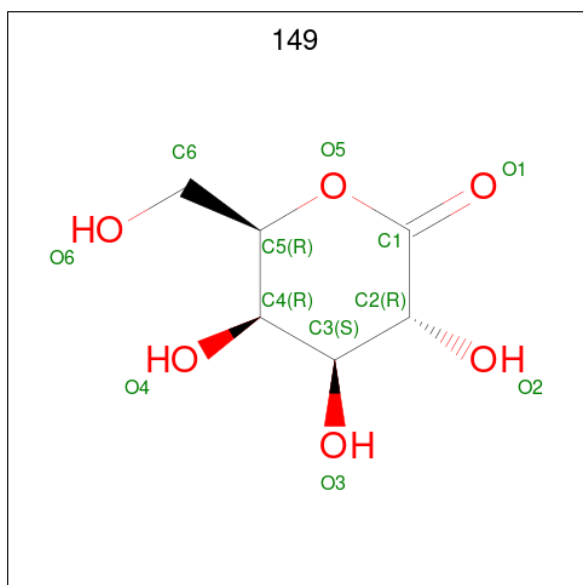
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP B8LFD6
A	2	SER	-	expression tag	UNP B8LFD6
A	3	HIS	-	expression tag	UNP B8LFD6
A	4	MET	-	expression tag	UNP B8LFD6
A	5	LEU	-	expression tag	UNP B8LFD6
A	6	GLU	-	expression tag	UNP B8LFD6
A	7	ASP	-	expression tag	UNP B8LFD6
A	8	PRO	-	expression tag	UNP B8LFD6
A	542	ALA	MET	engineered mutation	UNP B8LFD6
B	1	GLY	-	expression tag	UNP B8LFD6
B	2	SER	-	expression tag	UNP B8LFD6
B	3	HIS	-	expression tag	UNP B8LFD6
B	4	MET	-	expression tag	UNP B8LFD6
B	5	LEU	-	expression tag	UNP B8LFD6
B	6	GLU	-	expression tag	UNP B8LFD6
B	7	ASP	-	expression tag	UNP B8LFD6
B	8	PRO	-	expression tag	UNP B8LFD6
B	542	ALA	MET	engineered mutation	UNP B8LFD6
C	1	GLY	-	expression tag	UNP B8LFD6
C	2	SER	-	expression tag	UNP B8LFD6
C	3	HIS	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	-	expression tag	UNP B8LFD6
C	5	LEU	-	expression tag	UNP B8LFD6
C	6	GLU	-	expression tag	UNP B8LFD6
C	7	ASP	-	expression tag	UNP B8LFD6
C	8	PRO	-	expression tag	UNP B8LFD6
C	542	ALA	MET	engineered mutation	UNP B8LFD6
D	1	GLY	-	expression tag	UNP B8LFD6
D	2	SER	-	expression tag	UNP B8LFD6
D	3	HIS	-	expression tag	UNP B8LFD6
D	4	MET	-	expression tag	UNP B8LFD6
D	5	LEU	-	expression tag	UNP B8LFD6
D	6	GLU	-	expression tag	UNP B8LFD6
D	7	ASP	-	expression tag	UNP B8LFD6
D	8	PRO	-	expression tag	UNP B8LFD6
D	542	ALA	MET	engineered mutation	UNP B8LFD6

- Molecule 2 is D-galactonolactone (CCD ID: 149) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		

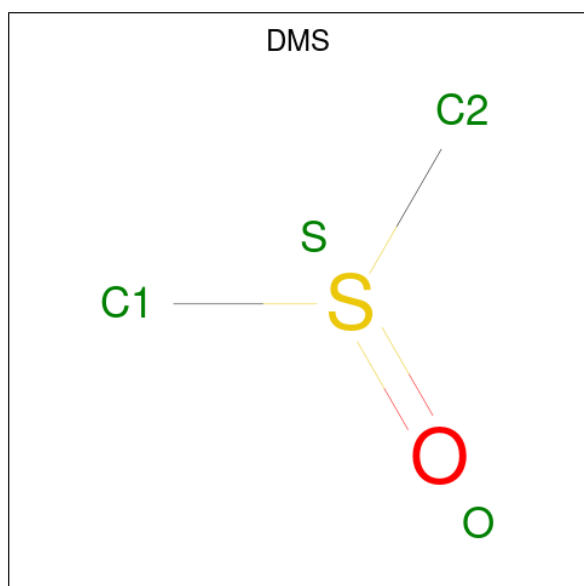
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

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

- 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		

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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	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0
5	B	1	Total 4	C 2	O 1	S 1	0	0

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

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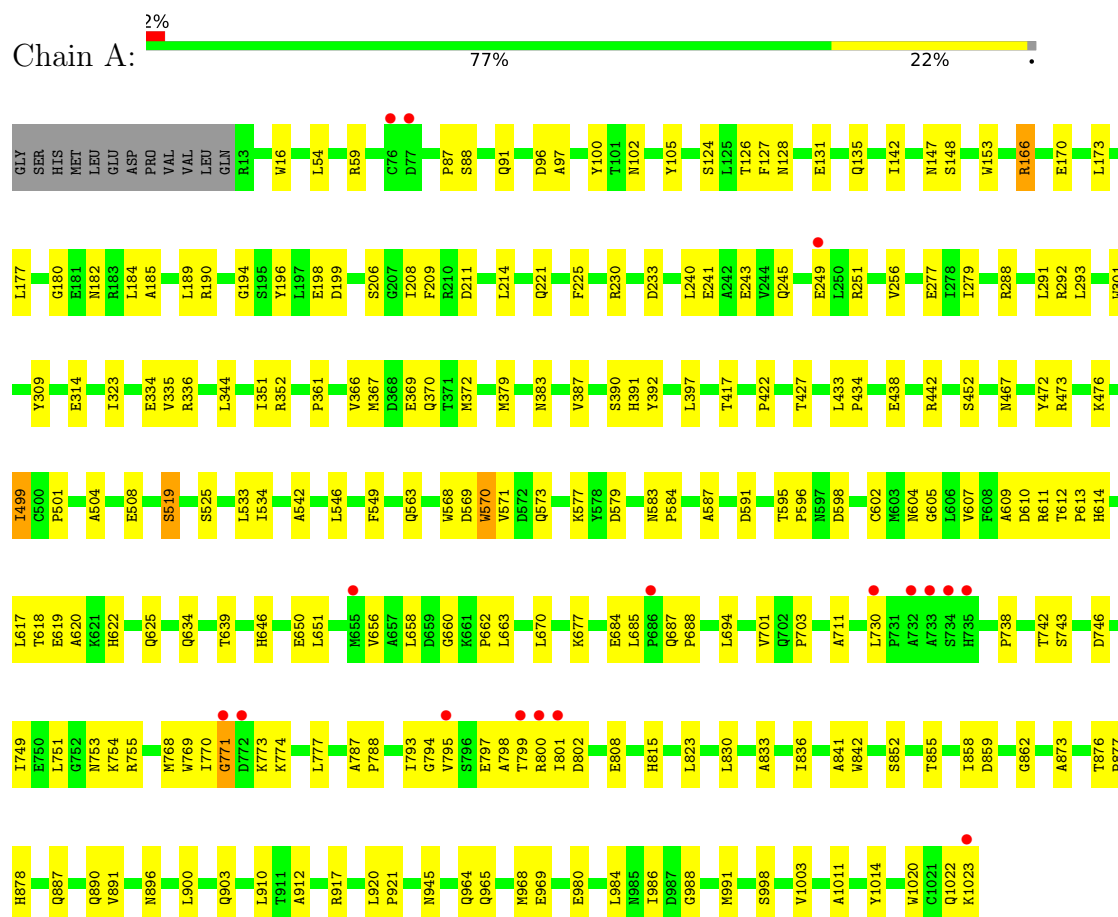
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	798	Total 798	O 798	0	0
6	B	821	Total 821	O 821	0	0
6	C	785	Total 785	O 785	0	0
6	D	804	Total 804	O 804	0	0

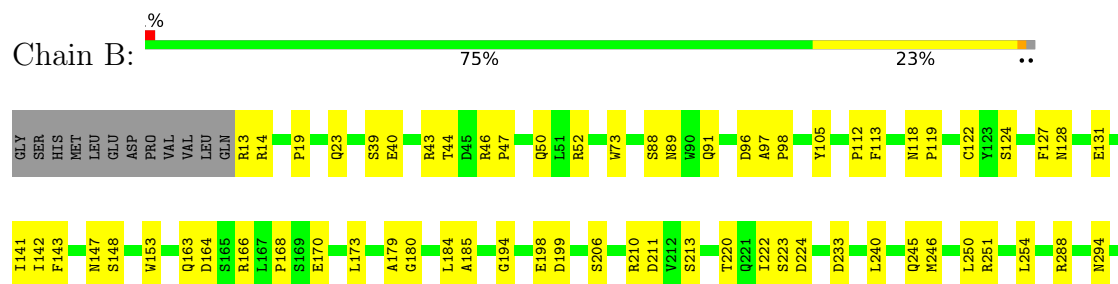
3 Residue-property plots [i](#)

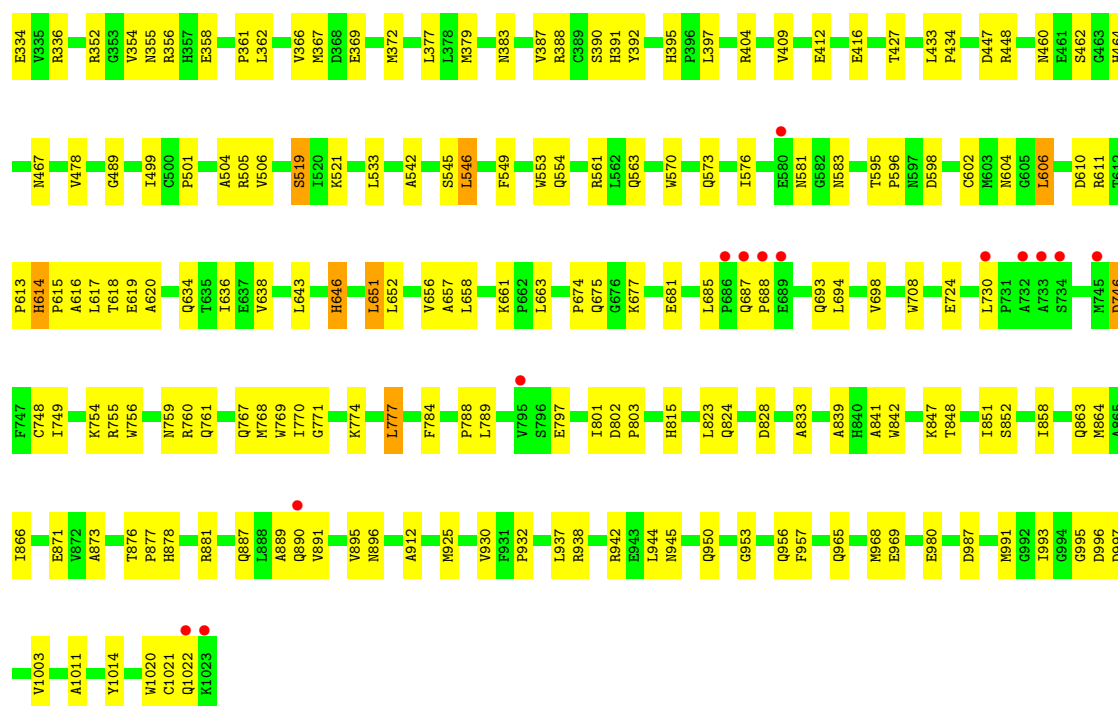
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-galactosidase

