



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:07 AM UTC

PDB ID : 3MUZ / pdb_00003muz
Title : E.Coli (lacZ) beta-galactosidase (R599A) in complex with IPTG
Authors : Dugdale, M.L.; Vance, M.L.; Driedger, M.R.; Nibber, A.; Tran, A.; Huber, R.E.
Deposited on : 2010-05-03
Resolution : 1.90 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

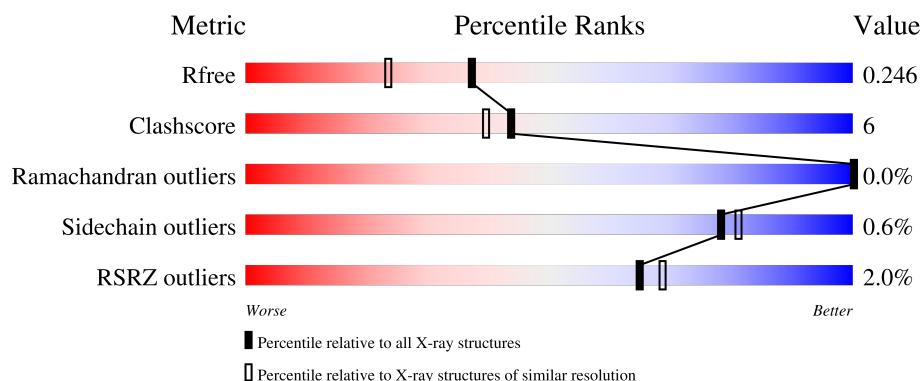
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	1	1052	2% 78% 18% .
1	2	1052	2% 82% 13% ..
1	3	1052	2% 81% 14% ..
1	4	1052	2% 79% 16% .

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	2	6026	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 37334 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	1	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	2	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	3	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			
1	4	1011	Total	C	N	O	S	0	0	0
			8119	5135	1437	1509	38			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	-28	MET	-	expression tag	UNP B8LFD6
1	-27	GLY	-	expression tag	UNP B8LFD6
1	-26	GLY	-	expression tag	UNP B8LFD6
1	-25	SER	-	expression tag	UNP B8LFD6
1	-24	HIS	-	expression tag	UNP B8LFD6
1	-23	HIS	-	expression tag	UNP B8LFD6
1	-22	HIS	-	expression tag	UNP B8LFD6
1	-21	HIS	-	expression tag	UNP B8LFD6
1	-20	HIS	-	expression tag	UNP B8LFD6
1	-19	HIS	-	expression tag	UNP B8LFD6
1	-18	GLY	-	expression tag	UNP B8LFD6
1	-17	MET	-	expression tag	UNP B8LFD6
1	-16	ALA	-	expression tag	UNP B8LFD6
1	-15	SER	-	expression tag	UNP B8LFD6
1	-14	MET	-	expression tag	UNP B8LFD6
1	-13	THR	-	expression tag	UNP B8LFD6
1	-12	GLY	-	expression tag	UNP B8LFD6
1	-11	GLY	-	expression tag	UNP B8LFD6
1	-10	GLN	-	expression tag	UNP B8LFD6
1	-9	GLN	-	expression tag	UNP B8LFD6
1	-8	MET	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
1	-7	GLY	-	expression tag	UNP B8LFD6
1	-6	ARG	-	expression tag	UNP B8LFD6
1	-5	ASP	-	expression tag	UNP B8LFD6
1	-4	LEU	-	expression tag	UNP B8LFD6
1	-3	TYR	-	expression tag	UNP B8LFD6
1	-2	ASP	-	expression tag	UNP B8LFD6
1	-1	ASP	-	expression tag	UNP B8LFD6
1	0	ASP	-	expression tag	UNP B8LFD6
1	1	ASP	-	expression tag	UNP B8LFD6
1	2	LYS	-	expression tag	UNP B8LFD6
1	3	ASP	-	expression tag	UNP B8LFD6
1	4	PRO	-	expression tag	UNP B8LFD6
1	5	MET	-	expression tag	UNP B8LFD6
1	6	ILE	-	expression tag	UNP B8LFD6
1	7	ASP	-	expression tag	UNP B8LFD6
1	8	PRO	-	expression tag	UNP B8LFD6
1	599	ALA	ARG	conflict	UNP B8LFD6
2	-28	MET	-	expression tag	UNP B8LFD6
2	-27	GLY	-	expression tag	UNP B8LFD6
2	-26	GLY	-	expression tag	UNP B8LFD6
2	-25	SER	-	expression tag	UNP B8LFD6
2	-24	HIS	-	expression tag	UNP B8LFD6
2	-23	HIS	-	expression tag	UNP B8LFD6
2	-22	HIS	-	expression tag	UNP B8LFD6
2	-21	HIS	-	expression tag	UNP B8LFD6
2	-20	HIS	-	expression tag	UNP B8LFD6
2	-19	HIS	-	expression tag	UNP B8LFD6
2	-18	GLY	-	expression tag	UNP B8LFD6
2	-17	MET	-	expression tag	UNP B8LFD6
2	-16	ALA	-	expression tag	UNP B8LFD6
2	-15	SER	-	expression tag	UNP B8LFD6
2	-14	MET	-	expression tag	UNP B8LFD6
2	-13	THR	-	expression tag	UNP B8LFD6
2	-12	GLY	-	expression tag	UNP B8LFD6
2	-11	GLY	-	expression tag	UNP B8LFD6
2	-10	GLN	-	expression tag	UNP B8LFD6
2	-9	GLN	-	expression tag	UNP B8LFD6
2	-8	MET	-	expression tag	UNP B8LFD6
2	-7	GLY	-	expression tag	UNP B8LFD6
2	-6	ARG	-	expression tag	UNP B8LFD6
2	-5	ASP	-	expression tag	UNP B8LFD6
2	-4	LEU	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
2	-3	TYR	-	expression tag	UNP B8LFD6
2	-2	ASP	-	expression tag	UNP B8LFD6
2	-1	ASP	-	expression tag	UNP B8LFD6
2	0	ASP	-	expression tag	UNP B8LFD6
2	1	ASP	-	expression tag	UNP B8LFD6
2	2	LYS	-	expression tag	UNP B8LFD6
2	3	ASP	-	expression tag	UNP B8LFD6
2	4	PRO	-	expression tag	UNP B8LFD6
2	5	MET	-	expression tag	UNP B8LFD6
2	6	ILE	-	expression tag	UNP B8LFD6
2	7	ASP	-	expression tag	UNP B8LFD6
2	8	PRO	-	expression tag	UNP B8LFD6
2	599	ALA	ARG	conflict	UNP B8LFD6
3	-28	MET	-	expression tag	UNP B8LFD6
3	-27	GLY	-	expression tag	UNP B8LFD6
3	-26	GLY	-	expression tag	UNP B8LFD6
3	-25	SER	-	expression tag	UNP B8LFD6
3	-24	HIS	-	expression tag	UNP B8LFD6
3	-23	HIS	-	expression tag	UNP B8LFD6
3	-22	HIS	-	expression tag	UNP B8LFD6
3	-21	HIS	-	expression tag	UNP B8LFD6
3	-20	HIS	-	expression tag	UNP B8LFD6
3	-19	HIS	-	expression tag	UNP B8LFD6
3	-18	GLY	-	expression tag	UNP B8LFD6
3	-17	MET	-	expression tag	UNP B8LFD6
3	-16	ALA	-	expression tag	UNP B8LFD6
3	-15	SER	-	expression tag	UNP B8LFD6
3	-14	MET	-	expression tag	UNP B8LFD6
3	-13	THR	-	expression tag	UNP B8LFD6
3	-12	GLY	-	expression tag	UNP B8LFD6
3	-11	GLY	-	expression tag	UNP B8LFD6
3	-10	GLN	-	expression tag	UNP B8LFD6
3	-9	GLN	-	expression tag	UNP B8LFD6
3	-8	MET	-	expression tag	UNP B8LFD6
3	-7	GLY	-	expression tag	UNP B8LFD6
3	-6	ARG	-	expression tag	UNP B8LFD6
3	-5	ASP	-	expression tag	UNP B8LFD6
3	-4	LEU	-	expression tag	UNP B8LFD6
3	-3	TYR	-	expression tag	UNP B8LFD6
3	-2	ASP	-	expression tag	UNP B8LFD6
3	-1	ASP	-	expression tag	UNP B8LFD6
3	0	ASP	-	expression tag	UNP B8LFD6

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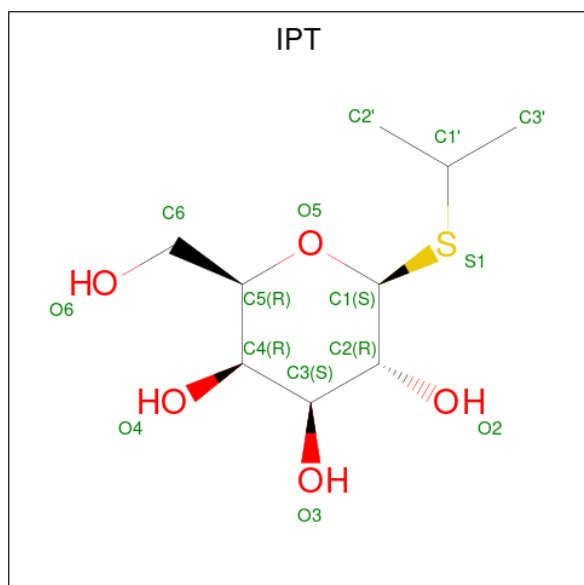
Chain	Residue	Modelled	Actual	Comment	Reference
3	1	ASP	-	expression tag	UNP B8LFD6
3	2	LYS	-	expression tag	UNP B8LFD6
3	3	ASP	-	expression tag	UNP B8LFD6
3	4	PRO	-	expression tag	UNP B8LFD6
3	5	MET	-	expression tag	UNP B8LFD6
3	6	ILE	-	expression tag	UNP B8LFD6
3	7	ASP	-	expression tag	UNP B8LFD6
3	8	PRO	-	expression tag	UNP B8LFD6
3	599	ALA	ARG	conflict	UNP B8LFD6
4	-28	MET	-	expression tag	UNP B8LFD6
4	-27	GLY	-	expression tag	UNP B8LFD6
4	-26	GLY	-	expression tag	UNP B8LFD6
4	-25	SER	-	expression tag	UNP B8LFD6
4	-24	HIS	-	expression tag	UNP B8LFD6
4	-23	HIS	-	expression tag	UNP B8LFD6
4	-22	HIS	-	expression tag	UNP B8LFD6
4	-21	HIS	-	expression tag	UNP B8LFD6
4	-20	HIS	-	expression tag	UNP B8LFD6
4	-19	HIS	-	expression tag	UNP B8LFD6
4	-18	GLY	-	expression tag	UNP B8LFD6
4	-17	MET	-	expression tag	UNP B8LFD6
4	-16	ALA	-	expression tag	UNP B8LFD6
4	-15	SER	-	expression tag	UNP B8LFD6
4	-14	MET	-	expression tag	UNP B8LFD6
4	-13	THR	-	expression tag	UNP B8LFD6
4	-12	GLY	-	expression tag	UNP B8LFD6
4	-11	GLY	-	expression tag	UNP B8LFD6
4	-10	GLN	-	expression tag	UNP B8LFD6
4	-9	GLN	-	expression tag	UNP B8LFD6
4	-8	MET	-	expression tag	UNP B8LFD6
4	-7	GLY	-	expression tag	UNP B8LFD6
4	-6	ARG	-	expression tag	UNP B8LFD6
4	-5	ASP	-	expression tag	UNP B8LFD6
4	-4	LEU	-	expression tag	UNP B8LFD6
4	-3	TYR	-	expression tag	UNP B8LFD6
4	-2	ASP	-	expression tag	UNP B8LFD6
4	-1	ASP	-	expression tag	UNP B8LFD6
4	0	ASP	-	expression tag	UNP B8LFD6
4	1	ASP	-	expression tag	UNP B8LFD6
4	2	LYS	-	expression tag	UNP B8LFD6
4	3	ASP	-	expression tag	UNP B8LFD6
4	4	PRO	-	expression tag	UNP B8LFD6