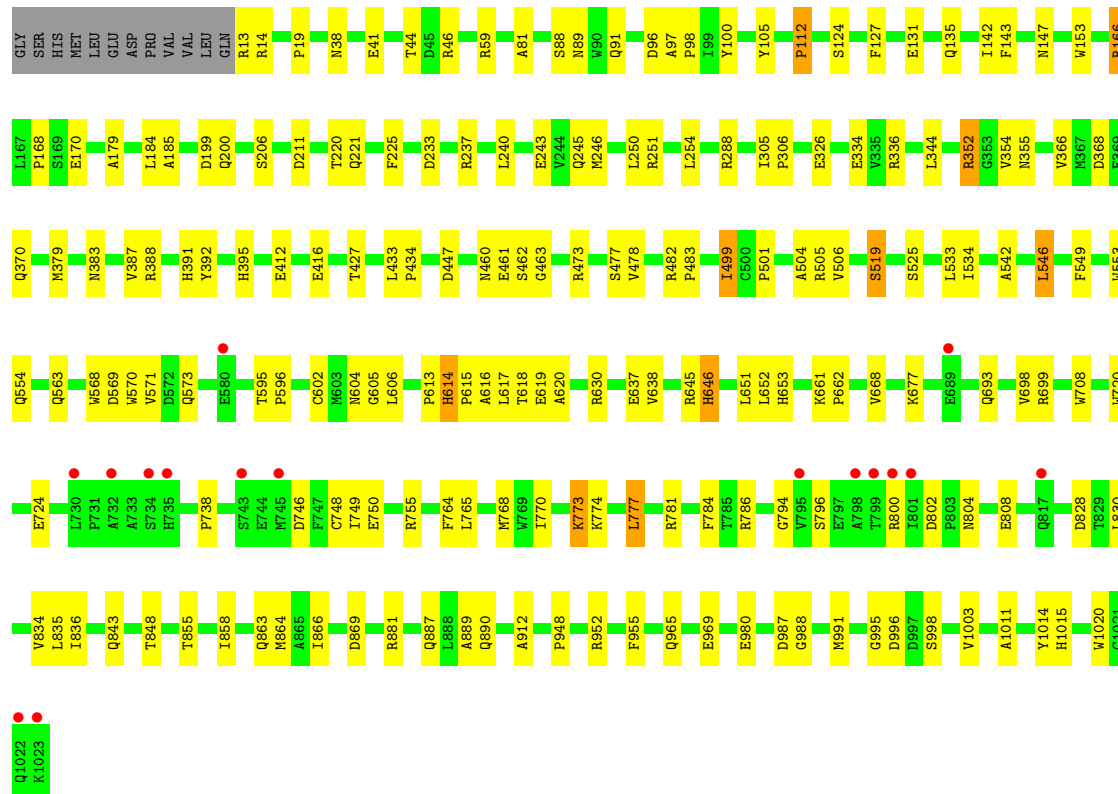
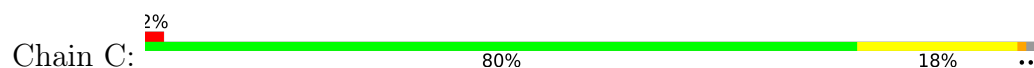


• Molecule 1: Beta-galactosidase





• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	149.60Å 168.42Å 201.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.18 – 2.20 14.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (14.18-2.20) 95.3 (14.18-2.20)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.00Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.244 0.191 , 0.242	Depositor DCC
R_{free} test set	3517 reflections (1.08%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.381	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36275	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.26 % 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 5.1383e-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: 149, NA, 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	0.37	0/8364	0.90	27/11412 (0.2%)
1	B	0.37	0/8364	0.90	31/11412 (0.3%)
1	C	0.37	0/8364	0.89	30/11412 (0.3%)
1	D	0.37	0/8364	0.89	28/11412 (0.2%)
All	All	0.37	0/33456	0.89	116/45648 (0.3%)

There are no bond length outliers.

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	771	GLY	N-CA-C	-10.12	102.36	111.67
1	B	614	HIS	N-CA-C	-8.63	99.09	110.40
1	C	614	HIS	N-CA-C	-8.59	98.85	110.36
1	A	614	HIS	N-CA-C	-8.21	99.36	110.36
1	C	570	TRP	N-CA-C	8.00	119.91	111.03
1	A	570	TRP	N-CA-C	7.86	119.75	111.03
1	C	988	GLY	N-CA-C	-7.76	102.23	113.86
1	D	614	HIS	N-CA-C	-7.51	100.30	110.36
1	B	233	ASP	N-CA-C	7.39	120.20	111.71
1	D	570	TRP	N-CA-C	7.24	119.06	111.03
1	B	746	ASP	N-CA-C	7.14	119.59	108.96
1	A	988	GLY	N-CA-C	-7.02	103.33	113.86
1	D	988	GLY	N-CA-C	-6.90	103.51	113.86
1	C	504	ALA	N-CA-C	-6.86	100.13	110.28
1	D	504	ALA	N-CA-C	-6.78	100.24	110.28
1	C	777	LEU	N-CA-C	-6.66	105.69	113.88
1	D	97	ALA	N-CA-C	6.65	118.45	110.07
1	C	770	ILE	N-CA-C	-6.56	97.28	106.53
1	B	570	TRP	N-CA-C	6.49	119.61	111.24
1	A	233	ASP	N-CA-C	6.30	118.95	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ASP	N-CA-C	6.26	118.38	110.24
1	A	97	ALA	N-CA-C	6.25	118.94	110.31
1	B	97	ALA	N-CA-C	6.23	117.65	109.93
1	C	97	ALA	N-CA-C	6.22	117.91	110.07
1	B	519	SER	N-CA-C	-6.21	101.23	110.23
1	B	222	ILE	N-CA-C	-6.20	99.37	108.54
1	A	504	ALA	N-CA-C	-6.17	101.15	110.28
1	C	383	ASN	N-CA-C	6.17	120.14	112.24
1	C	233	ASP	N-CA-C	6.15	118.77	111.33
1	A	519	SER	N-CA-C	-6.11	101.38	110.23
1	D	98	PRO	N-CA-C	-6.10	101.50	111.68
1	C	519	SER	N-CA-C	-6.04	101.48	110.23
1	C	605	GLY	N-CA-C	6.03	121.14	112.82
1	D	383	ASN	N-CA-C	5.93	119.75	111.74
1	C	166	ARG	N-CA-C	5.92	120.51	112.88
1	A	352	ARG	N-CA-C	-5.91	100.71	109.11
1	D	352	ARG	N-CA-C	-5.91	100.71	109.11
1	D	221	GLN	N-CA-C	5.88	117.90	109.14
1	C	211	ASP	N-CA-C	5.88	117.88	110.24
1	C	89	ASN	N-CA-C	-5.87	99.67	109.24
1	B	777	LEU	N-CA-C	-5.87	106.25	113.41
1	D	606	LEU	N-CA-C	-5.86	106.09	113.18
1	C	221	GLN	N-CA-C	5.86	117.86	109.14
1	D	499	ILE	N-CA-C	-5.84	100.29	108.12
1	A	903	GLN	N-CA-C	5.83	118.42	110.55
1	D	612	THR	N-CA-C	-5.81	102.46	109.83
1	D	777	LEU	N-CA-C	-5.80	106.55	113.97
1	D	233	ASP	N-CA-C	5.77	118.31	111.33
1	A	777	LEU	N-CA-C	-5.76	106.79	113.88
1	B	504	ALA	N-CA-C	-5.75	101.77	110.28
1	B	89	ASN	N-CA-C	-5.74	99.89	109.24
1	C	447	ASP	N-CA-C	5.70	120.94	113.30
1	A	646	HIS	N-CA-C	-5.68	102.11	110.52
1	D	563	GLN	N-CA-C	5.68	118.99	112.57
1	A	771	GLY	N-CA-C	-5.66	99.76	113.18
1	A	571	VAL	N-CA-C	5.66	116.89	108.46
1	D	220	THR	N-CA-C	-5.58	99.43	108.41
1	C	395	HIS	N-CA-C	-5.57	103.20	109.60
1	C	796	SER	N-CA-C	-5.56	106.16	113.17
1	B	554	GLN	N-CA-C	-5.54	105.32	111.36
1	C	506	VAL	N-CA-C	5.53	115.73	110.53
1	B	39	SER	N-CA-C	5.52	117.38	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	166	ARG	N-CA-C	5.52	119.59	112.41
1	A	383	ASN	N-CA-C	5.52	119.30	112.24
1	B	878	HIS	CA-C-N	5.51	125.41	119.85
1	B	878	HIS	C-N-CA	5.51	125.41	119.85
1	D	519	SER	N-CA-C	-5.49	102.27	110.23
1	D	571	VAL	N-CA-C	5.46	116.60	108.46
1	C	554	GLN	N-CA-C	-5.43	105.36	111.28
1	B	447	ASP	N-CA-C	5.41	119.99	113.17
1	D	447	ASP	N-CA-C	5.41	119.85	112.88
1	B	545	SER	N-CA-C	5.36	115.47	108.07
1	C	98	PRO	N-CA-C	-5.36	102.72	111.68
1	A	605	GLY	N-CA-C	5.36	120.21	112.82
1	B	646	HIS	N-CA-C	-5.35	102.61	110.52
1	D	166	ARG	N-CA-C	5.33	119.76	112.88
1	D	646	HIS	N-CA-C	-5.33	102.63	110.52
1	C	646	HIS	N-CA-C	-5.33	102.64	110.52
1	D	448	ARG	N-CA-C	5.32	118.86	112.38
1	C	352	ARG	N-CA-C	-5.31	101.57	109.11
1	A	746	ASP	N-CA-C	5.29	117.11	109.07
1	C	220	THR	N-CA-C	-5.29	99.90	108.41
1	A	309	TYR	N-CA-C	-5.28	101.73	109.81
1	C	563	GLN	N-CA-C	5.28	118.53	112.57
1	B	802	ASP	CA-C-N	5.27	125.08	119.28
1	B	802	ASP	C-N-CA	5.27	125.08	119.28
1	B	383	ASN	N-CA-C	5.25	118.96	112.24
1	A	499	ILE	N-CA-C	-5.25	101.09	108.12
1	A	323	ILE	N-CA-C	-5.22	106.59	111.45
1	B	98	PRO	N-CA-C	-5.22	102.40	111.32
1	A	211	ASP	N-CA-C	5.19	116.99	110.24
1	C	955	PHE	N-CA-C	5.19	116.18	108.86
1	D	956	GLN	N-CA-C	-5.18	101.43	109.72
1	B	606	LEU	N-CA-C	-5.18	106.47	112.89
1	C	412	GLU	N-CA-C	5.18	117.41	109.07
1	C	746	ASP	N-CA-C	5.17	116.93	109.07
1	D	788	PRO	N-CA-C	5.16	119.68	111.26
1	A	351	ILE	N-CA-C	5.16	115.03	108.12
1	A	612	THR	N-CA-C	-5.14	103.18	109.65
1	D	395	HIS	N-CA-C	-5.12	103.13	109.64
1	B	113	PHE	N-CA-C	5.12	118.05	110.48
1	D	309	TYR	N-CA-C	-5.11	101.99	109.81
1	C	571	VAL	N-CA-C	5.11	116.08	108.46
1	D	113	PHE	N-CA-C	5.11	117.71	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	GLU	N-CA-C	5.09	117.27	109.07
1	C	499	ILE	N-CA-C	-5.07	101.33	108.12
1	B	563	GLN	N-CA-C	5.05	118.28	112.57
1	B	395	HIS	N-CA-C	-5.05	103.79	109.60
1	A	563	GLN	N-CA-C	5.05	118.27	112.57
1	B	409	VAL	N-CA-C	5.03	115.73	108.48
1	A	878	HIS	CA-C-N	5.03	124.93	119.85
1	A	878	HIS	C-N-CA	5.03	124.93	119.85
1	D	525	SER	N-CA-C	5.02	119.09	112.92
1	B	220	THR	N-CA-C	-5.01	100.35	108.41
1	B	448	ARG	N-CA-C	5.00	118.48	112.38
1	A	787	ALA	N-CA-C	-5.00	100.83	109.58

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	8122	0	7711	142	0
1	B	8122	0	7712	145	0
1	C	8122	0	7712	120	0
1	D	8122	0	7712	114	0
2	A	12	0	9	0	0
2	B	12	0	9	0	0
2	C	12	0	9	0	0
2	D	12	0	9	0	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	120	0	180	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	132	0	198	5	0
5	C	132	0	198	5	0
5	D	120	0	180	2	0
6	A	798	0	0	2	0
6	B	821	0	0	4	0
6	C	785	0	0	2	0
6	D	804	0	0	4	0
All	All	36275	0	31639	509	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 8.

All (509) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HG12	1:A:170:GLU:HG2	1.42	1.01
1:A:249:GLU:CD	1:A:251:ARG:HE	1.68	1.01
1:C:142:ILE:HG12	1:C:170:GLU:HG2	1.59	0.82
1:A:730:LEU:HD21	1:B:823:LEU:O	1.82	0.80
1:A:147:ASN:HB3	1:A:206:SER:HA	1.63	0.79
1:A:102:ASN:HD21	5:A:5130:DMS:H22	1.47	0.79
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.63	0.79
1:B:767:GLN:NE2	1:B:774:LYS:HB3	2.00	0.77
1:C:765:LEU:HD21	1:C:768:MET:HE2	1.68	0.76
1:B:245:GLN:HG2	1:B:288:ARG:HG2	1.69	0.75
1:B:991:MET:HE3	1:B:1003:VAL:HG21	1.67	0.75
1:C:773:LYS:HE2	1:C:774:LYS:N	2.01	0.75
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.53	0.74
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.69	0.74
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.03	0.74
1:B:863:GLN:HG2	1:B:1021:CYS:HB3	1.69	0.74
1:C:44:THR:OG1	1:C:46:ARG:HD3	1.88	0.73
1:C:864:MET:HE3	1:C:866:ILE:HD11	1.70	0.73
1:D:88:SER:HA	1:D:366:VAL:HG21	1.71	0.72
1:D:863:GLN:HE22	1:D:952:ARG:HH21	1.37	0.70
1:A:241:GLU:HG2	1:A:292:ARG:HG2	1.73	0.70
1:A:245:GLN:HG2	1:A:288:ARG:HG2	1.74	0.70
1:A:768:MET:HE1	1:A:1020:TRP:CH2	2.26	0.69
1:B:52:ARG:O	1:B:213:SER:HB2	1.94	0.68
1:D:147:ASN:HB3	1:D:206:SER:HA	1.75	0.68
1:C:245:GLN:HG2	1:C:288:ARG:HG2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:HB3	1:A:1023:LYS:NZ	2.11	0.66
1:C:81:ALA:HA	5:C:5030:DMS:H12	1.77	0.66
1:B:890:GLN:HG2	1:B:891:VAL:N	2.12	0.65
1:D:965:GLN:O	1:D:969:GLU:HG3	1.95	0.65
1:A:54:LEU:HD11	1:A:214:LEU:HD13	1.78	0.65
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.31	0.65
1:C:473:ARG:HH12	1:C:477:SER:HB2	1.62	0.65
1:C:991:MET:HE3	1:C:1003:VAL:HG21	1.79	0.64
1:B:864:MET:HE3	1:B:866:ILE:HD11	1.79	0.64
1:C:1011:ALA:HB3	1:C:1014:TYR:CZ	2.33	0.64
1:A:579:ASP:OD2	1:A:583:ASN:HB2	1.97	0.64
1:C:237:ARG:NH1	1:C:237:ARG:HB3	2.12	0.64
1:D:749:ILE:HD12	1:D:749:ILE:N	2.13	0.64
1:A:88:SER:HA	1:A:366:VAL:HG21	1.79	0.64
1:A:788:PRO:HD2	1:A:968:MET:HG3	1.81	0.63
1:C:147:ASN:HB3	1:C:206:SER:HA	1.79	0.63
1:A:749:ILE:HD12	1:A:858:ILE:HD12	1.81	0.63
1:A:249:GLU:HG2	1:A:251:ARG:HG2	1.79	0.62
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.79	0.62
1:D:844:HIS:ND1	1:D:845:GLN:HG2	2.14	0.62
1:B:651:LEU:C	1:B:651:LEU:HD12	2.25	0.62
1:A:823:LEU:O	1:B:730:LEU:HD11	2.00	0.62
1:C:131:GLU:O	1:C:135:GLN:HG3	1.99	0.62
1:D:578:TYR:CE1	1:D:584:PRO:HB3	2.35	0.62
1:D:768:MET:HE1	1:D:1020:TRP:CH2	2.35	0.61
1:C:91:GLN:HG3	1:C:96:ASP:OD1	2.00	0.61
1:C:533:LEU:C	1:C:533:LEU:HD23	2.25	0.61
1:D:573:GLN:HB2	1:D:602:CYS:O	2.01	0.61
1:B:777:LEU:HG	1:B:889:ALA:HA	1.82	0.61
1:C:355:ASN:OD1	1:C:388:ARG:HD3	2.01	0.60
1:D:863:GLN:HE22	1:D:952:ARG:NH2	1.99	0.60
1:A:801:ILE:HD12	1:A:801:ILE:N	2.16	0.60
1:B:334:GLU:OE1	1:B:336:ARG:NH1	2.33	0.60
1:A:751:LEU:HD23	1:A:862:GLY:HA2	1.83	0.60
1:B:873:ALA:O	1:B:876:THR:HG22	2.01	0.59
1:C:887:GLN:NE2	1:C:980:GLU:O	2.35	0.59
1:A:965:GLN:O	1:A:969:GLU:HG3	2.02	0.59
1:B:1011:ALA:HB3	1:B:1014:TYR:CZ	2.37	0.59
1:C:473:ARG:NH1	1:C:477:SER:HB2	2.18	0.59
1:B:355:ASN:OD1	1:B:388:ARG:HD3	2.01	0.59
1:B:643:LEU:HD23	1:B:675:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LEU:HD12	6:D:4828:HOH:O	2.03	0.59
1:C:131:GLU:OE1	1:C:179:ALA:HB2	2.03	0.59
1:B:774:LYS:HB2	6:B:4851:HOH:O	2.03	0.59
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.85	0.58
1:A:131:GLU:O	1:A:135:GLN:HG2	2.03	0.58
1:C:166:ARG:HG3	1:C:392:TYR:HB2	1.84	0.58
1:D:793:ILE:HG22	1:D:795:VAL:HG22	1.84	0.58
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.83	0.58
1:D:379:MET:HE1	1:D:387:VAL:HB	1.83	0.58
1:D:656:VAL:HG21	1:D:685:LEU:HD13	1.84	0.58
1:A:102:ASN:ND2	5:A:5130:DMS:H22	2.17	0.58
1:B:754:LYS:HE2	1:B:1022:GLN:OE1	2.04	0.58
1:B:754:LYS:HE3	1:B:770:ILE:HG23	1.85	0.58
1:C:777:LEU:HG	1:C:889:ALA:HA	1.86	0.58
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.34	0.58
1:A:334:GLU:OE1	1:A:336:ARG:NH1	2.37	0.58
1:C:749:ILE:N	1:C:749:ILE:HD12	2.18	0.58
1:A:249:GLU:CG	1:A:251:ARG:HE	2.17	0.57
1:D:245:GLN:HG2	1:D:288:ARG:HG2	1.85	0.57
1:A:613:PRO:HB3	1:A:617:LEU:HD23	1.86	0.57
1:B:890:GLN:HG2	1:B:891:VAL:H	1.69	0.57
1:A:279:ILE:HD11	1:D:422:PRO:HG3	1.86	0.56
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.87	0.56
1:B:595:THR:HA	1:B:596:PRO:C	2.29	0.56
1:B:823:LEU:HD11	1:B:841:ALA:HB2	1.88	0.56
1:A:194:GLY:O	1:A:198:GLU:HG3	2.06	0.56
1:B:246:MET:HE3	1:B:250:LEU:HD23	1.87	0.56
1:A:292:ARG:HH12	5:A:5012:DMS:H13	1.71	0.56
1:B:759:ASN:OD1	1:B:761:GLN:HB3	2.06	0.56
1:D:615:PRO:O	1:D:618:THR:HG22	2.06	0.56
1:A:823:LEU:HD11	1:A:841:ALA:HB2	1.86	0.56
1:B:131:GLU:OE1	1:B:179:ALA:HB2	2.05	0.56
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.88	0.55
1:B:746:ASP:HA	1:B:760:ARG:HG3	1.88	0.55
1:D:595:THR:HA	1:D:596:PRO:C	2.32	0.55
1:B:769:TRP:NE1	1:B:774:LYS:HG2	2.22	0.55
1:D:768:MET:HE1	1:D:1020:TRP:CZ2	2.42	0.55
1:A:96:ASP:OD2	1:A:190:ARG:NH1	2.40	0.55
1:D:863:GLN:NE2	1:D:952:ARG:HH21	2.04	0.55
1:B:749:ILE:N	1:B:749:ILE:HD12	2.21	0.55
1:B:965:GLN:O	1:B:969:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:634:GLN:NE2	1:A:684:GLU:HA	2.21	0.55
1:B:573:GLN:HB2	1:B:602:CYS:O	2.06	0.55
1:C:240:LEU:C	1:C:240:LEU:HD23	2.31	0.55
1:D:499:ILE:HG22	1:D:501:PRO:HD3	1.88	0.55
1:B:688:PRO:HD3	1:B:694:LEU:HD11	1.89	0.55
1:D:881:ARG:HE	1:D:987:ASP:CG	2.14	0.55
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.17	0.55
1:A:533:LEU:C	1:A:533:LEU:HD23	2.32	0.54
1:A:472:TYR:O	1:A:476:LYS:HG2	2.07	0.54