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Chain	Residue	Modelled	Actual	Comment	Reference
4	5	MET	-	expression tag	UNP B8LFD6
4	6	ILE	-	expression tag	UNP B8LFD6
4	7	ASP	-	expression tag	UNP B8LFD6
4	8	PRO	-	expression tag	UNP B8LFD6
4	599	ALA	ARG	conflict	UNP B8LFD6

- Molecule 2 is 1-methylethyl 1-thio-beta-D-galactopyranoside (CCD ID: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	1	1	Total	C	O	S	0	0
			15	9	5	1		
2	1	1	Total	C	O	S	0	0
			15	9	5	1		
2	2	1	Total	C	O	S	0	0
			15	9	5	1		
2	2	1	Total	C	O	S	0	0
			15	9	5	1		
2	3	1	Total	C	O	S	0	0
			15	9	5	1		
2	3	1	Total	C	O	S	0	0
			15	9	5	1		
2	4	1	Total	C	O	S	0	0
			15	9	5	1		
2	4	1	Total	C	O	S	0	0
			15	9	5	1		

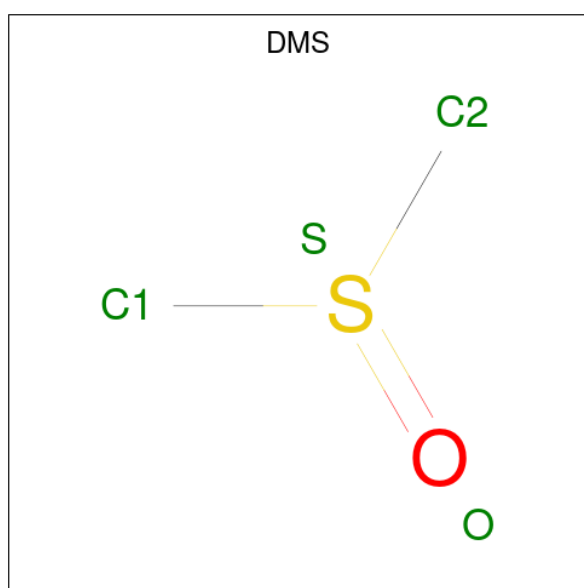
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	4	Total	Mg	0	0
			4	4		
3	2	4	Total	Mg	0	0
			4	4		
3	3	3	Total	Mg	0	0
			3	3		
3	4	3	Total	Mg	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	4	Total	Na	0	0
			4	4		
4	2	4	Total	Na	0	0
			4	4		
4	3	4	Total	Na	0	0
			4	4		
4	4	4	Total	Na	0	0
			4	4		

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



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

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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	2	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	3	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0
5	4	1	Total 4	C 2	O 1	S 1	0	0

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1	1022	Total	O	0	0
			1022	1022		
6	2	1089	Total	O	0	0
			1089	1089		
6	3	1051	Total	O	0	0
			1051	1051		
6	4	946	Total	O	0	0
			946	946		

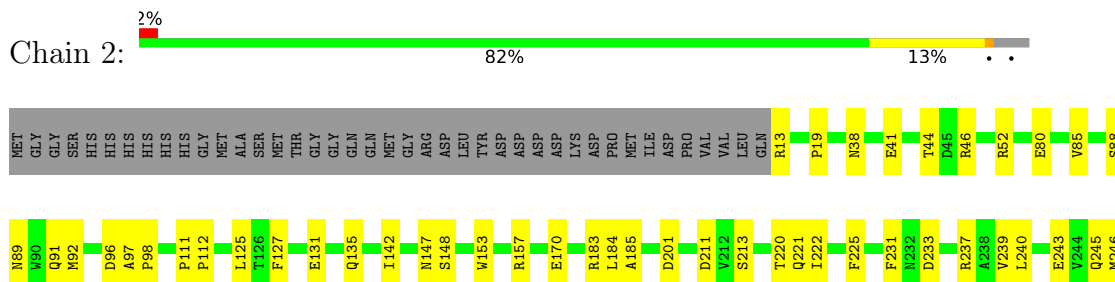
3 Residue-property plots

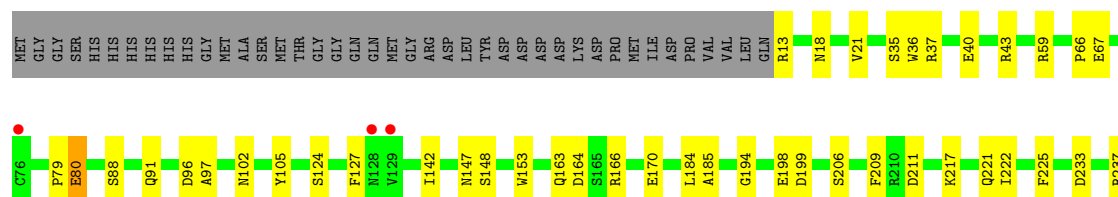
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

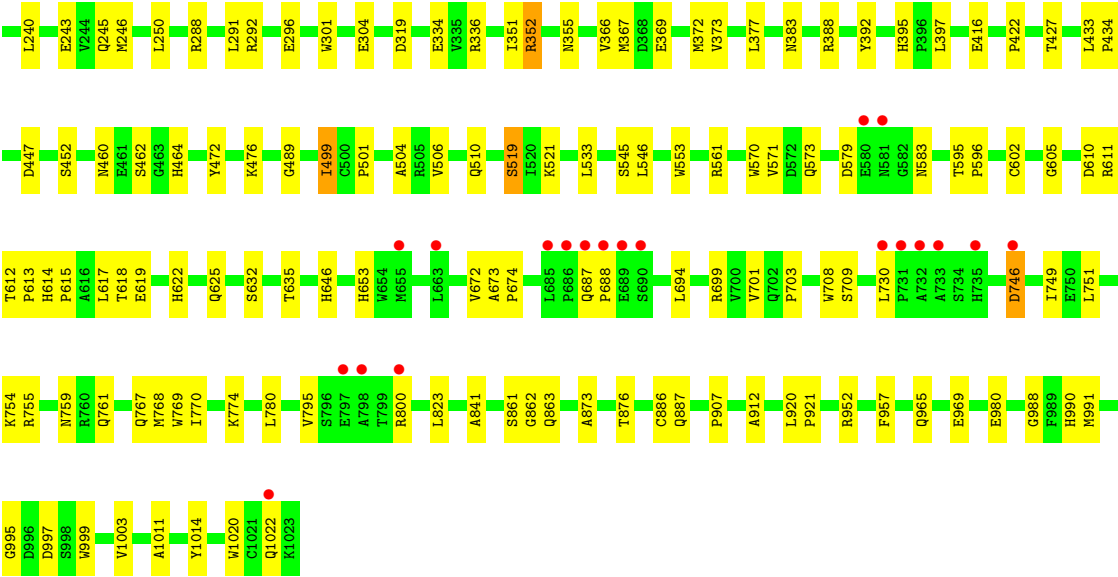
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase







4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.83Å 163.28Å 204.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.42 – 1.90 12.42 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.0 (12.42-1.90) 93.6 (12.42-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.90Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.248 0.217 , 0.246	Depositor DCC
R_{free} test set	5355 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å ²)	17.0	Xtrriage
Anisotropy	0.203	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 65.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	37334	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 41.77 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2481e-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: IPT, DMS, NA, 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	1	0.33	0/8361	0.86	25/11408 (0.2%)
1	2	0.35	0/8361	0.88	26/11408 (0.2%)
1	3	0.35	0/8361	0.89	29/11408 (0.3%)
1	4	0.32	0/8361	0.86	26/11408 (0.2%)
All	All	0.34	0/33444	0.87	106/45632 (0.2%)

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	1	0	1

There are no bond length outliers.