1:C:88:SER:HA	1:C:366:VAL:HG21	1.90	0.54
1:C:863:GLN:NE2	1:C:952:ARG:NH2	2.55	0.54
1:B:88:SER:HA	1:B:366:VAL:HG21	1.87	0.54
1:A:651:LEU:C	1:A:651:LEU:HD12	2.32	0.54
1:B:784:PHE:HA	1:B:881:ARG:O	2.08	0.54
1:C:334:GLU:OE1	1:C:336:ARG:NH1	2.39	0.54
1:B:851:ILE:HB	1:B:871:GLU:HB2	1.90	0.53
1:D:890:GLN:HE22	1:D:948:PRO:HD3	1.73	0.53
1:B:404:ARG:HB3	5:B:5132:DMS:H12	1.89	0.53
1:D:945:ASN:OD1	1:D:950:GLN:HG3	2.09	0.53
1:A:105:TYR:CE1	1:A:199:ASP:HB2	2.44	0.53
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.43	0.53
1:A:292:ARG:C	1:A:293:LEU:HD12	2.33	0.53
1:B:369:GLU:HA	1:B:372:MET:HE3	1.91	0.53
1:C:750:GLU:OE2	1:C:755:ARG:HD2	2.09	0.53
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.53
1:B:652:LEU:HD11	1:B:698:VAL:HB	1.91	0.53
1:C:773:LYS:HE2	1:C:774:LYS:H	1.72	0.53
1:D:823:LEU:HD11	1:D:841:ALA:HB2	1.91	0.53
1:A:663:LEU:HD11	1:A:688:PRO:HB3	1.91	0.53
1:A:984:LEU:HD21	1:A:986:ILE:HD11	1.91	0.53
1:B:748:CYS:C	1:B:749:ILE:HD12	2.34	0.53
1:C:352:ARG:HG2	1:C:553:TRP:CH2	2.43	0.53
1:A:196:TYR:O	1:A:417:THR:HG22	2.09	0.53
1:B:887:GLN:NE2	1:B:980:GLU:O	2.40	0.53
1:C:863:GLN:HE22	1:C:952:ARG:NH2	2.07	0.53
1:D:73:TRP:HB2	1:D:78:LEU:HD11	1.91	0.53
1:B:606:LEU:O	1:B:614:HIS:HB2	2.09	0.52
1:C:646:HIS:HB3	6:C:4937:HOH:O	2.09	0.52
1:D:887:GLN:NE2	1:D:980:GLU:O	2.42	0.52
1:B:755:ARG:HD3	1:B:769:TRP:CE3	2.45	0.52
1:C:843:GLN:HG2	1:C:848:THR:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:PHE:CE2	1:A:620:ALA:HA	2.45	0.52
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.92	0.52
1:D:473:ARG:O	1:D:473:ARG:NH1	2.42	0.52
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.45	0.52
1:B:433:LEU:HB3	1:B:434:PRO:HD3	1.92	0.52
1:B:542:ALA:HA	1:B:604:ASN:HA	1.91	0.52
1:A:873:ALA:O	1:A:876:THR:HG22	2.09	0.52
1:A:945:ASN:HB3	1:A:1023:LYS:HZ3	1.75	0.51
1:C:237:ARG:HH11	1:C:237:ARG:CB	2.22	0.51
1:A:991:MET:HE3	1:A:1003:VAL:HG21	1.92	0.51
1:B:777:LEU:HD11	1:B:980:GLU:HG2	1.92	0.51
1:B:863:GLN:HG2	1:B:1021:CYS:CB	2.38	0.51
1:C:251:ARG:HB2	1:C:254:LEU:HG	1.92	0.51
1:D:19:PRO:HD3	1:D:112:PRO:CB	2.41	0.51
1:B:73:TRP:CE2	1:B:122:CYS:HB3	2.45	0.51
1:B:369:GLU:HG3	1:B:397:LEU:HD21	1.93	0.51
1:C:595:THR:HA	1:C:596:PRO:C	2.36	0.51
1:A:595:THR:HA	1:A:596:PRO:C	2.35	0.51
1:C:237:ARG:HB3	1:C:237:ARG:HH11	1.75	0.51
1:D:105:TYR:CE1	1:D:199:ASP:HB2	2.45	0.51
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.93	0.51
1:B:427:THR:HG21	1:B:462:SER:HB3	1.93	0.51
1:B:937:LEU:HA	1:B:957:PHE:O	2.11	0.51
1:B:246:MET:C	1:B:246:MET:SD	2.94	0.50
1:B:930:VAL:O	1:B:932:PRO:HD3	2.11	0.50
1:A:749:ILE:CD1	1:A:858:ILE:HD12	2.41	0.50
1:B:44:THR:OG1	1:B:46:ARG:HG3	2.11	0.50
1:D:91:GLN:HG3	1:D:96:ASP:OD1	2.11	0.50
1:A:688:PRO:HD3	1:A:694:LEU:HD11	1.92	0.50
1:B:464:HIS:HB2	1:B:489:GLY:HA3	1.92	0.50
1:B:416:GLU:HG3	1:B:460:ASN:O	2.12	0.50
1:B:615:PRO:O	1:B:618:THR:HG22	2.12	0.50
1:C:427:THR:HG21	1:C:462:SER:HB3	1.93	0.50
1:D:801:ILE:HD12	1:D:801:ILE:N	2.26	0.50
1:D:464:HIS:HB2	1:D:489:GLY:HA3	1.93	0.50
1:B:533:LEU:HD23	1:B:533:LEU:C	2.37	0.49
1:C:433:LEU:HB3	1:C:434:PRO:HD3	1.93	0.49
1:A:687:GLN:CD	1:A:687:GLN:H	2.20	0.49
1:A:797:GLU:C	1:A:799:THR:H	2.20	0.49
1:D:334:GLU:OE1	1:D:336:ARG:NH1	2.45	0.49
1:A:650:GLU:HB3	1:A:670:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:GLY:O	1:B:198:GLU:HG3	2.12	0.49
1:B:651:LEU:HD12	1:B:651:LEU:O	2.12	0.49
1:A:240:LEU:C	1:A:240:LEU:HD23	2.36	0.49
1:B:124:SER:HA	1:B:184:LEU:O	2.13	0.49
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.47	0.49
1:D:240:LEU:HD23	1:D:240:LEU:C	2.38	0.49
1:A:279:ILE:HD11	1:D:422:PRO:CG	2.42	0.49
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.95	0.49
1:B:354:VAL:HG22	1:B:355:ASN:O	2.13	0.48
1:D:246:MET:SD	1:D:246:MET:C	2.96	0.48
1:A:438:GLU:HG2	1:A:442:ARG:HD2	1.94	0.48
1:A:833:ALA:HB1	1:A:858:ILE:O	2.12	0.48
1:B:619:GLU:HA	1:B:912:ALA:HB2	1.95	0.48
1:C:630:ARG:HD3	1:C:637:GLU:OE1	2.13	0.48
1:D:890:GLN:NE2	1:D:947:GLY:HA3	2.27	0.48
1:A:433:LEU:HB3	1:A:434:PRO:HD3	1.94	0.48
1:A:573:GLN:HB2	1:A:602:CYS:O	2.13	0.48
1:C:738:PRO:HG2	1:C:858:ILE:O	2.14	0.48
1:A:887:GLN:NE2	1:A:980:GLU:O	2.44	0.48
1:B:842:TRP:HZ3	1:B:852:SER:HB3	1.79	0.48
1:C:546:LEU:HA	6:C:4132:HOH:O	2.13	0.48
1:C:166:ARG:HG3	1:C:392:TYR:CB	2.43	0.48
1:C:830:LEU:CD2	1:D:830:LEU:HD21	2.44	0.48
1:D:687:GLN:H	1:D:687:GLN:CD	2.22	0.48
1:A:755:ARG:HB2	1:A:769:TRP:HB2	1.96	0.48
1:C:615:PRO:O	1:C:618:THR:HG22	2.14	0.48
1:D:542:ALA:HA	1:D:604:ASN:HA	1.96	0.48
1:D:895:VAL:HG21	1:D:925:MET:HG3	1.96	0.48
1:A:833:ALA:HB2	1:A:859:ASP:HA	1.96	0.48
1:B:549:PHE:CE2	1:B:620:ALA:HA	2.49	0.48
1:C:652:LEU:HD11	1:C:698:VAL:HB	1.95	0.48
1:C:786:ARG:NH2	1:C:991:MET:HE2	2.29	0.48
1:B:636:ILE:HD13	1:B:698:VAL:HG11	1.96	0.47
1:A:830:LEU:HD22	1:B:828:ASP:HB3	1.97	0.47
1:A:619:GLU:HA	1:A:912:ALA:HB2	1.97	0.47
1:B:143:PHE:O	1:B:168:PRO:HA	2.14	0.47
1:B:708:TRP:CZ2	5:B:5003:DMS:H23	2.49	0.47
1:C:38:ASN:OD1	1:C:41:GLU:HG3	2.14	0.47
1:C:765:LEU:CD2	1:C:768:MET:HE2	2.42	0.47
1:D:942:ARG:HA	1:D:953:GLY:O	2.14	0.47
1:A:1011:ALA:HB3	1:A:1014:TYR:CZ	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PRO:HB2	1:B:576:ILE:HG12	1.95	0.47
1:D:225:PHE:HA	1:D:243:GLU:O	2.14	0.47
1:C:549:PHE:CE2	1:C:620:ALA:HA	2.49	0.47
1:C:828:ASP:HB3	1:D:830:LEU:HD22	1.95	0.47
1:D:836:ILE:O	1:D:855:THR:HA	2.14	0.47
1:A:815:HIS:HE1	1:A:877:PRO:O	1.97	0.47
1:B:656:VAL:HG21	1:B:685:LEU:CD1	2.44	0.47
1:B:661:LYS:O	1:B:663:LEU:HD22	2.15	0.47
1:A:570:TRP:O	1:A:607:VAL:HG22	2.14	0.47
1:A:836:ILE:O	1:A:855:THR:HA	2.15	0.47
1:B:147:ASN:HA	1:B:148:SER:HA	1.56	0.47
1:B:613:PRO:HB3	1:B:617:LEU:HD23	1.96	0.47
1:D:117:GLU:HG2	6:D:4257:HOH:O	2.15	0.47
1:D:372:MET:HE1	1:D:395:HIS:HB3	1.97	0.47
1:D:794:GLY:HA2	1:D:998:SER:O	2.15	0.47
1:C:738:PRO:HB2	1:C:834:VAL:HG23	1.97	0.47
1:D:533:LEU:C	1:D:533:LEU:HD23	2.40	0.47
1:D:636:ILE:HD11	1:D:682:LEU:HD11	1.97	0.47
1:C:368:ASP:OD2	1:C:370:GLN:HB3	2.15	0.46
1:C:764:PHE:CE2	1:C:781:ARG:NH1	2.82	0.46
1:D:128:ASN:HB3	1:D:180:GLY:O	2.15	0.46
1:A:542:ALA:HA	1:A:604:ASN:HA	1.98	0.46
1:B:13:ARG:NH1	1:C:13:ARG:HD2	2.30	0.46
1:C:416:GLU:HA	1:C:460:ASN:O	2.15	0.46
1:C:651:LEU:HD12	1:C:668:VAL:O	2.15	0.46
1:D:301:TRP:CH2	1:D:452:SER:HA	2.49	0.46
1:D:476:LYS:HD2	6:D:4195:HOH:O	2.14	0.46
1:B:693:GLN:OE1	1:B:724:GLU:HB2	2.15	0.46
1:B:777:LEU:CD1	1:B:980:GLU:HG2	2.44	0.46
1:C:573:GLN:HB2	1:C:602:CYS:O	2.15	0.46
1:D:784:PHE:HA	1:D:881:ARG:O	2.15	0.46
1:C:460:ASN:ND2	1:C:461:GLU:HG3	2.31	0.46
1:D:352:ARG:HG2	1:D:553:TRP:CH2	2.51	0.46
1:D:577:LYS:O	1:D:584:PRO:HA	2.15	0.46
1:A:794:GLY:HA2	1:A:998:SER:O	2.16	0.46
1:B:362:LEU:HD23	1:B:576:ILE:HB	1.97	0.46
1:C:379:MET:HE1	1:C:387:VAL:HB	1.96	0.46
1:A:100:TYR:CZ	1:A:602:CYS:HB3	2.51	0.46
1:C:131:GLU:HG3	1:C:135:GLN:HG3	1.98	0.46
1:C:246:MET:SD	1:C:246:MET:C	2.99	0.46
1:D:144:ASP:OD2	1:D:211:ASP:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:945:ASN:HB3	1:A:1023:LYS:HZ2	1.81	0.46
1:D:26:ARG:HD2	1:D:169:SER:HA	1.98	0.46
1:D:142:ILE:HG12	1:D:170:GLU:HG2	1.97	0.46
1:B:942:ARG:HA	1:B:953:GLY:O	2.16	0.46
1:A:100:TYR:CE1	1:A:602:CYS:HB3	2.51	0.45
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.97	0.45
1:C:606:LEU:O	1:C:614:HIS:HB2	2.16	0.45
1:C:693:GLN:OE1	1:C:724:GLU:HB2	2.16	0.45
1:A:390:SER:HA	1:A:391:HIS:HA	1.71	0.45
1:B:210:ARG:NH2	1:B:358:GLU:OE1	2.46	0.45
1:B:506:VAL:HG12	1:B:521:LYS:HE3	1.98	0.45
1:B:646:HIS:HB3	6:B:4983:HOH:O	2.15	0.45
1:C:613:PRO:HB3	1:C:617:LEU:HD23	1.99	0.45
1:D:598:ASP:OD1	1:D:797:GLU:HA	2.16	0.45
1:D:656:VAL:HG21	1:D:685:LEU:CD1	2.46	0.45
1:D:1008:GLN:HE22	5:D:5007:DMS:H13	1.81	0.45
1:A:379:MET:HE1	1:A:387:VAL:HB	1.98	0.45
1:B:246:MET:CE	1:B:250:LEU:HD23	2.46	0.45
1:C:835:LEU:HD11	1:C:855:THR:HB	1.98	0.45
1:A:753:ASN:O	1:A:771:GLY:N	2.48	0.45
1:B:47:PRO:HA	5:B:5029:DMS:H12	1.97	0.45
1:B:546:LEU:HA	6:B:4129:HOH:O	2.16	0.45
1:C:800:ARG:HG2	1:C:800:ARG:HH11	1.81	0.45
1:A:230:ARG:NH2	1:A:241:GLU:OE2	2.49	0.45
1:A:577:LYS:O	1:A:584:PRO:HA	2.17	0.45
1:B:801:ILE:O	1:B:803:PRO:HD3	2.17	0.45
1:C:246:MET:HE3	1:C:250:LEU:HD23	1.98	0.45
1:D:390:SER:HA	1:D:391:HIS:HA	1.73	0.45
1:D:873:ALA:O	1:D:876:THR:HG22	2.17	0.45
1:A:87:PRO:HB2	1:A:209:PHE:C	2.42	0.45
1:B:166:ARG:HG3	1:B:392:TYR:HB2	1.98	0.45
1:B:505:ARG:O	1:B:519:SER:HA	2.16	0.45
1:B:610:ASP:O	1:B:611:ARG:HB2	2.16	0.45
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.98	0.45
1:C:830:LEU:HD21	1:D:830:LEU:HD21	1.99	0.45
1:D:19:PRO:HD3	1:D:112:PRO:HB3	1.98	0.45
1:C:225:PHE:HA	1:C:243:GLU:O	2.16	0.45
1:D:292:ARG:C	1:D:293:LEU:HD12	2.42	0.45
1:A:658:LEU:HD22	1:A:688:PRO:HB2	1.99	0.45
1:D:368:ASP:OD2	1:D:370:GLN:HB3	2.17	0.45
1:D:756:TRP:CD2	1:D:858:ILE:HD13	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:GLN:O	1:A:968:MET:HB2	2.17	0.45
1:C:965:GLN:O	1:C:969:GLU:HG3	2.16	0.45
1:A:301:TRP:CH2	1:A:452:SER:HA	2.52	0.44
1:A:367:MET:HB3	1:A:372:MET:HE2	1.99	0.44
1:B:756:TRP:CD2	1:B:858:ILE:HD13	2.51	0.44
1:C:568:TRP:CD2	1:C:569:ASP:HB3	2.52	0.44
1:C:952:ARG:NH1	1:C:952:ARG:HB2	2.32	0.44
1:D:196:TYR:O	1:D:417:THR:HG22	2.17	0.44
1:B:240:LEU:C	1:B:240:LEU:HD23	2.42	0.44
1:B:427:THR:O	1:B:467:ASN:HB2	2.17	0.44
1:D:147:ASN:HA	1:D:148:SER:HA	1.62	0.44
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.52	0.44
1:A:730:LEU:HD12	1:A:730:LEU:N	2.32	0.44
1:B:1020:TRP:HD1	1:B:1021:CYS:N	2.15	0.44
1:C:881:ARG:HE	1:C:987:ASP:CG	2.25	0.44
1:A:249:GLU:CD	1:A:251:ARG:NE	2.53	0.44
1:A:587:ALA:HB1	1:A:591:ASP:CB	2.47	0.44
1:D:577:LYS:HD3	1:D:585:TRP:CH2	2.52	0.44
1:D:635:THR:OG1	1:D:681:GLU:OE2	2.29	0.44
1:A:147:ASN:HA	1:A:148:SER:HA	1.61	0.44
1:B:40:GLU:OE2	1:B:43:ARG:NH2	2.50	0.44
1:C:143:PHE:O	1:C:168:PRO:HA	2.17	0.44
1:C:653:HIS:HB3	1:C:699:ARG:NH2	2.32	0.44
1:D:688:PRO:HG3	1:D:694:LEU:HD21	2.00	0.44
1:D:755:ARG:HB2	1:D:769:TRP:HB2	2.00	0.44
1:A:370:GLN:HG3	6:A:4474:HOH:O	2.16	0.44
1:B:50:GLN:N	1:B:50:GLN:CD	2.76	0.44
1:C:200:GLN:HA	1:C:416:GLU:OE1	2.17	0.44
1:C:708:TRP:CZ2	5:C:5003:DMS:H23	2.53	0.44
1:D:80:GLU:CD	1:D:80:GLU:H	2.25	0.44
1:A:369:GLU:HG3	1:A:397:LEU:HD21	2.00	0.44
1:A:422:PRO:CG	1:D:279:ILE:HD11	2.48	0.44
1:A:473:ARG:NH1	1:A:476:LYS:HB2	2.33	0.44
1:A:800:ARG:HG2	1:A:800:ARG:HH11	1.83	0.44
1:A:249:GLU:CG	1:A:251:ARG:NE	2.79	0.44
1:B:546:LEU:HD22	1:B:616:ALA:HB1	1.99	0.44
1:C:131:GLU:HG3	1:C:135:GLN:CG	2.48	0.44
1:A:660:GLY:O	1:A:662:PRO:HD3	2.18	0.44
1:A:770:ILE:HG23	1:A:1022:GLN:OE1	2.17	0.44
1:A:920:LEU:HB3	1:A:921:PRO:HD2	2.00	0.44
1:C:505:ARG:O	1:C:519:SER:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:768:MET:HE1	1:C:1020:TRP:CH2	2.53	0.44
1:D:610:ASP:O	1:D:611:ARG:HB2	2.18	0.44
1:A:687:GLN:CD	1:A:687:GLN:N	2.76	0.43
1:A:802:ASP:O	1:A:808:GLU:HG3	2.18	0.43
1:A:945:ASN:OD1	1:A:1023:LYS:HD3	2.18	0.43
1:C:326:GLU:OE1	1:C:326:GLU:HA	2.18	0.43
1:A:842:TRP:HZ3	1:A:852:SER:HB3	1.82	0.43
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.17	0.43
1:C:525:SER:O	1:D:561:ARG:HD3	2.18	0.43
1:D:390:SER:HB2	1:D:391:HIS:CE1	2.54	0.43
1:A:610:ASP:O	1:A:611:ARG:HB2	2.18	0.43
1:B:824:GLN:HB3	1:B:839:ALA:HB3	2.00	0.43
1:C:869:ASP:CG	1:C:1015:HIS:HD1	2.26	0.43
1:D:355:ASN:OD1	1:D:388:ARG:HD3	2.18	0.43
1:B:147:ASN:HB3	1:B:206:SER:HA	2.01	0.43
1:B:833:ALA:HB1	1:B:858:ILE:O	2.19	0.43
1:C:777:LEU:HB2	1:C:887:GLN:HG2	2.00	0.43
1:D:673:ALA:HB1	1:D:674:PRO:HD2	2.00	0.43
1:B:598:ASP:OD1	1:B:797:GLU:HA	2.17	0.43
1:D:568:TRP:HA	1:D:569:ASP:HA	1.78	0.43
1:C:59:ARG:HB2	1:C:124:SER:OG	2.19	0.43
1:D:192:SER:C	1:D:194:GLY:N	2.77	0.43
1:D:524:LEU:HD11	1:D:562:LEU:HG	2.01	0.43
1:D:843:GLN:HA	1:D:847:LYS:O	2.18	0.43
1:A:634:GLN:HE21	1:A:684:GLU:HA	1.82	0.43
1:B:937:LEU:O	1:B:938:ARG:HD2	2.17	0.43
1:C:777:LEU:HD11	1:C:980:GLU:HG2	2.01	0.43
1:A:91:GLN:HG3	1:A:96:ASP:OD1	2.19	0.43
1:A:427:THR:O	1:A:467:ASN:HB2	2.19	0.43
1:B:19:PRO:HD3	1:B:112:PRO:CB	2.48	0.43
1:B:352:ARG:HG2	1:B:553:TRP:CH2	2.54	0.43
1:A:622:HIS:ND1	1:A:625:GLN:OE1	2.49	0.43
1:D:427:THR:O	1:D:467:ASN:HB2	2.18	0.43