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	614	HIS	N-CA-C	-8.23	99.33	110.36
1	2	570	TRP	N-CA-C	8.17	120.10	111.03
1	3	97	ALA	N-CA-C	8.16	120.35	110.07
1	4	570	TRP	N-CA-C	8.12	120.05	111.03
1	1	570	TRP	N-CA-C	7.85	119.74	111.03
1	3	614	HIS	N-CA-C	-7.81	99.90	110.36
1	3	988	GLY	N-CA-C	-7.54	102.55	113.86
1	2	988	GLY	N-CA-C	-7.47	102.66	113.86
1	1	614	HIS	N-CA-C	-7.45	100.38	110.36
1	3	605	GLY	N-CA-C	7.32	124.66	113.02
1	4	614	HIS	N-CA-C	-7.23	100.67	110.36
1	2	519	SER	N-CA-C	-7.09	99.95	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	233	ASP	N-CA-C	7.08	118.99	111.28
1	2	233	ASP	N-CA-C	6.90	118.80	111.28
1	4	988	GLY	N-CA-C	-6.88	103.54	113.86
1	3	570	TRP	N-CA-C	6.79	118.57	111.03
1	4	97	ALA	N-CA-C	6.50	118.26	110.07
1	2	646	HIS	N-CA-C	-6.49	100.92	110.52
1	3	571	VAL	N-CA-C	6.48	118.11	108.46
1	2	351	ILE	N-CA-C	6.48	116.80	108.12
1	3	447	ASP	N-CA-C	6.45	121.30	113.17
1	1	166	ARG	N-CA-C	6.34	121.06	112.88
1	1	777	LEU	N-CA-C	-6.32	106.10	113.88
1	1	352	ARG	N-CA-C	-6.31	100.82	109.71
1	3	519	SER	N-CA-C	-6.27	101.14	110.23
1	4	519	SER	N-CA-C	-6.25	101.42	110.24
1	2	352	ARG	N-CA-C	-6.21	100.96	109.71
1	1	519	SER	N-CA-C	-6.17	101.28	110.23
1	1	383	ASN	N-CA-C	6.14	120.10	112.24
1	2	211	ASP	N-CA-C	6.14	118.22	110.24
1	2	323	ILE	N-CA-C	-6.12	105.86	111.67
1	3	222	ILE	N-CA-C	-6.08	99.55	108.54
1	2	98	PRO	N-CA-C	-6.05	101.57	111.68
1	1	504	ALA	N-CA-C	-6.03	101.36	110.28
1	4	504	ALA	N-CA-C	-6.02	101.37	110.28
1	2	383	ASN	N-CA-C	6.01	119.94	112.24
1	3	383	ASN	N-CA-C	5.97	119.88	112.24
1	2	605	GLY	N-CA-C	5.92	122.44	113.02
1	3	211	ASP	N-CA-C	5.89	117.89	110.24
1	3	233	ASP	N-CA-C	5.87	118.43	111.33
1	3	934	GLU	N-CA-C	-5.86	101.98	110.24
1	3	98	PRO	N-CA-C	-5.82	101.96	111.68
1	1	97	ALA	N-CA-C	5.81	117.39	110.07
1	2	612	THR	N-CA-C	-5.79	102.47	109.83
1	1	605	GLY	N-CA-C	5.79	122.22	113.02
1	2	97	ALA	N-CA-C	5.74	117.30	110.07
1	2	499	ILE	N-CA-C	-5.73	100.45	108.12
1	4	746	ASP	N-CA-C	5.73	117.78	109.07
1	4	233	ASP	N-CA-C	5.70	118.23	111.33
1	1	646	HIS	N-CA-C	-5.70	102.09	110.52
1	2	395	HIS	N-CA-C	-5.67	102.44	109.64
1	2	89	ASN	N-CA-C	-5.66	99.96	109.07
1	2	571	VAL	N-CA-C	5.64	116.86	108.46
1	3	221	GLN	N-CA-C	5.61	117.49	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	323	ILE	N-CA-C	-5.60	106.35	111.67
1	1	447	ASP	N-CA-C	5.59	120.21	113.17
1	4	605	GLY	N-CA-C	5.59	121.90	113.02
1	1	545	SER	N-CA-C	5.57	115.76	108.07
1	4	383	ASN	N-CA-C	5.57	119.37	112.24
1	4	352	ARG	N-CA-C	-5.57	101.20	109.11
1	1	211	ASP	N-CA-C	5.55	117.46	110.24
1	4	646	HIS	N-CA-C	-5.55	102.30	110.52
1	3	499	ILE	N-CA-C	-5.54	100.69	108.12
1	4	447	ASP	N-CA-C	5.50	119.97	112.88
1	3	777	LEU	N-CA-C	-5.47	107.15	113.88
1	1	499	ILE	N-CA-C	-5.46	100.80	108.12
1	2	220	THR	N-CA-C	-5.46	99.62	108.41
1	3	746	ASP	N-CA-C	5.46	117.36	109.07
1	3	351	ILE	N-CA-C	5.41	115.37	108.12
1	1	746	ASP	N-CA-C	5.39	117.26	109.07
1	2	746	ASP	N-CA-C	5.37	117.23	109.07
1	3	299	LYS	N-CA-C	-5.36	101.06	109.25
1	3	89	ASN	N-CA-C	-5.35	100.46	109.07
1	1	98	PRO	N-CA-C	-5.33	102.78	111.68
1	4	545	SER	N-CA-C	5.33	115.42	108.07
1	2	504	ALA	N-CA-C	-5.32	101.80	110.20
1	2	777	LEU	N-CA-C	-5.31	106.94	113.41
1	1	571	VAL	N-CA-C	5.28	116.33	108.46
1	4	571	VAL	N-CA-C	5.28	116.33	108.46
1	2	787	ALA	N-CA-C	-5.26	100.38	109.58
1	1	409	VAL	N-CA-C	5.25	116.05	108.48
1	4	612	THR	N-CA-C	-5.23	103.06	109.65
1	3	612	THR	N-CA-C	-5.21	103.22	109.83
1	3	771	GLY	N-CA-C	-5.20	103.50	111.24
1	2	222	ILE	N-CA-C	-5.19	100.85	108.54
1	4	211	ASP	N-CA-C	5.18	116.97	110.24
1	4	351	ILE	N-CA-C	5.18	115.06	108.12
1	4	209	PHE	N-CA-C	5.17	119.57	113.16
1	3	504	ALA	N-CA-C	-5.17	102.03	110.20
1	2	221	GLN	N-CA-C	5.16	117.04	109.24
1	4	510	GLN	CA-C-N	5.16	126.29	119.84
1	4	510	GLN	C-N-CA	5.16	126.29	119.84
1	1	472	TYR	N-CA-C	-5.14	105.57	111.07
1	1	563	GLN	N-CA-C	5.13	118.37	112.57
1	4	221	GLN	N-CA-C	5.12	116.78	109.14
1	4	499	ILE	N-CA-C	-5.12	101.26	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	770	ILE	N-CA-C	-5.09	98.62	106.72
1	3	166	ARG	N-CA-C	5.09	120.12	112.94
1	1	150	PHE	N-CA-C	5.09	116.25	108.52
1	3	563	GLN	N-CA-C	5.08	118.31	112.57
1	1	934	GLU	N-CA-C	-5.07	103.09	110.24
1	4	222	ILE	N-CA-C	-5.04	100.51	108.23
1	3	545	SER	N-CA-C	5.04	115.02	108.07
1	3	472	TYR	N-CA-C	-5.02	105.70	111.07
1	4	635	THR	N-CA-C	5.02	116.91	108.73
1	1	635	THR	N-CA-C	5.02	117.42	109.24

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	100	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	8119	0	7708	113	0
1	2	8119	0	7707	101	0
1	3	8119	0	7707	91	0
1	4	8119	0	7708	103	0
2	1	30	0	35	0	0
2	2	30	0	35	2	0
2	3	30	0	35	2	0
2	4	30	0	35	1	0
3	1	4	0	0	0	0
3	2	4	0	0	0	0
3	3	3	0	0	0	0
3	4	3	0	0	0	0
4	1	4	0	0	0	0
4	2	4	0	0	0	0
4	3	4	0	0	0	0
4	4	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1	132	0	198	7	0
5	2	172	0	258	15	0
5	3	172	0	258	12	0
5	4	124	0	186	5	0
6	1	1022	0	0	13	0
6	2	1089	0	0	5	0
6	3	1051	0	0	6	0
6	4	946	0	0	3	0
All	All	37334	0	31870	397	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 6.