1:B:788:PRO:HD2	1:B:968:MET:HG3	2.01	0.42
1:C:245:GLN:HG2	1:C:288:ARG:CG	2.48	0.42
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.53	0.42
1:B:657:ALA:HA	1:B:663:LEU:HD22	2.00	0.42
1:A:128:ASN:HA	1:A:180:GLY:O	2.19	0.42
1:A:256:VAL:HA	1:A:314:GLU:O	2.19	0.42
1:A:508:GLU:OE2	5:A:5007:DMS:H21	2.18	0.42
1:C:749:ILE:N	1:C:749:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:890:GLN:HB2	6:D:4659:HOH:O	2.18	0.42
1:B:638:VAL:O	1:B:677:LYS:HA	2.19	0.42
1:D:52:ARG:O	1:D:213:SER:HB2	2.19	0.42
1:D:100:TYR:CE1	1:D:602:CYS:HB3	2.54	0.42
1:A:173:LEU:O	1:A:177:LEU:HG	2.20	0.42
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.01	0.42
1:A:225:PHE:HA	1:A:243:GLU:O	2.20	0.42
1:A:361:PRO:HB3	1:A:609:ALA:HB1	2.02	0.42
1:A:622:HIS:CE1	5:A:5002:DMS:H22	2.54	0.42
1:C:13:ARG:O	1:C:14:ARG:C	2.62	0.42
1:C:354:VAL:CG1	1:C:379:MET:HE3	2.50	0.42
1:C:720:TRP:NE1	5:C:5024:DMS:H23	2.35	0.42
1:D:984:LEU:HD21	1:D:986:ILE:HD11	2.01	0.42
1:A:16:TRP:CG	1:A:189:LEU:HD13	2.55	0.42
1:A:87:PRO:HA	1:A:208:ILE:O	2.20	0.42
1:D:340:GLY:O	1:D:561:ARG:HG2	2.20	0.42
1:B:23:GLN:C	1:B:23:GLN:CD	2.88	0.42
1:C:748:CYS:C	1:C:749:ILE:HD12	2.45	0.42
1:A:618:THR:HG22	1:A:912:ALA:HB1	2.01	0.42
1:A:703:PRO:O	1:A:711:ALA:HB1	2.20	0.42
1:B:896:ASN:HB3	1:B:945:ASN:HB2	2.01	0.42
1:B:944:LEU:O	1:B:950:GLN:HA	2.20	0.42
1:C:661:LYS:HA	1:C:662:PRO:HD3	1.92	0.42
1:C:890:GLN:HE22	1:C:948:PRO:HD3	1.84	0.42
1:D:995:GLY:C	1:D:997:ASP:N	2.75	0.42
1:A:598:ASP:OD1	1:A:797:GLU:HA	2.20	0.41
1:B:815:HIS:HE1	1:B:877:PRO:O	2.02	0.41
1:A:433:LEU:N	1:A:434:PRO:CD	2.83	0.41
1:A:738:PRO:HD2	1:A:833:ALA:HA	2.03	0.41
1:A:773:LYS:HG2	1:A:774:LYS:O	2.20	0.41
1:B:13:ARG:O	1:B:14:ARG:C	2.61	0.41
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.35	0.41
1:C:105:TYR:CE1	1:C:199:ASP:HB2	2.54	0.41
1:A:797:GLU:C	1:A:799:THR:N	2.78	0.41
1:B:105:TYR:CE1	1:B:199:ASP:HB2	2.56	0.41
1:B:506:VAL:CG1	1:B:521:LYS:HE3	2.50	0.41
1:B:634:GLN:HB2	1:B:681:GLU:OE2	2.21	0.41
1:B:658:LEU:HD22	1:B:688:PRO:HB2	2.02	0.41
1:B:995:GLY:O	1:B:996:ASP:C	2.64	0.41
1:C:19:PRO:HD3	1:C:112:PRO:CB	2.50	0.41
1:C:200:GLN:HG3	1:C:416:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:656:VAL:HG21	1:A:685:LEU:CD1	2.50	0.41
1:A:754:LYS:HA	1:A:769:TRP:O	2.19	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:A:525:SER:O	1:B:561:ARG:HD3	2.21	0.41
1:B:390:SER:HA	1:B:391:HIS:HA	1.81	0.41
1:C:784:PHE:HA	1:C:881:ARG:O	2.21	0.41
1:C:995:GLY:O	1:C:996:ASP:C	2.63	0.41
1:D:738:PRO:HG3	1:D:751:LEU:HD13	2.01	0.41
1:C:482:ARG:HA	1:C:483:PRO:HD3	1.97	0.41
1:C:773:LYS:HE2	1:C:773:LYS:C	2.45	0.41
1:C:952:ARG:HH11	1:C:952:ARG:CB	2.33	0.41
1:D:87:PRO:HB2	1:D:209:PHE:C	2.46	0.41
1:D:166:ARG:HG3	1:D:392:TYR:HB2	2.02	0.41
1:D:458:LEU:HD11	1:D:472:TYR:HB2	2.03	0.41
1:A:390:SER:HB2	1:A:391:HIS:CE1	2.56	0.41
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.56	0.41
1:B:223:SER:O	1:B:224:ASP:HB2	2.21	0.41
1:B:674:PRO:O	1:B:675:GLN:HB2	2.21	0.41
1:B:895:VAL:HG21	1:B:925:MET:HG3	2.03	0.41
1:C:306:PRO:HD2	5:C:5033:DMS:H23	2.01	0.41
1:D:863:GLN:NE2	1:D:952:ARG:NH2	2.67	0.41
1:A:126:THR:HA	1:A:182:ASN:O	2.21	0.41
1:A:292:ARG:HH12	5:A:5012:DMS:C1	2.34	0.41
1:A:335:VAL:HG22	1:A:344:LEU:HD12	2.03	0.41
1:A:587:ALA:HB1	1:A:591:ASP:HB2	2.03	0.41
1:A:793:ILE:HG22	1:A:795:VAL:HG22	2.03	0.41
6:A:4541:HOH:O	1:D:463:GLY:HA2	2.20	0.41
1:B:19:PRO:HD3	1:B:112:PRO:HB3	2.02	0.41
1:B:141:ILE:HB	1:B:173:LEU:HD11	2.03	0.41
1:B:294:ASN:HD22	5:B:5028:DMS:H22	1.86	0.41
1:B:356:ARG:HH22	1:B:367:MET:HE2	1.86	0.41
1:B:768:MET:HE1	1:B:1020:TRP:CZ2	2.55	0.41
1:B:995:GLY:C	1:B:997:ASP:N	2.78	0.41
5:B:5018:DMS:H22	1:C:478:VAL:HB	2.03	0.41
1:C:100:TYR:CE1	1:C:602:CYS:HB3	2.56	0.41
1:C:638:VAL:O	1:C:677:LYS:HA	2.21	0.41
1:D:482:ARG:HA	1:D:483:PRO:HD3	1.96	0.41
1:A:701:VAL:O	1:A:703:PRO:HD3	2.20	0.41
1:A:890:GLN:HG2	1:A:891:VAL:N	2.35	0.41
1:A:499:ILE:HG22	1:A:501:PRO:HD3	2.03	0.40
1:A:651:LEU:HD12	1:A:651:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASN:O	1:B:119:PRO:C	2.64	0.40
1:B:379:MET:HE1	1:B:387:VAL:HB	2.02	0.40
1:B:881:ARG:HE	1:B:987:ASP:CG	2.28	0.40
1:C:542:ALA:HA	1:C:604:ASN:HA	2.03	0.40
1:C:749:ILE:HD11	1:C:836:ILE:HD11	2.03	0.40
1:C:794:GLY:HA2	1:C:998:SER:O	2.21	0.40
1:C:802:ASP:O	1:C:808:GLU:HG3	2.21	0.40
1:A:896:ASN:HD21	1:A:917:ARG:HD2	1.86	0.40
1:A:900:LEU:CD1	1:A:910:LEU:HD22	2.51	0.40
1:B:163:GLN:O	1:B:164:ASP:HB3	2.21	0.40
1:B:251:ARG:HB2	1:B:254:LEU:HG	2.03	0.40
1:B:658:LEU:N	1:B:663:LEU:CD2	2.84	0.40
1:D:429:ASP:OD1	1:D:431:ARG:HG3	2.21	0.40
1:D:742:THR:HG22	1:D:743:SER:N	2.37	0.40
1:D:811:LYS:HD2	5:D:5229:DMS:H11	2.02	0.40
1:A:291:LEU:N	1:A:291:LEU:HD22	2.37	0.40
1:B:478:VAL:HG12	5:C:5018:DMS:H22	2.03	0.40
1:B:847:LYS:HE2	1:B:848:THR:O	2.21	0.40
1:C:619:GLU:HA	1:C:912:ALA:HB2	2.02	0.40
1:C:952:ARG:HB2	1:C:952:ARG:HH11	1.87	0.40
1:D:773:LYS:HA	1:D:773:LYS:HD2	1.94	0.40
1:A:59:ARG:HB2	1:A:124:SER:OG	2.21	0.40
1:A:88:SER:HA	1:A:366:VAL:CG2	2.48	0.40
1:A:533:LEU:HD23	1:A:534:ILE:N	2.36	0.40
1:A:639:THR:OG1	1:A:677:LYS:NZ	2.49	0.40
1:A:742:THR:HG22	1:A:743:SER:N	2.36	0.40
1:B:687:GLN:N	1:B:687:GLN:CD	2.80	0.40
1:C:533:LEU:HD23	1:C:534:ILE:N	2.36	0.40
1:C:546:LEU:HD22	1:C:616:ALA:HB1	2.04	0.40
1:B:372:MET:CE	1:B:397:LEU:HD23	2.52	0.40
1:B:789:LEU:HD11	1:B:993:ILE:HG22	2.03	0.40
6:B:4559:HOH:O	1:C:463:GLY:HA2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1009/1023 (99%)	963 (95%)	45 (4%)	1 (0%)	48	57
1	B	1009/1023 (99%)	961 (95%)	48 (5%)	0	100	100
1	C	1009/1023 (99%)	962 (95%)	47 (5%)	0	100	100
1	D	1009/1023 (99%)	965 (96%)	43 (4%)	1 (0%)	48	57
All	All	4036/4092 (99%)	3851 (95%)	183 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	798	ALA
1	D	211	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	863/874 (99%)	859 (100%)	4 (0%)	81	90
1	B	863/874 (99%)	860 (100%)	3 (0%)	86	93
1	C	863/874 (99%)	858 (99%)	5 (1%)	78	89
1	D	863/874 (99%)	859 (100%)	4 (0%)	81	90
All	All	3452/3496 (99%)	3436 (100%)	16 (0%)	81	90

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	A	277	GLU
1	A	519	SER
1	A	546	LEU

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Mol	Chain	Res	Type
1	B	546	LEU
1	B	651	LEU
1	B	956	GLN
1	C	112	PRO
1	C	344	LEU
1	C	546	LEU
1	C	773	LYS
1	C	804	ASN
1	D	546	LEU
1	D	655	MET
1	D	663	LEU
1	D	885	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	135	GLN
1	A	138	GLN
1	A	221	GLN
1	A	226	HIS
1	A	445	GLN
1	A	485	GLN
1	A	817	GLN
1	A	824	GLN
1	A	843	GLN
1	A	885	ASN
1	A	1017	GLN
1	B	128	ASN
1	B	262	GLN
1	B	294	ASN
1	B	464	HIS
1	B	485	GLN
1	B	583	ASN
1	B	624	GLN
1	B	675	GLN
1	B	702	GLN
1	B	718	GLN
1	B	804	ASN
1	B	824	GLN
1	B	950	GLN
1	C	50	GLN

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Mol	Chain	Res	Type
1	C	128	ASN
1	C	297	ASN
1	C	624	GLN
1	C	687	GLN
1	C	824	GLN
1	C	863	GLN
1	C	1017	GLN
1	D	128	ASN
1	D	485	GLN
1	D	702	GLN
1	D	718	GLN
1	D	817	GLN
1	D	843	GLN
1	D	863	GLN
1	D	903	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 157 ligands modelled in this entry, 27 are monoatomic - leaving 130 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	D	5229	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	A	5010	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	C	5032	-	3,3,3	0.22	0	3,3,3	0.62	0
2	149	A	2001	4	12,12,12	1.11	1 (8%)	15,17,17	0.88	0
5	DMS	B	5006	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	C	5007	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	5023	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	A	5126	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	A	5015	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	A	5012	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	B	5001	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	D	5001	-	3,3,3	0.23	0	3,3,3	0.67	0
5	DMS	B	5009	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	A	5022	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	B	5002	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	B	5003	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	D	5007	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	A	5001	-	3,3,3	0.21	0	3,3,3	0.64	0
5	DMS	B	5004	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	B	5021	4	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	C	5010	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	A	5008	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	A	5020	-	3,3,3	0.19	0	3,3,3	0.63	0
5	DMS	D	5028	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	B	5008	-	3,3,3	0.19	0	3,3,3	0.63	0
5	DMS	A	5007	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	B	5028	-	3,3,3	0.24	0	3,3,3	0.64	0
2	149	B	2001	4	12,12,12	1.02	1 (8%)	15,17,17	0.88	1 (6%)
5	DMS	A	5128	-	3,3,3	0.27	0	3,3,3	0.65	0
2	149	D	2001	4	12,12,12	1.01	1 (8%)	15,17,17	0.85	0
5	DMS	A	5024	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	C	5015	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	A	5232	-	3,3,3	0.25	0	3,3,3	0.67	0
5	DMS	C	5006	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	5027	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	A	5129	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	B	5022	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	D	5022	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	A	5018	4	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	B	5133	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	5006	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	B	5005	-	3,3,3	0.22	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	5031	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	1024	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	B	5015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	5020	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	5027	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	D	5009	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	C	5033	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	C	5001	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	D	5002	-	3,3,3	0.19	0	3,3,3	0.55	0
5	DMS	D	5013	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	C	5013	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	A	5130	-	3,3,3	0.15	0	3,3,3	0.61	0
5	DMS	A	5009	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	B	5132	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	D	5021	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	C	5024	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	B	5016	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	B	5034	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	A	5002	-	3,3,3	0.20	0	3,3,3	0.57	0
5	DMS	B	5029	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	D	5018	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	D	5014	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5016	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	D	5004	-	3,3,3	0.18	0	3,3,3	0.63	0
5	DMS	B	5018	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	B	5007	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	5011	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	C	5025	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	5014	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	B	5026	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	B	5010	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	D	5017	-	3,3,3	0.25	0	3,3,3	0.64	0
2	149	C	2001	4	12,12,12	1.16	1 (8%)	15,17,17	0.80	0
5	DMS	C	5011	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	5231	-	3,3,3	0.21	0	3,3,3	0.64	0
5	DMS	C	5023	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	A	5016	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	B	5025	-	3,3,3	0.25	0	3,3,3	0.66	0
5	DMS	C	5012	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	C	5134	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	C	5002	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	D	5012	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	C	5004	-	3,3,3	0.22	0	3,3,3	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	5003	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	D	5011	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	5006	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	B	5023	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	D	5008	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	C	5028	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	A	5125	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	D	5005	-	3,3,3	0.26	0	3,3,3	0.60	0
5	DMS	B	5012	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	A	5017	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	C	5014	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	B	5013	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	C	5018	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	C	5019	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	D	5027	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	A	5003	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	A	5011	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	C	5030	-	3,3,3	0.28	0	3,3,3	0.64	0
5	DMS	D	5230	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	A	5005	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	D	5003	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	5017	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	D	5016	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	A	5004	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	D	5020	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	B	5014	-	3,3,3	0.21	0	3,3,3	0.64	0
5	DMS	D	5010	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	A	5019	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5020	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5017	-	3,3,3	0.27	0	3,3,3	0.63	0
5	DMS	C	5009	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	B	5131	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	B	5024	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	C	5022	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	D	5024	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	C	5021	4	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	5026	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	A	5127	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	C	5005	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	B	5019	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	D	5023	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	D	5015	-	3,3,3	0.22	0	3,3,3	0.63	0
5	DMS	D	5019	-	3,3,3	0.25	0	3,3,3	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	C	5008	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	D	5025	-	3,3,3	0.26	0	3,3,3	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	149	A	2001	4	-	1/2/22/22	0/1/1/1
2	149	C	2001	4	-	1/2/22/22	0/1/1/1
2	149	D	2001	4	-	1/2/22/22	0/1/1/1
2	149	B	2001	4	-	1/2/22/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2001	149	O5-C1	2.92	1.39	1.34
2	C	2001	149	O5-C1	2.80	1.38	1.34
2	B	2001	149	O5-C1	2.72	1.38	1.34
2	D	2001	149	O5-C1	2.71	1.38	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	149	O5-C5-C6	2.00	108.06	106.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2001	149	O5-C5-C6-O6
2	D	2001	149	O5-C5-C6-O6
2	B	2001	149	O5-C5-C6-O6
2	A	2001	149	O5-C5-C6-O6

There are no ring outliers.