All (397) 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)
1:2:431:ARG:HB2	1:2:431:ARG:HH21	1.33	0.93
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.52	0.91
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.53	0.89
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.59	0.84
1:2:770:ILE:HG21	1:2:1022:GLN:HE22	1.42	0.84
1:4:153:TRP:HB2	1:4:185:ALA:HB3	1.60	0.82
1:3:125:LEU:HA	5:3:6029:DMS:H22	1.62	0.81
1:1:153:TRP:HB2	1:1:185:ALA:HB3	1.64	0.79
1:2:142:ILE:HG12	1:2:170:GLU:HG2	1.65	0.77
1:1:765:LEU:HD21	1:1:768:MET:HE2	1.67	0.77
1:2:770:ILE:HG21	1:2:1022:GLN:NE2	2.03	0.73
1:4:653:HIS:HD1	1:4:699:ARG:NH2	1.86	0.73
1:3:768:MET:HE1	1:3:1020:TRP:CH2	2.24	0.73
1:3:59:ARG:HG2	5:3:6029:DMS:H23	1.73	0.71
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.73	0.70
1:4:754:LYS:HE2	1:4:1022:GLN:NE2	2.06	0.69
1:2:239:VAL:HG23	2:2:2002:IPT:H2'1	1.75	0.69
1:1:372:MET:HE1	1:1:395:HIS:HB3	1.75	0.68
1:3:131:GLU:O	1:3:135:GLN:HG3	1.92	0.68
1:2:965:GLN:O	1:2:969:GLU:HG3	1.95	0.67
1:1:230:ARG:HG3	6:1:4904:HOH:O	1.95	0.67
1:2:245:GLN:HG2	1:2:288:ARG:HG2	1.77	0.65
1:2:749:ILE:HD12	1:2:858:ILE:HD12	1.78	0.65
1:4:754:LYS:HE2	1:4:1022:GLN:HE21	1.60	0.65
1:4:372:MET:HE1	1:4:395:HIS:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:768:MET:HE1	1:4:1020:TRP:CZ2	2.31	0.65
1:1:737:ILE:HD12	1:1:738:PRO:HD2	1.80	0.64
1:1:579:ASP:OD2	1:1:583:ASN:HB2	1.98	0.64
1:4:377:LEU:HD22	1:4:708:TRP:HA	1.80	0.64
1:1:304:GLU:HA	6:1:4948:HOH:O	1.97	0.64
1:1:127:PHE:HE2	1:1:184:LEU:HG	1.62	0.64
1:4:965:GLN:O	1:4:969:GLU:HG3	1.98	0.64
1:3:127:PHE:CE2	1:3:184:LEU:HG	2.34	0.63
1:1:245:GLN:HG2	1:1:288:ARG:HG2	1.80	0.63
1:2:768:MET:HE1	1:2:1020:TRP:CH2	2.33	0.63
1:4:91:GLN:HG3	1:4:96:ASP:OD1	1.99	0.63
1:2:127:PHE:CE2	1:2:184:LEU:HG	2.35	0.62
1:4:823:LEU:HD11	1:4:841:ALA:HB2	1.80	0.62
1:2:431:ARG:HH21	1:2:431:ARG:CB	2.11	0.61
1:2:372:MET:HE2	6:2:4190:HOH:O	2.00	0.61
1:3:703:PRO:HG2	5:3:6016:DMS:H11	1.81	0.61
1:3:749:ILE:HD12	1:3:858:ILE:HD12	1.82	0.61
1:2:770:ILE:HD13	1:2:1022:GLN:NE2	2.16	0.61
1:1:965:GLN:O	1:1:969:GLU:HG3	2.00	0.60
1:4:367:MET:HB3	1:4:372:MET:HE3	1.83	0.60
1:4:88:SER:HA	1:4:366:VAL:HG21	1.82	0.60
1:3:58:TRP:HA	5:3:6029:DMS:H21	1.82	0.60
1:1:873:ALA:O	1:1:876:THR:HG22	2.01	0.60
1:3:245:GLN:HB3	6:3:4956:HOH:O	2.01	0.60
1:1:573:GLN:HB2	1:1:602:CYS:O	2.02	0.59
1:3:372:MET:HE1	1:3:395:HIS:HB3	1.83	0.59
1:3:377:LEU:HD22	1:3:708:TRP:HA	1.84	0.59
1:2:424:ASN:OD1	1:3:279:ILE:HD11	2.02	0.59
1:3:774:LYS:HD2	1:3:774:LYS:O	2.02	0.59
1:2:127:PHE:HE2	1:2:184:LEU:HG	1.66	0.59
1:1:127:PHE:CE2	1:1:184:LEU:HG	2.38	0.59
1:3:823:LEU:O	1:4:730:LEU:HD21	2.03	0.59
1:1:714:ILE:HD13	5:1:6032:DMS:H13	1.86	0.58
1:3:984:LEU:HD21	1:3:986:ILE:HD11	1.85	0.58
1:2:237:ARG:HD2	5:2:6040:DMS:H12	1.85	0.58
1:4:355:ASN:OD1	1:4:388:ARG:HD3	2.03	0.58
1:3:75:GLU:HG2	6:3:5024:HOH:O	2.04	0.57
1:1:194:GLY:O	1:1:198:GLU:HG3	2.03	0.57
1:2:372:MET:HE1	1:2:395:HIS:HB3	1.86	0.57
1:2:595:THR:HA	1:2:596:PRO:C	2.30	0.57
1:3:127:PHE:HE2	1:3:184:LEU:HG	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:292:ARG:HH12	5:1:6009:DMS:H13	1.69	0.57
1:2:1014:TYR:HA	5:2:6026:DMS:H12	1.86	0.57
1:1:79:PRO:HG2	1:1:80:GLU:OE2	2.05	0.57
1:2:598:ASP:OD1	5:2:6032:DMS:H12	2.04	0.57
1:3:245:GLN:HG2	1:3:288:ARG:HG2	1.84	0.57
1:4:304:GLU:HA	6:4:4892:HOH:O	2.05	0.56
1:2:499:ILE:HG22	1:2:501:PRO:HD3	1.87	0.56
1:4:755:ARG:HD3	6:4:4870:HOH:O	2.04	0.56
1:2:765:LEU:HD21	1:2:768:MET:HE2	1.88	0.56
1:3:573:GLN:HB2	1:3:602:CYS:O	2.05	0.56
1:1:131:GLU:O	1:1:135:GLN:HG3	2.06	0.56
1:2:88:SER:HA	1:2:366:VAL:HG21	1.88	0.56
1:1:299:LYS:HD2	6:1:4745:HOH:O	2.05	0.56
1:4:615:PRO:O	1:4:618:THR:HG22	2.06	0.56
1:3:965:GLN:O	1:3:969:GLU:HG3	2.05	0.56
1:1:59:ARG:HB2	1:1:124:SER:OG	2.06	0.56
1:4:730:LEU:N	1:4:730:LEU:HD12	2.21	0.55
1:1:595:THR:HA	1:1:596:PRO:C	2.31	0.55
1:2:367:MET:HA	1:2:367:MET:HE2	1.88	0.55
1:1:355:ASN:OD1	1:1:388:ARG:HD3	2.05	0.55
1:1:749:ILE:N	1:1:749:ILE:HD12	2.22	0.55
1:1:18:ASN:ND2	1:1:21:VAL:HG23	2.22	0.55
1:3:730:LEU:N	1:3:730:LEU:HD12	2.23	0.55
1:4:708:TRP:CZ2	5:4:6002:DMS:H23	2.41	0.55
1:4:240:LEU:C	1:4:240:LEU:HD23	2.32	0.54
1:3:431:ARG:HH21	1:3:431:ARG:HB2	1.72	0.54
1:4:952:ARG:HH11	1:4:952:ARG:HB2	1.72	0.54
1:2:375:ASP:O	1:2:379:MET:HG3	2.07	0.54
1:2:397:LEU:HD11	5:2:6018:DMS:H13	1.88	0.54
1:4:147:ASN:HB3	1:4:206:SER:HA	1.90	0.54
1:4:237:ARG:HD2	1:4:296:GLU:OE1	2.08	0.54
1:3:499:ILE:HG22	1:3:501:PRO:HD3	1.90	0.54
1:3:88:SER:HA	1:3:366:VAL:HG21	1.90	0.54
1:1:768:MET:HB3	6:1:4926:HOH:O	2.08	0.53
1:3:372:MET:HE2	6:3:4190:HOH:O	2.08	0.53
1:3:749:ILE:CD1	1:3:858:ILE:HD12	2.39	0.53
1:4:613:PRO:HB3	1:4:617:LEU:HD23	1.90	0.53
1:4:767:GLN:HE22	1:4:774:LYS:HE3	1.74	0.53
1:2:749:ILE:CD1	1:2:858:ILE:HD12	2.39	0.53
1:3:355:ASN:OD1	1:3:388:ARG:HD3	2.08	0.53
1:2:615:PRO:O	1:2:618:THR:HG22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:88:SER:HA	1:1:366:VAL:HG21	1.91	0.52
1:4:749:ILE:N	1:4:749:ILE:HD12	2.24	0.52
1:4:127:PHE:HE2	1:4:184:LEU:HG	1.75	0.52
1:3:887:GLN:NE2	1:3:980:GLU:O	2.42	0.52
1:1:372:MET:HE2	6:1:4186:HOH:O	2.09	0.52
1:2:240:LEU:C	1:2:240:LEU:HD23	2.35	0.52
1:4:499:ILE:HG22	1:4:501:PRO:HD3	1.92	0.52
1:3:619:GLU:HA	1:3:912:ALA:HB2	1.91	0.52
1:2:730:LEU:HD12	1:2:730:LEU:N	2.24	0.52
1:3:615:PRO:O	1:3:618:THR:HG22	2.10	0.52
1:1:91:GLN:HG3	1:1:96:ASP:OD1	2.10	0.51
1:2:632:SER:HB2	5:2:6022:DMS:H23	1.92	0.51
1:4:127:PHE:CE2	1:4:184:LEU:HG	2.45	0.51
1:4:625:GLN:HB2	5:4:6001:DMS:H21	1.92	0.51
1:2:863:GLN:NE2	1:2:952:ARG:HH21	2.08	0.51
1:3:147:ASN:HB3	1:3:206:SER:HA	1.92	0.51
1:3:632:SER:HB3	5:3:6020:DMS:H12	1.93	0.51
1:2:433:LEU:HB3	1:2:434:PRO:HD3	1.91	0.51
1:4:334:GLU:OE1	1:4:336:ARG:NH1	2.44	0.51
1:4:873:ALA:O	1:4:876:THR:HG22	2.11	0.51
1:1:765:LEU:CD2	1:1:768:MET:HE2	2.39	0.51
1:1:379:MET:HE1	1:1:387:VAL:HB	1.92	0.51
1:2:1015:HIS:H	5:2:6026:DMS:H12	1.75	0.51
1:4:579:ASP:OD2	1:4:583:ASN:HB2	2.11	0.51
1:1:499:ILE:HG22	1:1:501:PRO:HD3	1.93	0.51
1:1:619:GLU:HA	1:1:912:ALA:HB2	1.92	0.51
1:1:240:LEU:C	1:1:240:LEU:HD23	2.36	0.50
1:1:368:ASP:OD2	1:1:370:GLN:HB3	2.11	0.50
1:2:201:ASP:OD2	2:2:2001:IPT:H62	2.10	0.50
1:2:730:LEU:HD12	1:2:730:LEU:H	1.76	0.50
1:3:91:GLN:HG3	1:3:96:ASP:OD1	2.11	0.50
1:1:890:GLN:HG2	1:1:891:VAL:N	2.27	0.50
1:4:102:ASN:ND2	2:4:2001:IPT:H2'3	2.27	0.50
1:1:13:ARG:NH1	1:4:13:ARG:HG3	2.26	0.50
1:3:576:ILE:O	5:3:6040:DMS:H21	2.11	0.50
1:4:863:GLN:OE1	1:4:952:ARG:NH2	2.45	0.50
1:3:672:VAL:HG22	1:3:678:GLN:HB2	1.94	0.50
1:1:706:THR:HG22	6:1:4518:HOH:O	2.12	0.49
1:2:864:MET:HE3	1:2:866:ILE:HD11	1.94	0.49
1:3:102:ASN:ND2	5:3:6030:DMS:H22	2.27	0.49
1:3:240:LEU:HD23	1:3:240:LEU:C	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:348:PRO:HB2	6:1:4921:HOH:O	2.12	0.49
1:4:768:MET:HE1	1:4:1020:TRP:CH2	2.48	0.49
1:4:369:GLU:HG3	1:4:397:LEU:HD21	1.95	0.49
1:3:1011:ALA:HB3	1:3:1014:TYR:CZ	2.47	0.49
1:1:710:GLU:HG3	5:1:6021:DMS:H11	1.95	0.49
1:3:246:MET:SD	1:3:246:MET:C	2.96	0.49
1:4:36:TRP:O	1:4:37:ARG:HD3	2.13	0.49
1:4:246:MET:SD	1:4:246:MET:C	2.96	0.49
1:4:920:LEU:HB3	1:4:921:PRO:HD2	1.95	0.49
1:4:291:LEU:N	1:4:291:LEU:HD22	2.28	0.49
1:4:595:THR:HA	1:4:596:PRO:C	2.38	0.49
1:4:699:ARG:HD3	5:4:6027:DMS:H21	1.93	0.49
1:2:867:THR:HG23	1:2:1015:HIS:HE1	1.77	0.49
1:3:128:ASN:HA	1:3:180:GLY:O	2.12	0.49
1:4:751:LEU:HD23	1:4:862:GLY:HA2	1.95	0.49
1:4:952:ARG:HB2	1:4:952:ARG:NH1	2.27	0.48
1:3:200:GLN:HG2	1:3:391:HIS:HB2	1.95	0.48
1:3:266:GLN:O	5:3:6018:DMS:H22	2.12	0.48
1:3:595:THR:HA	1:3:596:PRO:C	2.37	0.48
1:3:765:LEU:HD21	1:3:768:MET:HE2	1.95	0.48
1:2:739:HIS:HB2	6:2:4974:HOH:O	2.14	0.48
1:4:105:TYR:CE2	1:4:199:ASP:HB2	2.49	0.48
1:2:687:GLN:N	1:2:687:GLN:OE1	2.47	0.48
1:2:153:TRP:HB2	1:2:185:ALA:HB3	1.96	0.48
1:2:157:ARG:HD3	6:2:4673:HOH:O	2.13	0.48
1:2:1011:ALA:HB3	1:2:1014:TYR:CZ	2.49	0.48
1:4:887:GLN:NE2	1:4:980:GLU:O	2.41	0.48
1:4:66:PRO:HG2	1:4:67:GLU:OE1	2.13	0.48
1:4:194:GLY:O	1:4:198:GLU:HG3	2.14	0.48
1:4:730:LEU:HD12	1:4:730:LEU:H	1.79	0.48
1:3:431:ARG:HD2	6:3:4509:HOH:O	2.13	0.47
1:4:319:ASP:OD1	1:4:319:ASP:N	2.44	0.47
1:1:724:GLU:O	1:2:847:LYS:NZ	2.47	0.47
1:1:354:VAL:CG1	1:1:379:MET:HE3	2.44	0.47
1:4:472:TYR:O	1:4:476:LYS:HG2	2.14	0.47
1:4:991:MET:HE3	1:4:1003:VAL:HG21	1.97	0.47
1:1:317:THR:OG1	1:1:319:ASP:OD1	2.32	0.47
1:1:1017:GLN:HB2	6:1:4900:HOH:O	2.14	0.47
1:2:91:GLN:HG3	1:2:96:ASP:OD1	2.15	0.47
1:2:621:LYS:NZ	5:2:6043:DMS:H13	2.30	0.47
1:2:800:ARG:HG2	1:2:800:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1013:ARG:O	5:2:6026:DMS:H23	2.15	0.47
1:3:892:ALA:HB3	1:3:946:TYR:CE1	2.49	0.47
1:1:748:CYS:C	1:1:749:ILE:HD12	2.39	0.47
1:1:751:LEU:HD23	1:1:862:GLY:HA2	1.97	0.47
1:1:1023:LYS:NZ	1:1:1023:LYS:HB3	2.29	0.47
1:2:619:GLU:HA	1:2:912:ALA:HB2	1.95	0.47
1:3:369:GLU:HG3	1:3:397:LEU:HD21	1.96	0.47
1:4:573:GLN:HB2	1:4:602:CYS:O	2.15	0.47
1:1:147:ASN:HB3	1:1:206:SER:HA	1.97	0.47
1:1:615:PRO:O	1:1:618:THR:HG22	2.14	0.47
1:2:125:LEU:HD21	5:2:6027:DMS:H13	1.96	0.47
1:3:613:PRO:HB3	1:3:617:LEU:HD23	1.96	0.47
1:3:688:PRO:HG3	1:3:694:LEU:HD21	1.96	0.47
1:1:427:THR:HG21	1:1:462:SER:HB3	1.96	0.47