16 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	5229	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	5012	DMS	2	0
5	B	5003	DMS	1	0
5	D	5007	DMS	1	0
5	A	5007	DMS	1	0
5	B	5028	DMS	1	0
5	C	5033	DMS	1	0
5	A	5130	DMS	2	0
5	B	5132	DMS	1	0
5	C	5024	DMS	1	0
5	A	5002	DMS	1	0
5	B	5029	DMS	1	0
5	B	5018	DMS	1	0
5	C	5003	DMS	1	0
5	C	5018	DMS	1	0
5	C	5030	DMS	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1011/1023 (98%)	-0.31	17 (1%) 69 66	7, 20, 41, 66	0
1	B	1011/1023 (98%)	-0.39	14 (1%) 73 71	5, 18, 39, 66	0
1	C	1011/1023 (98%)	-0.45	16 (1%) 70 67	6, 17, 37, 73	0
1	D	1011/1023 (98%)	-0.42	13 (1%) 75 73	6, 18, 38, 66	0
All	All	4044/4092 (98%)	-0.39	60 (1%) 72 69	5, 18, 39, 73	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	795	VAL	4.5
1	D	732	ALA	3.7
1	B	795	VAL	3.4
1	B	1022	GLN	3.4
1	D	686	PRO	3.3
1	D	689	GLU	3.3
1	A	686	PRO	3.2
1	C	801	ILE	3.1
1	C	745	MET	3.1
1	A	1023	LYS	3.1
1	C	1022	GLN	3.0
1	C	1023	LYS	3.0
1	A	735	HIS	3.0
1	A	249	GLU	2.9
1	B	688	PRO	2.9
1	C	735	HIS	2.9
1	A	771	GLY	2.9
1	B	687	GLN	2.9
1	B	732	ALA	2.8
1	B	733	ALA	2.8
1	A	799	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	734	SER	2.7
1	A	732	ALA	2.7
1	A	772	ASP	2.7
1	C	795	VAL	2.7
1	D	735	HIS	2.6
1	C	730	LEU	2.5
1	C	799	THR	2.5
1	D	730	LEU	2.5
1	A	734	SER	2.5
1	C	580	GLU	2.4
1	D	801	ILE	2.4
1	D	734	SER	2.4
1	C	800	ARG	2.4
1	B	1023	LYS	2.3
1	A	76	CYS	2.3
1	C	732	ALA	2.3
1	A	730	LEU	2.3
1	D	772	ASP	2.3
1	B	745	MET	2.3
1	D	687	GLN	2.3
1	A	800	ARG	2.2
1	A	655	MET	2.2
1	D	733	ALA	2.2
1	C	817	GLN	2.2
1	A	801	ILE	2.2
1	D	795	VAL	2.2
1	B	890	GLN	2.2
1	C	743	SER	2.2
1	D	685	LEU	2.1
1	B	689	GLU	2.1
1	C	798	ALA	2.1
1	A	733	ALA	2.1
1	A	77	ASP	2.1
1	B	730	LEU	2.1
1	D	1022	GLN	2.1
1	C	734	SER	2.0
1	C	689	GLU	2.0
1	B	580	GLU	2.0
1	B	686	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	B	5013	4/4	0.42	0.25	109,109,109,109	0
5	DMS	A	5024	4/4	0.66	0.23	79,79,79,79	0
5	DMS	C	5012	4/4	0.66	0.19	97,97,97,97	0
5	DMS	D	5015	4/4	0.66	0.21	78,79,79,79	0
5	DMS	D	5007	4/4	0.69	0.23	86,87,87,87	0
5	DMS	B	5017	4/4	0.70	0.23	74,74,74,75	0
5	DMS	D	5024	4/4	0.70	0.26	85,85,86,86	0
5	DMS	C	5024	4/4	0.71	0.23	66,66,66,67	0
5	DMS	C	5016	4/4	0.71	0.19	68,68,69,69	0
5	DMS	C	5009	4/4	0.72	0.21	90,90,90,91	0
5	DMS	A	5232	4/4	0.73	0.17	58,58,58,59	0
5	DMS	C	5028	4/4	0.74	0.21	84,85,85,85	0
5	DMS	D	5023	4/4	0.75	0.23	81,82,82,82	0
3	MG	A	3005	1/1	0.76	0.19	70,70,70,70	0
5	DMS	B	5007	4/4	0.77	0.19	75,75,76,76	0
5	DMS	C	5017	4/4	0.77	0.17	65,65,66,67	0
5	DMS	B	5025	4/4	0.78	0.19	70,70,70,72	0
5	DMS	D	5013	4/4	0.79	0.15	87,87,87,88	0
5	DMS	A	5017	4/4	0.79	0.17	59,59,59,60	0
5	DMS	D	5229	4/4	0.79	0.16	67,67,69,69	0
5	DMS	B	5026	4/4	0.80	0.17	55,55,55,56	0
5	DMS	A	5010	4/4	0.81	0.17	71,71,71,72	0
3	MG	B	3003	1/1	0.81	0.12	59,59,59,59	0
5	DMS	A	5022	4/4	0.81	0.19	65,65,66,66	0
4	NA	D	3104	1/1	0.81	0.12	29,29,29,29	0
5	DMS	D	5026	4/4	0.81	0.19	113,113,113,113	0
5	DMS	C	5014	4/4	0.81	0.18	65,65,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	A	5125	4/4	0.82	0.17	72,72,72,73	0
5	DMS	D	5230	4/4	0.82	0.15	54,54,54,55	0
5	DMS	C	5018	4/4	0.83	0.18	66,67,67,67	0
5	DMS	C	1024	4/4	0.83	0.18	63,64,64,65	0
5	DMS	B	5133	4/4	0.84	0.18	70,70,70,71	0
5	DMS	A	5231	4/4	0.84	0.16	57,57,57,58	0
5	DMS	C	5033	4/4	0.84	0.13	58,58,59,60	0
5	DMS	A	5016	4/4	0.84	0.17	57,57,57,58	0
5	DMS	D	5010	4/4	0.84	0.15	71,71,71,72	0
5	DMS	B	5015	4/4	0.84	0.18	59,59,60,60	0
5	DMS	B	5020	4/4	0.85	0.15	67,68,68,68	0
5	DMS	B	5010	4/4	0.85	0.16	72,72,73,73	0
5	DMS	A	5128	4/4	0.85	0.18	54,54,55,55	0
5	DMS	D	5018	4/4	0.85	0.15	71,71,71,72	0
5	DMS	D	5021	4/4	0.85	0.20	83,83,83,83	0
5	DMS	B	5006	4/4	0.86	0.16	63,63,64,64	0
5	DMS	C	5027	4/4	0.86	0.14	65,66,66,66	0
5	DMS	D	5027	4/4	0.86	0.17	75,75,76,76	0
5	DMS	A	5004	4/4	0.86	0.12	57,57,58,59	0
5	DMS	C	5021	4/4	0.86	0.17	60,60,60,61	0
5	DMS	B	5022	4/4	0.87	0.16	89,89,89,90	0
5	DMS	A	5007	4/4	0.87	0.15	65,66,66,66	0
5	DMS	D	5004	4/4	0.87	0.14	52,52,53,54	0
5	DMS	C	5004	4/4	0.88	0.14	36,37,39,39	0
5	DMS	B	5009	4/4	0.88	0.15	39,40,41,41	0
5	DMS	C	5031	4/4	0.88	0.14	69,69,70,70	0
5	DMS	C	5020	4/4	0.88	0.12	68,68,68,69	0
5	DMS	C	5134	4/4	0.88	0.13	40,41,41,43	0
5	DMS	A	5002	4/4	0.88	0.18	45,46,46,47	0
5	DMS	C	5022	4/4	0.88	0.15	65,65,65,66	0
5	DMS	D	5028	4/4	0.88	0.13	63,63,63,63	0
5	DMS	A	5015	4/4	0.88	0.11	65,65,65,66	0
5	DMS	B	5021	4/4	0.88	0.17	66,66,66,67	0
5	DMS	D	5020	4/4	0.89	0.12	65,66,66,66	0
5	DMS	A	5009	4/4	0.89	0.14	44,45,46,47	0
5	DMS	D	5022	4/4	0.89	0.14	62,62,62,63	0
5	DMS	A	5019	4/4	0.89	0.15	84,84,84,84	0
5	DMS	A	5127	4/4	0.89	0.15	51,53,53,53	0
5	DMS	B	5132	4/4	0.89	0.12	58,58,59,59	0
4	NA	B	3104	1/1	0.89	0.08	31,31,31,31	0
5	DMS	C	5030	4/4	0.89	0.14	62,63,63,64	0
5	DMS	A	5023	4/4	0.89	0.14	60,61,61,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	5006	4/4	0.89	0.15	56,57,58,58	0
5	DMS	D	5017	4/4	0.90	0.16	70,70,71,72	0
4	NA	C	3104	1/1	0.90	0.08	32,32,32,32	0
5	DMS	B	5028	4/4	0.90	0.13	53,53,54,55	0
5	DMS	A	5018	4/4	0.90	0.14	55,55,55,56	0
5	DMS	C	5019	4/4	0.90	0.11	51,52,52,52	0
5	DMS	C	5015	4/4	0.90	0.14	56,57,57,57	0
5	DMS	A	5020	4/4	0.91	0.12	56,57,57,58	0
5	DMS	B	5018	4/4	0.91	0.12	45,46,46,48	0
4	NA	B	3103	1/1	0.91	0.07	23,23,23,23	0
5	DMS	A	5006	4/4	0.91	0.13	57,58,58,58	0
5	DMS	B	5131	4/4	0.91	0.12	58,58,58,59	0
5	DMS	A	5129	4/4	0.92	0.10	60,61,61,61	0
5	DMS	D	5009	4/4	0.92	0.11	44,45,45,46	0
4	NA	A	3103	1/1	0.92	0.09	39,39,39,39	0
5	DMS	A	5014	4/4	0.92	0.11	49,51,51,51	0
5	DMS	C	5032	4/4	0.92	0.12	61,62,62,63	0
5	DMS	B	5027	4/4	0.92	0.12	52,52,52,52	0
5	DMS	B	5003	4/4	0.92	0.13	39,40,41,41	0
5	DMS	D	5019	4/4	0.92	0.12	56,57,57,57	0
5	DMS	B	5004	4/4	0.92	0.13	51,52,53,53	0
5	DMS	B	5008	4/4	0.93	0.11	40,41,41,42	0
5	DMS	D	5014	4/4	0.93	0.12	58,59,60,60	0
5	DMS	B	5034	4/4	0.93	0.11	45,46,46,48	0
5	DMS	C	5025	4/4	0.93	0.12	55,55,55,56	0
5	DMS	B	5012	4/4	0.94	0.09	37,37,38,39	0
5	DMS	C	5003	4/4	0.94	0.11	36,37,38,39	0
5	DMS	D	5012	4/4	0.94	0.12	53,53,53,54	0
5	DMS	B	5002	4/4	0.94	0.12	38,38,40,41	0
5	DMS	A	5126	4/4	0.94	0.12	45,46,46,47	0
5	DMS	C	5008	4/4	0.94	0.11	55,55,55,55	0
5	DMS	D	5016	4/4	0.94	0.11	43,44,44,45	0
5	DMS	A	5012	4/4	0.94	0.10	46,46,47,47	0
5	DMS	A	5008	4/4	0.94	0.10	48,49,49,50	0
5	DMS	D	5008	4/4	0.94	0.10	44,45,45,46	0
4	NA	C	3103	1/1	0.95	0.08	29,29,29,29	0
5	DMS	C	5007	4/4	0.95	0.09	38,39,41,42	0
2	149	D	2001	12/12	0.95	0.06	8,13,15,20	0
5	DMS	B	5019	4/4	0.95	0.10	60,60,60,61	0
5	DMS	B	5014	4/4	0.95	0.09	40,40,41,42	0
5	DMS	C	5013	4/4	0.95	0.11	38,40,40,40	0
5	DMS	C	5023	4/4	0.95	0.10	47,47,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	5002	4/4	0.95	0.10	32,33,34,35	0
2	149	A	2001	12/12	0.95	0.07	11,13,18,18	0
5	DMS	B	5029	4/4	0.95	0.10	57,57,58,59	0
5	DMS	D	5002	4/4	0.96	0.10	30,31,32,32	0
3	MG	A	3001	1/1	0.96	0.03	17,17,17,17	0
3	MG	D	3001	1/1	0.96	0.04	13,13,13,13	0
5	DMS	B	5023	4/4	0.96	0.11	41,42,42,43	0
5	DMS	B	5024	4/4	0.96	0.12	62,62,62,62	0
5	DMS	B	5005	4/4	0.96	0.07	34,36,37,38	0
3	MG	D	3002	1/1	0.96	0.05	23,23,23,23	0
5	DMS	D	5025	4/4	0.96	0.08	40,41,41,41	0
5	DMS	A	5130	4/4	0.96	0.08	27,27,29,31	0
2	149	B	2001	12/12	0.96	0.06	11,13,16,17	0
4	NA	A	3104	1/1	0.96	0.04	28,28,28,28	0
3	MG	A	1024	1/1	0.96	0.08	44,44,44,44	0
5	DMS	C	5011	4/4	0.96	0.09	41,41,41,42	0
4	NA	D	3102	1/1	0.97	0.03	16,16,16,16	0
4	NA	D	3103	1/1	0.97	0.07	33,33,33,33	0
3	MG	A	3002	1/1	0.97	0.04	19,19,19,19	0
5	DMS	A	5011	4/4	0.97	0.08	39,39,40,41	0
4	NA	C	3101	1/1	0.97	0.04	13,13,13,13	0
5	DMS	A	5003	4/4	0.97	0.09	38,38,38,39	0
5	DMS	B	5016	4/4	0.97	0.08	41,42,42,42	0
4	NA	C	3102	1/1	0.97	0.04	14,14,14,14	0
5	DMS	A	5005	4/4	0.97	0.07	32,32,33,34	0
4	NA	B	3102	1/1	0.97	0.03	16,16,16,16	0
3	MG	B	3002	1/1	0.97	0.03	19,19,19,19	0
5	DMS	D	5003	4/4	0.97	0.08	32,33,33,33	0
5	DMS	A	5001	4/4	0.98	0.07	22,22,24,24	0
5	DMS	C	5005	4/4	0.98	0.06	36,36,37,38	0
2	149	C	2001	12/12	0.98	0.04	9,12,13,15	0
3	MG	C	3002	1/1	0.98	0.05	17,17,17,17	0
5	DMS	D	5011	4/4	0.98	0.08	32,32,33,34	0
5	DMS	B	5011	4/4	0.98	0.08	28,28,29,29	0
5	DMS	D	5001	4/4	0.98	0.07	21,21,22,24	0
4	NA	A	3101	1/1	0.98	0.02	13,13,13,13	0
4	NA	A	3102	1/1	0.98	0.04	21,21,21,21	0
5	DMS	B	5001	4/4	0.98	0.07	19,21,23,24	0
5	DMS	D	5005	4/4	0.98	0.07	27,27,28,29	0
5	DMS	D	5006	4/4	0.98	0.06	30,32,33,33	0
5	DMS	C	5010	4/4	0.99	0.06	34,35,35,36	0
4	NA	B	3101	1/1	0.99	0.02	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	C	5001	4/4	0.99	0.06	23,25,25,26	0
3	MG	C	3001	1/1	0.99	0.01	12,12,12,12	0
4	NA	D	3101	1/1	0.99	0.04	12,12,12,12	0
3	MG	B	3001	1/1	0.99	0.02	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.