1:2:131:GLU:HG3	1:2:135:GLN:HG3	1.97	0.47
1:4:755:ARG:HB2	1:4:769:TRP:HB2	1.96	0.47
1:2:424:ASN:CG	1:3:279:ILE:HD11	2.40	0.46
1:2:431:ARG:HB2	1:2:431:ARG:NH2	2.15	0.46
1:4:292:ARG:HH12	5:4:6009:DMS:H13	1.80	0.46
1:1:52:ARG:O	1:1:213:SER:HB2	2.15	0.46
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.96	0.46
1:2:674:PRO:O	1:2:675:GLN:HB2	2.16	0.46
1:2:630:ARG:NH1	1:2:637:GLU:OE1	2.49	0.46
1:2:751:LEU:HD21	1:2:860:GLY:O	2.15	0.46
1:3:147:ASN:HA	1:3:148:SER:HA	1.61	0.46
1:3:646:HIS:ND1	1:3:673:ALA:HA	2.31	0.46
1:4:59:ARG:HB2	1:4:124:SER:OG	2.16	0.46
1:3:379:MET:HE1	1:3:387:VAL:HB	1.97	0.46
1:1:730:LEU:N	1:1:730:LEU:HD12	2.30	0.46
1:4:619:GLU:HA	1:4:912:ALA:HB2	1.97	0.46
1:1:147:ASN:HA	1:1:148:SER:HA	1.61	0.46
1:2:52:ARG:O	1:2:213:SER:HB2	2.16	0.46
1:2:225:PHE:HA	1:2:243:GLU:O	2.16	0.46
1:4:746:ASP:OD1	1:4:759:ASN:HA	2.16	0.46
1:2:573:GLN:HB2	1:2:602:CYS:O	2.16	0.46
1:1:105:TYR:CE2	1:1:199:ASP:HB2	2.51	0.45
1:1:632:SER:HB3	5:1:6019:DMS:H12	1.98	0.45
1:1:380:LYS:O	5:1:6002:DMS:H21	2.16	0.45
1:1:701:VAL:O	1:1:703:PRO:HD3	2.15	0.45
1:2:601:PHE:CD2	5:2:6032:DMS:H13	2.51	0.45
1:3:636:ILE:HD11	1:3:682:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:13:ARG:HG3	1:4:13:ARG:NH1	2.31	0.45
1:2:131:GLU:O	1:2:135:GLN:HG3	2.16	0.45
1:1:887:GLN:NE2	1:1:980:GLU:O	2.49	0.45
1:2:1015:HIS:H	5:2:6026:DMS:C1	2.29	0.45
1:3:674:PRO:O	1:3:675:GLN:HB2	2.16	0.45
1:4:246:MET:HE3	1:4:250:LEU:HD23	1.99	0.45
1:2:38:ASN:CG	1:2:41:GLU:HG3	2.42	0.45
1:2:746:ASP:HA	1:2:760:ARG:HG3	1.99	0.45
1:2:549:PHE:CE2	1:2:620:ALA:HA	2.51	0.45
1:4:225:PHE:HA	1:4:243:GLU:O	2.17	0.45
1:1:367:MET:HB3	1:1:372:MET:HE3	1.99	0.45
1:2:568:TRP:CD2	1:2:569:ASP:HB3	2.52	0.45
1:3:19:PRO:HD3	1:3:112:PRO:CB	2.47	0.45
1:4:952:ARG:HH11	1:4:952:ARG:CB	2.30	0.45
1:3:873:ALA:O	1:3:876:THR:HG22	2.16	0.45
1:1:737:ILE:HD13	1:1:832:ASP:HA	1.99	0.45
1:2:111:PRO:HA	1:2:112:PRO:HA	1.83	0.45
1:3:279:ILE:HG23	1:3:284:GLY:HA2	1.99	0.45
1:3:533:LEU:C	1:3:533:LEU:HD23	2.41	0.44
1:1:200:GLN:HG2	1:1:391:HIS:HB2	1.99	0.44
1:1:634:GLN:HB2	1:1:681:GLU:OE2	2.17	0.44
1:2:995:GLY:C	1:2:997:ASP:N	2.75	0.44
1:3:431:ARG:NH2	6:3:4869:HOH:O	2.50	0.44
1:1:768:MET:HE1	1:1:1020:TRP:CH2	2.52	0.44
1:3:730:LEU:HD12	1:3:730:LEU:H	1.81	0.44
1:4:464:HIS:HB2	1:4:489:GLY:HA3	1.99	0.44
1:1:131:GLU:HG3	1:1:135:GLN:HG3	2.00	0.44
1:3:428:ASP:O	5:3:6013:DMS:H11	2.17	0.44
1:1:225:PHE:HA	1:1:243:GLU:O	2.18	0.44
1:2:887:GLN:NE2	1:2:980:GLU:O	2.50	0.44
1:3:40:GLU:OE2	1:3:43:ARG:NH2	2.46	0.44
1:3:433:LEU:HB3	1:3:434:PRO:HD3	2.00	0.44
1:1:737:ILE:HD12	1:1:738:PRO:CD	2.46	0.44
1:4:767:GLN:NE2	1:4:774:LYS:HE3	2.32	0.44
1:1:1011:ALA:HB3	1:1:1014:TYR:CZ	2.53	0.44
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.99	0.44
1:4:632:SER:HB3	5:4:6021:DMS:H12	1.99	0.44
1:4:861:SER:OG	1:4:863:GLN:HG3	2.18	0.44
1:1:777:LEU:HG	1:1:889:ALA:HA	1.99	0.44
1:2:246:MET:SD	1:2:246:MET:C	3.01	0.44
1:3:721:ARG:NH1	5:3:1024:DMS:H21	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:40:GLU:OE2	1:4:43:ARG:NH2	2.51	0.44
1:1:49:GLN:HG2	6:1:4584:HOH:O	2.17	0.44
1:1:262:GLN:HG2	6:1:4786:HOH:O	2.16	0.44
1:4:688:PRO:HD3	1:4:694:LEU:HD11	1.99	0.44
1:1:125:LEU:O	1:1:183:ARG:HA	2.18	0.43
1:3:630:ARG:NH1	1:3:637:GLU:OE1	2.51	0.43
1:1:830:LEU:HD22	1:2:828:ASP:HB3	2.00	0.43
1:4:997:ASP:HB2	1:4:999:TRP:CZ2	2.53	0.43
1:2:92:MET:HE2	1:2:92:MET:HA	2.00	0.43
1:3:995:GLY:C	1:3:997:ASP:N	2.74	0.43
1:4:166:ARG:HG3	1:4:392:TYR:HB2	1.99	0.43
1:4:427:THR:HG21	1:4:462:SER:HB3	2.00	0.43
1:1:486:TYR:CE2	1:1:488:GLY:HA3	2.53	0.43
1:1:823:LEU:HD11	1:1:841:ALA:HB2	2.01	0.43
1:4:416:GLU:HG3	1:4:460:ASN:O	2.17	0.43
1:1:305:ILE:HD11	1:1:645:ARG:HB3	1.99	0.43
1:1:610:ASP:O	1:1:611:ARG:HB2	2.17	0.43
1:1:995:GLY:C	1:1:997:ASP:N	2.74	0.43
1:2:13:ARG:HG3	1:3:13:ARG:CZ	2.48	0.43
1:2:800:ARG:HG3	6:2:4921:HOH:O	2.17	0.43
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.54	0.43
1:4:1011:ALA:HB3	1:4:1014:TYR:CZ	2.54	0.43
1:1:372:MET:CE	1:1:395:HIS:HB3	2.45	0.43
1:4:673:ALA:HB1	1:4:674:PRO:HD2	2.00	0.43
1:1:369:GLU:HG3	1:1:397:LEU:HD21	2.00	0.43
1:1:650:GLU:HB3	1:1:670:LEU:HD12	2.00	0.43
1:2:85:VAL:HG23	5:2:6010:DMS:O	2.19	0.43
1:2:125:LEU:O	1:2:183:ARG:HA	2.19	0.43
1:2:770:ILE:O	1:2:770:ILE:HG22	2.19	0.43
1:1:131:GLU:HG3	1:1:135:GLN:CG	2.49	0.43
1:2:867:THR:HG23	1:2:1015:HIS:CE1	2.54	0.43
1:3:239:VAL:HG23	2:3:2002:IPT:H2'1	2.01	0.43
1:3:372:MET:CE	1:3:395:HIS:HB3	2.46	0.43
1:4:163:GLN:O	1:4:164:ASP:HB3	2.19	0.43
1:3:957:PHE:CD1	1:3:957:PHE:C	2.96	0.42
1:2:147:ASN:HA	1:2:148:SER:HA	1.58	0.42
1:3:231:PHE:CD1	1:3:231:PHE:N	2.88	0.42
1:3:577:LYS:O	1:3:584:PRO:HA	2.19	0.42
1:1:19:PRO:HD3	1:1:112:PRO:HB3	2.01	0.42
1:1:533:LEU:HD23	1:1:533:LEU:C	2.44	0.42
1:2:19:PRO:HD3	1:2:112:PRO:CB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:353:GLY:HA2	1:2:386:ALA:O	2.20	0.42
1:4:433:LEU:HB3	1:4:434:PRO:HD3	2.00	0.42
1:1:720:TRP:NE1	5:1:6014:DMS:H23	2.35	0.42
1:1:861:SER:OG	1:1:863:GLN:HG3	2.19	0.42
1:4:795:VAL:HG12	6:4:4965:HOH:O	2.19	0.42
1:2:464:HIS:HB2	1:2:489:GLY:HA3	2.02	0.42
1:3:13:ARG:O	1:3:14:ARG:C	2.62	0.42
1:4:352:ARG:HG2	1:4:553:TRP:CH2	2.55	0.42
1:4:533:LEU:C	1:4:533:LEU:HD23	2.44	0.42
1:4:780:LEU:HA	1:4:886:CYS:HB3	2.01	0.42
1:1:708:TRP:CZ2	5:1:6002:DMS:H23	2.55	0.42
1:3:475:ILE:HA	1:3:478:VAL:HG22	2.02	0.42
1:1:13:ARG:O	1:1:14:ARG:C	2.62	0.42
1:2:533:LEU:C	1:2:533:LEU:HD23	2.45	0.42
1:4:18:ASN:ND2	1:4:21:VAL:HG23	2.34	0.42
1:1:754:LYS:HE2	1:1:1022:GLN:HE21	1.84	0.42
1:4:800:ARG:HG2	1:4:800:ARG:HH11	1.85	0.42
1:4:759:ASN:OD1	1:4:761:GLN:HB3	2.18	0.42
1:1:373:VAL:O	1:1:377:LEU:HG	2.20	0.41
1:1:768:MET:HE1	1:1:1020:TRP:CZ2	2.55	0.41
1:1:784:PHE:HA	1:1:881:ARG:O	2.20	0.41
1:2:995:GLY:O	1:2:996:ASP:C	2.62	0.41
1:3:807:VAL:HG21	5:3:6026:DMS:H21	2.02	0.41
1:1:326:GLU:HA	1:1:326:GLU:OE1	2.20	0.41
1:2:358:GLU:HB3	1:2:367:MET:CG	2.50	0.41
1:1:285:TYR:CE1	1:4:422:PRO:HG3	2.54	0.41
1:2:231:PHE:CD1	1:2:231:PHE:N	2.88	0.41
1:4:995:GLY:C	1:4:997:ASP:N	2.77	0.41
1:1:66:PRO:HG2	1:1:67:GLU:OE1	2.21	0.41
1:1:883:GLY:HA3	1:1:987:ASP:HA	2.02	0.41
1:2:974:HIS:HA	5:2:6015:DMS:H22	2.02	0.41
1:3:525:SER:O	1:4:561:ARG:HD3	2.21	0.41
1:4:79:PRO:HG2	1:4:80:GLU:OE2	2.21	0.41
1:4:147:ASN:HA	1:4:148:SER:HA	1.63	0.41
1:2:237:ARG:HD2	5:2:6040:DMS:H23	2.01	0.41
1:2:372:MET:CE	1:2:395:HIS:HB3	2.48	0.41
1:3:431:ARG:HB2	6:3:4869:HOH:O	2.20	0.41
1:3:857:ARG:HG2	1:3:857:ARG:HH11	1.86	0.41
1:4:708:TRP:CE3	1:4:709:SER:HB3	2.54	0.41
1:1:301:TRP:CH2	1:1:452:SER:HA	2.55	0.41
1:1:788:PRO:HD2	1:1:968:MET:HG3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:92:MET:SD	5:2:6039:DMS:H12	2.61	0.41
1:1:71:GLU:N	1:1:71:GLU:CD	2.78	0.41
1:1:390:SER:HA	1:1:391:HIS:HA	1.83	0.41
1:1:910:LEU:C	1:1:910:LEU:HD12	2.45	0.41
1:2:44:THR:OG1	1:2:46:ARG:HG3	2.21	0.41
1:2:291:LEU:N	1:2:291:LEU:HD22	2.35	0.41
1:4:622:HIS:O	1:4:625:GLN:HG3	2.20	0.41
1:1:506:VAL:HG12	1:1:521:LYS:HE3	2.02	0.41
1:1:800:ARG:HG3	6:1:4829:HOH:O	2.20	0.41
1:1:843:GLN:HA	1:1:847:LYS:O	2.21	0.41
1:3:246:MET:HE3	1:3:250:LEU:HD23	2.03	0.41
1:4:373:VAL:O	1:4:377:LEU:HG	2.20	0.41
1:1:26:ARG:HD2	1:1:169:SER:HA	2.02	0.41
1:1:472:TYR:O	1:1:476:LYS:HG2	2.20	0.41
1:1:581:ASN:HB2	1:1:583:ASN:ND2	2.35	0.41
1:2:730:LEU:H	1:2:730:LEU:CD1	2.33	0.41
1:3:701:VAL:O	1:3:703:PRO:HD3	2.21	0.41
1:4:35:SER:HB2	1:4:217:LYS:HG2	2.01	0.41
1:4:301:TRP:CH2	1:4:452:SER:HA	2.56	0.41
1:4:610:ASP:O	1:4:611:ARG:HB2	2.21	0.41
1:4:907:PRO:HG2	1:4:990:HIS:O	2.20	0.41
1:4:957:PHE:CD1	1:4:957:PHE:C	2.99	0.41
1:3:79:PRO:HG2	1:3:80:GLU:OE2	2.21	0.41
1:3:608:PHE:CD1	1:3:614:HIS:HD2	2.39	0.41
1:3:784:PHE:HA	1:3:881:ARG:O	2.21	0.41
1:2:473:ARG:HA	1:2:473:ARG:HD2	1.92	0.40
1:2:652:LEU:HD23	1:2:680:ILE:HD12	2.03	0.40
1:3:225:PHE:HA	1:3:243:GLU:O	2.21	0.40
1:4:506:VAL:HG12	1:4:521:LYS:HE3	2.03	0.40
1:2:1020:TRP:HD1	1:2:1021:CYS:N	2.18	0.40
1:1:118:ASN:O	1:1:119:PRO:C	2.64	0.40
1:1:561:ARG:HD3	1:2:525:SER:O	2.20	0.40
1:1:817:GLN:HG2	6:1:4323:HOH:O	2.19	0.40
1:1:99:ILE:HD13	6:1:4167:HOH:O	2.21	0.40
1:1:255:ARG:HB2	1:1:316:HIS:CE1	2.57	0.40
1:2:513:PRO:HD2	6:2:4947:HOH:O	2.20	0.40
1:2:569:ASP:O	1:2:605:GLY:HA2	2.21	0.40
1:3:568:TRP:CD2	1:3:569:ASP:HB3	2.56	0.40
1:3:1013:ARG:O	5:3:6027:DMS:H22	2.20	0.40
1:4:701:VAL:O	1:4:703:PRO:HD3	2.21	0.40
1:2:355:ASN:OD1	1:2:388:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:230:ARG:HG3	2:3:2002:IPT:H2'3	2.03	0.40
1:3:431:ARG:HB2	1:3:431:ARG:NH2	2.36	0.40
1:4:730:LEU:H	1:4:730:LEU:CD1	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	1009/1052 (96%)	968 (96%)	41 (4%)	0	100	100
1	2	1009/1052 (96%)	967 (96%)	42 (4%)	0	100	100
1	3	1009/1052 (96%)	972 (96%)	36 (4%)	1 (0%)	48	40
1	4	1009/1052 (96%)	969 (96%)	40 (4%)	0	100	100
All	All	4036/4208 (96%)	3876 (96%)	159 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	3	164	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	863/897 (96%)	858 (99%)	5 (1%)	78	81
1	2	863/897 (96%)	859 (100%)	4 (0%)	81	84
1	3	863/897 (96%)	855 (99%)	8 (1%)	70	73
1	4	863/897 (96%)	858 (99%)	5 (1%)	78	81
All	All	3452/3588 (96%)	3430 (99%)	22 (1%)	78	81

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	519	SER
1	1	546	LEU
1	1	672	VAL
1	1	687	GLN
1	1	750	GLU
1	2	80	GLU
1	2	431	ARG
1	2	519	SER
1	2	546	LEU
1	3	80	GLU
1	3	279	ILE
1	3	431	ARG
1	3	519	SER
1	3	546	LEU
1	3	687	GLN
1	3	761	GLN
1	3	774	LYS
1	4	80	GLU
1	4	519	SER
1	4	546	LEU
1	4	672	VAL
1	4	687	GLN

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

Mol	Chain	Res	Type
1	1	49	GLN
1	1	50	GLN
1	1	128	ASN
1	1	163	GLN
1	1	262	GLN

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Mol	Chain	Res	Type
1	1	307	ASN
1	1	485	GLN
1	1	583	ASN
1	1	624	GLN
1	1	634	GLN
1	1	653	HIS
1	1	702	GLN
1	1	903	GLN
1	1	1022	GLN
1	2	128	ASN
1	2	262	GLN
1	2	485	GLN
1	2	634	GLN
1	2	653	HIS
1	2	824	GLN
1	2	845	GLN
1	2	863	GLN
1	2	903	GLN
1	2	950	GLN
1	2	965	GLN
1	2	1022	GLN
1	3	128	ASN
1	3	262	GLN
1	3	266	GLN
1	3	374	GLN
1	3	485	GLN
1	3	634	GLN
1	3	653	HIS
1	3	718	GLN
1	3	844	HIS
1	3	863	GLN
1	3	890	GLN
1	3	903	GLN
1	3	950	GLN
1	4	50	GLN
1	4	262	GLN
1	4	374	GLN
1	4	485	GLN
1	4	583	ASN
1	4	624	GLN
1	4	675	GLN
1	4	757	GLN

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Mol	Chain	Res	Type
1	4	844	HIS
1	4	903	GLN
1	4	950	GLN
1	4	1022	GLN

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 188 ligands modelled in this entry, 30 are monoatomic - leaving 158 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	2	6042	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	4	2002	-	15,15,15	0.90	1 (6%)	18,21,21	0.70	0
5	DMS	1	6017	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	2	6035	-	3,3,3	0.24	0	3,3,3	0.63	0
2	IPT	3	2001	4	15,15,15	0.89	1 (6%)	18,21,21	0.73	0
5	DMS	3	6027	-	3,3,3	0.19	0	3,3,3	0.64	0
5	DMS	3	6041	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6006	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	6007	-	3,3,3	0.23	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	2	6043	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	3	6019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6002	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	6028	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6023	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	1	6001	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	3	6004	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	4	6021	-	3,3,3	0.24	0	3,3,3	0.64	0
2	IPT	4	2001	4	15,15,15	0.87	1 (6%)	18,21,21	0.71	0
5	DMS	4	6014	-	3,3,3	0.23	0	3,3,3	0.62	0
2	IPT	1	2001	4	15,15,15	0.83	1 (6%)	18,21,21	0.70	0
5	DMS	1	6014	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6012	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	6016	4	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6029	-	3,3,3	0.23	0	3,3,3	0.63	0
2	IPT	1	2002	-	15,15,15	0.98	1 (6%)	18,21,21	0.71	0
5	DMS	1	6016	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6006	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	6015	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	3	6020	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6038	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6030	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6000	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	2	6005	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6040	-	3,3,3	0.21	0	3,3,3	0.65	0
5	DMS	2	6007	-	3,3,3	0.27	0	3,3,3	0.64	0
5	DMS	2	6019	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	2	6023	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6017	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6005	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6014	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	4	6013	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	6025	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6018	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6017	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6035	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6036	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	2	6027	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	4	6002	-	3,3,3	0.29	0	3,3,3	0.61	0
5	DMS	4	6026	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	2	6031	-	3,3,3	0.22	0	3,3,3	0.64	0
5	DMS	1	6024	-	3,3,3	0.23	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	1	6030	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	6004	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	3	6031	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	2	6011	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	3	6021	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	4	6023	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	1	6031	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	6022	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	6022	-	3,3,3	0.26	0	3,3,3	0.66	0
5	DMS	2	6014	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6025	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	4	6005	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	6004	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	6005	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6016	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	6036	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	6012	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	6020	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	6018	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	3	6002	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	6019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6037	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6038	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	6008	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	6001	-	3,3,3	0.19	0	3,3,3	0.58	0
5	DMS	2	6010	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	1	6010	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	4	6015	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	6003	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	6026	-	3,3,3	0.35	0	3,3,3	0.66	0
5	DMS	2	6040	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6034	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	1	6032	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	6011	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	4	6018	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	6007	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	6022	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	4	6019	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6033	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	4	6008	-	3,3,3	0.28	0	3,3,3	0.62	0
5	DMS	2	6037	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	2	6029	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	6028	-	3,3,3	0.24	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	4	6024	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6010	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6001	-	3,3,3	0.19	0	3,3,3	0.59	0
5	DMS	2	6024	-	3,3,3	0.26	0	3,3,3	0.61	0
5	DMS	1	6012	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6003	-	3,3,3	0.22	0	3,3,3	0.66	0
5	DMS	1	6011	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	1	6000	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	4	6017	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	4	6004	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6002	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6025	-	3,3,3	0.27	0	3,3,3	0.61	0
5	DMS	4	6009	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	1024	-	3,3,3	0.12	0	3,3,3	0.64	0
2	IPT	3	2002	-	15,15,15	0.91	1 (6%)	18,21,21	0.72	0
5	DMS	2	6006	-	3,3,3	0.21	0	3,3,3	0.63	0
5	DMS	3	6026	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	6010	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6029	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	6006	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	1	6026	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6032	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	6030	-	3,3,3	0.27	0	3,3,3	0.60	0
5	DMS	4	6025	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	1	6003	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	6028	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	6021	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	1	6027	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	4	6000	-	3,3,3	0.22	0	3,3,3	0.60	0
2	IPT	2	2001	4	15,15,15	0.90	1 (6%)	18,21,21	0.76	0
5	DMS	2	6009	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	6034	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	6039	-	3,3,3	0.21	0	3,3,3	0.67	0
5	DMS	2	6012	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	6024	-	3,3,3	0.24	0	3,3,3	0.62	0
2	IPT	2	2002	-	15,15,15	0.88	1 (6%)	18,21,21	0.72	0
5	DMS	4	6020	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	1	6020	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	6029	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6013	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	4	6001	-	3,3,3	0.17	0	3,3,3	0.59	0
5	DMS	1	6009	-	3,3,3	0.24	0	3,3,3	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	1	6013	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	2	6015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	1	6015	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6003	-	3,3,3	0.26	0	3,3,3	0.67	0
5	DMS	2	6000	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6007	-	3,3,3	0.29	0	3,3,3	0.62	0
5	DMS	2	6008	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	3	6039	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	6021	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6016	4	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	6013	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	3	6009	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	6032	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	6030	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	3	6008	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	6011	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	4	6022	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	4	6027	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	6028	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	6033	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	2	6018	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	6023	-	3,3,3	0.25	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	IPT	2	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	4	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	1	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	3	2001	4	-	3/6/26/26	0/1/1/1
2	IPT	3	2002	-	-	0/6/26/26	0/1/1/1
2	IPT	4	2001	4	-	3/6/26/26	0/1/1/1
2	IPT	2	2001	4	-	1/6/26/26	0/1/1/1
2	IPT	1	2001	4	-	1/6/26/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	2002	IPT	O5-C1	2.65	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	2001	IPT	O5-C1	2.62	1.46	1.42
2	3	2002	IPT	O5-C1	2.51	1.46	1.42
2	4	2001	IPT	O5-C1	2.36	1.46	1.42
2	4	2002	IPT	O5-C1	2.32	1.46	1.42
2	2	2002	IPT	O5-C1	2.31	1.46	1.42
2	3	2001	IPT	O5-C1	2.23	1.46	1.42
2	1	2001	IPT	O5-C1	2.12	1.45	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	3	2001	IPT	C2'-C1'-S1-C1
2	3	2001	IPT	C3'-C1'-S1-C1
2	4	2001	IPT	C2'-C1'-S1-C1
2	2	2001	IPT	O5-C5-C6-O6
2	4	2001	IPT	O5-C5-C6-O6
2	1	2001	IPT	O5-C5-C6-O6
2	3	2001	IPT	O5-C5-C6-O6
2	4	2001	IPT	C3'-C1'-S1-C1

There are no ring outliers.

35 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	6027	DMS	1	0
5	2	6043	DMS	1	0
5	1	6002	DMS	2	0
5	4	6021	DMS	1	0
2	4	2001	IPT	1	0
5	1	6014	DMS	1	0
5	3	6020	DMS	1	0
5	3	6040	DMS	1	0
5	2	6027	DMS	1	0
5	4	6002	DMS	1	0
5	2	6022	DMS	1	0
5	3	6018	DMS	1	0
5	1	6019	DMS	1	0
5	2	6010	DMS	1	0
5	2	6026	DMS	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	2	6040	DMS	2	0
5	1	6032	DMS	1	0
5	4	6009	DMS	1	0
5	3	1024	DMS	1	0
2	3	2002	IPT	2	0
5	3	6026	DMS	1	0
5	2	6032	DMS	2	0
5	3	6030	DMS	1	0
2	2	2001	IPT	1	0
5	2	6039	DMS	1	0
2	2	2002	IPT	1	0
5	3	6029	DMS	3	0
5	4	6001	DMS	1	0
5	1	6009	DMS	1	0
5	2	6015	DMS	1	0
5	1	6021	DMS	1	0
5	3	6016	DMS	1	0
5	3	6013	DMS	1	0
5	4	6027	DMS	1	0
5	2	6018	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	1	1011/1052 (96%)	-0.07	21 (2%) 63 67	10, 20, 40, 66	0
1	2	1011/1052 (96%)	-0.29	20 (1%) 65 69	8, 16, 36, 68	0
1	3	1011/1052 (96%)	-0.32	17 (1%) 69 72	9, 16, 33, 67	0
1	4	1011/1052 (96%)	-0.07	23 (2%) 61 65	10, 21, 39, 70	0
All	All	4044/4208 (96%)	-0.19	81 (2%) 65 69	8, 19, 37, 70	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1	735	HIS	4.9
1	2	732	ALA	4.8
1	2	731	PRO	4.6
1	3	689	GLU	3.8
1	3	1023	LYS	3.8
1	4	735	HIS	3.7
1	4	686	PRO	3.6
1	4	689	GLU	3.5
1	4	730	LEU	3.5
1	2	1023	LYS	3.4
1	1	319	ASP	3.4
1	4	797	GLU	3.4
1	1	800	ARG	3.3
1	2	689	GLU	3.3
1	2	730	LEU	3.3
1	1	730	LEU	3.3
1	3	688	PRO	3.3
1	3	800	ARG	3.2
1	3	1022	GLN	3.2
1	1	684	GLU	3.2
1	4	687	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	4	580	GLU	3.1
1	2	771	GLY	3.1
1	4	581	ASN	3.0
1	2	1022	GLN	3.0
1	2	800	ARG	3.0
1	4	732	ALA	3.0
1	1	686	PRO	2.9
1	3	735	HIS	2.9
1	4	1022	GLN	2.9
1	1	1023	LYS	2.9
1	1	685	LEU	2.9
1	2	688	PRO	2.8
1	1	689	GLU	2.8
1	2	685	LEU	2.8
1	4	129	VAL	2.8
1	3	798	ALA	2.7
1	2	772	ASP	2.7
1	4	746	ASP	2.7
1	3	684	GLU	2.6
1	4	690	SER	2.6
1	3	686	PRO	2.6
1	3	799	THR	2.6
1	4	128	ASN	2.6
1	2	735	HIS	2.6
1	4	798	ALA	2.6
1	2	686	PRO	2.5
1	1	76	CYS	2.5
1	1	687	GLN	2.5
1	2	663	LEU	2.4
1	2	733	ALA	2.4
1	2	734	SER	2.4
1	4	688	PRO	2.4
1	1	79	PRO	2.3
1	3	771	GLY	2.3
1	1	71	GLU	2.3
1	1	681	GLU	2.3
1	2	774	LYS	2.3
1	1	178	ARG	2.3
1	1	130	ASP	2.3
1	4	685	LEU	2.3
1	4	800	ARG	2.2
1	1	136	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	3	733	ALA	2.2
1	4	733	ALA	2.2
1	1	737	ILE	2.2
1	3	655	MET	2.2
1	3	370	GLN	2.2
1	3	651	LEU	2.2
1	4	655	MET	2.1
1	3	731	PRO	2.1
1	4	731	PRO	2.1
1	1	733	ALA	2.1
1	1	80	GLU	2.1
1	2	684	GLU	2.1
1	3	744	GLU	2.1
1	2	736	ALA	2.1
1	4	76	CYS	2.1
1	2	655	MET	2.0
1	1	731	PRO	2.0
1	4	663	LEU	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	2	6040	4/4	0.37	0.32	92,92,93,93	0
5	DMS	2	6042	4/4	0.40	0.22	95,96,96,96	0
5	DMS	3	6040	4/4	0.40	0.29	51,53,55,56	0
5	DMS	1	6019	4/4	0.41	0.38	99,99,100,100	0
5	DMS	3	6035	4/4	0.43	0.28	88,88,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	1	6025	4/4	0.47	0.24	82,83,83,83	0
5	DMS	2	6016	4/4	0.50	0.28	91,92,92,92	0
5	DMS	2	6012	4/4	0.56	0.30	77,78,79,79	0
5	DMS	3	6026	4/4	0.56	0.26	97,97,98,98	0
5	DMS	2	6029	4/4	0.58	0.25	80,81,81,82	0
5	DMS	4	6017	4/4	0.58	0.26	75,76,76,76	0
5	DMS	1	6032	4/4	0.60	0.29	75,76,76,76	0
5	DMS	3	6036	4/4	0.60	0.25	97,97,98,98	0
5	DMS	2	6031	4/4	0.61	0.22	75,76,76,77	0
5	DMS	4	6027	4/4	0.62	0.22	60,60,60,61	0
5	DMS	1	6029	4/4	0.64	0.19	67,68,69,69	0
5	DMS	3	6032	4/4	0.65	0.25	85,86,86,86	0
5	DMS	3	6041	4/4	0.65	0.24	77,78,78,79	0
5	DMS	4	6021	4/4	0.66	0.27	82,82,82,82	0
5	DMS	3	6037	4/4	0.66	0.23	74,75,75,75	0
5	DMS	2	6035	4/4	0.67	0.25	75,75,76,76	0
5	DMS	2	6038	4/4	0.68	0.20	55,55,55,57	0
5	DMS	4	6016	4/4	0.69	0.27	93,94,94,94	0
5	DMS	4	6029	4/4	0.70	0.17	73,73,74,75	0
3	MG	4	3003	1/1	0.71	0.14	65,65,65,65	0
5	DMS	1	6024	4/4	0.72	0.24	80,81,81,81	0
5	DMS	2	6033	4/4	0.72	0.20	92,92,92,92	0
5	DMS	4	6013	4/4	0.73	0.15	66,66,66,67	0
5	DMS	2	6015	4/4	0.73	0.20	85,85,85,85	0
5	DMS	2	6026	4/4	0.73	0.23	40,42,45,45	0
5	DMS	1	6028	4/4	0.74	0.18	70,71,71,71	0
2	IPT	1	2002	15/15	0.74	0.14	27,31,34,35	15
5	DMS	4	6018	4/4	0.74	0.21	80,81,81,81	0
5	DMS	2	6028	4/4	0.75	0.20	44,45,46,49	0
5	DMS	4	6007	4/4	0.75	0.18	74,74,74,74	0
5	DMS	1	6014	4/4	0.75	0.25	94,94,94,94	0
5	DMS	3	6038	4/4	0.76	0.18	68,68,69,70	0
5	DMS	1	6023	4/4	0.76	0.18	59,60,61,61	0
5	DMS	3	6014	4/4	0.76	0.18	60,60,60,61	0
5	DMS	4	6026	4/4	0.76	0.19	67,68,68,68	0
5	DMS	3	6025	4/4	0.76	0.19	60,60,61,61	0
5	DMS	1	6011	4/4	0.76	0.18	84,84,84,84	0
5	DMS	2	6025	4/4	0.77	0.20	66,67,67,67	0
5	DMS	1	6031	4/4	0.77	0.20	73,74,74,74	0
5	DMS	3	6018	4/4	0.77	0.22	59,59,60,61	0
5	DMS	2	6043	4/4	0.77	0.17	56,56,57,57	0
5	DMS	4	6012	4/4	0.78	0.18	79,79,79,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	2	6034	4/4	0.78	0.16	67,68,69,69	0
5	DMS	4	6028	4/4	0.78	0.18	89,89,90,90	0
5	DMS	1	6030	4/4	0.78	0.17	66,66,66,67	0
5	DMS	1	6026	4/4	0.79	0.16	76,76,76,77	0
5	DMS	3	6022	4/4	0.80	0.16	74,75,75,75	0
5	DMS	2	6022	4/4	0.80	0.19	81,81,82,82	0
5	DMS	3	6039	4/4	0.80	0.18	59,59,60,61	0
5	DMS	3	6005	4/4	0.80	0.16	53,53,53,54	0
3	MG	1	3003	1/1	0.80	0.13	59,59,59,59	0
5	DMS	4	6011	4/4	0.80	0.16	56,57,57,58	0
5	DMS	3	6015	4/4	0.80	0.19	70,71,71,71	0
5	DMS	2	6039	4/4	0.80	0.20	47,48,48,48	0
5	DMS	3	6031	4/4	0.81	0.17	84,84,84,85	0
5	DMS	3	6020	4/4	0.81	0.19	64,65,65,65	0
5	DMS	4	6030	4/4	0.81	0.19	81,82,82,82	0
5	DMS	1	6027	4/4	0.82	0.18	49,49,49,51	0
5	DMS	1	6018	4/4	0.82	0.16	64,64,65,65	0
5	DMS	2	6036	4/4	0.82	0.18	52,52,53,54	0
5	DMS	2	6037	4/4	0.82	0.15	74,74,75,75	0
2	IPT	4	2002	15/15	0.82	0.11	27,30,32,32	0
5	DMS	1	6010	4/4	0.82	0.15	58,58,58,59	0
5	DMS	3	6030	4/4	0.82	0.18	51,51,52,52	0
5	DMS	4	6024	4/4	0.83	0.18	67,68,68,68	0
5	DMS	3	6029	4/4	0.83	0.22	55,55,56,57	0
5	DMS	1	6017	4/4	0.83	0.17	38,41,42,46	0
5	DMS	3	6017	4/4	0.84	0.18	57,57,57,58	0
5	DMS	3	6016	4/4	0.84	0.18	65,65,65,65	0
5	DMS	2	6018	4/4	0.85	0.20	65,65,66,66	0
5	DMS	2	6023	4/4	0.85	0.15	72,72,72,73	0
5	DMS	4	6022	4/4	0.85	0.16	54,55,55,56	0
5	DMS	3	6034	4/4	0.85	0.12	57,57,58,59	0
5	DMS	4	6025	4/4	0.85	0.17	68,69,69,69	0
5	DMS	1	6022	4/4	0.86	0.17	54,54,54,54	0
5	DMS	2	6030	4/4	0.86	0.13	64,64,65,65	0
5	DMS	1	6015	4/4	0.86	0.17	70,70,70,70	0
5	DMS	2	6007	4/4	0.86	0.15	43,44,45,46	0
5	DMS	4	6015	4/4	0.86	0.17	63,63,63,64	0
5	DMS	1	6007	4/4	0.86	0.17	51,51,51,51	0
5	DMS	3	6019	4/4	0.86	0.15	77,77,77,77	0
5	DMS	3	6007	4/4	0.86	0.13	49,50,50,51	0
5	DMS	4	6019	4/4	0.86	0.15	63,64,64,64	0
5	DMS	3	6027	4/4	0.87	0.14	41,41,42,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	2	6019	4/4	0.87	0.14	63,63,64,64	0
5	DMS	2	6005	4/4	0.87	0.18	50,51,51,51	0
5	DMS	2	6006	4/4	0.87	0.14	43,44,44,45	0
2	IPT	2	2002	15/15	0.87	0.10	32,37,39,39	0
5	DMS	3	6033	4/4	0.87	0.17	66,67,67,67	0
2	IPT	4	2001	15/15	0.87	0.11	20,25,32,34	0
5	DMS	4	6014	4/4	0.87	0.17	91,91,91,91	0
5	DMS	1	6003	4/4	0.87	0.13	55,56,57,57	0
5	DMS	1	6020	4/4	0.87	0.14	63,63,63,63	0
2	IPT	1	2001	15/15	0.87	0.11	17,21,28,30	0
5	DMS	2	6032	4/4	0.88	0.15	42,46,47,48	0
4	NA	4	3103	1/1	0.88	0.07	37,37,37,37	0
3	MG	3	3003	1/1	0.88	0.19	74,74,74,74	0
5	DMS	2	6010	4/4	0.88	0.15	40,40,42,43	0
5	DMS	2	6020	4/4	0.88	0.15	60,60,60,61	0
5	DMS	1	6006	4/4	0.88	0.15	61,61,61,62	0
3	MG	2	3003	1/1	0.88	0.13	52,52,52,52	0
5	DMS	4	6002	4/4	0.88	0.18	43,45,45,46	0
5	DMS	3	6011	4/4	0.88	0.13	39,41,41,43	0
2	IPT	3	2002	15/15	0.89	0.10	32,36,38,39	0
5	DMS	3	6023	4/4	0.89	0.15	51,52,52,53	0
5	DMS	3	6024	4/4	0.89	0.14	60,60,60,60	0
5	DMS	3	1024	4/4	0.89	0.12	58,58,58,60	0
5	DMS	3	6001	4/4	0.89	0.15	29,31,33,33	0
5	DMS	1	6009	4/4	0.89	0.14	57,57,57,58	0
5	DMS	1	6002	4/4	0.90	0.15	39,40,40,41	0
5	DMS	1	6012	4/4	0.90	0.13	69,69,70,70	0
5	DMS	3	6012	4/4	0.90	0.14	57,57,57,57	0
5	DMS	1	6013	4/4	0.90	0.13	55,55,56,56	0
4	NA	3	3104	1/1	0.90	0.12	28,28,28,28	0
5	DMS	1	6021	4/4	0.90	0.15	59,59,59,60	0
4	NA	3	3103	1/1	0.90	0.07	34,34,34,34	0
5	DMS	4	6009	4/4	0.91	0.13	45,46,46,47	0
5	DMS	2	6001	4/4	0.91	0.17	27,29,29,30	0
5	DMS	1	6001	4/4	0.91	0.16	28,31,31,31	0
5	DMS	2	6011	4/4	0.91	0.12	59,59,60,60	0
5	DMS	4	6020	4/4	0.91	0.13	36,38,39,41	0
5	DMS	1	6016	4/4	0.91	0.12	66,66,66,66	0
5	DMS	3	6010	4/4	0.91	0.13	33,35,36,37	0
5	DMS	3	6013	4/4	0.92	0.11	54,54,55,55	0
5	DMS	2	6013	4/4	0.92	0.12	43,43,44,44	0
5	DMS	2	6017	4/4	0.92	0.13	61,61,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	3	6021	4/4	0.92	0.11	44,45,45,46	0
5	DMS	3	6003	4/4	0.92	0.11	37,37,38,39	0
4	NA	4	3104	1/1	0.92	0.07	35,35,35,35	0
5	DMS	4	6005	4/4	0.92	0.12	50,50,51,52	0
3	MG	1	3002	1/1	0.93	0.05	24,24,24,24	0
5	DMS	4	6001	4/4	0.93	0.15	35,36,36,37	0
5	DMS	2	6014	4/4	0.93	0.10	55,56,56,56	0
4	NA	2	3103	1/1	0.93	0.08	36,36,36,36	0
5	DMS	4	6006	4/4	0.93	0.11	45,46,46,46	0
2	IPT	2	2001	15/15	0.93	0.08	10,16,21,21	0
5	DMS	3	6006	4/4	0.93	0.10	46,47,47,47	0
5	DMS	4	6010	4/4	0.93	0.11	55,55,55,55	0
5	DMS	2	6027	4/4	0.93	0.11	44,44,44,45	0
4	NA	4	3102	1/1	0.94	0.07	16,16,16,16	0
5	DMS	4	6023	4/4	0.94	0.10	41,41,42,42	0
2	IPT	3	2001	15/15	0.94	0.08	12,18,23,26	0
4	NA	2	3104	1/1	0.94	0.08	31,31,31,31	0
5	DMS	2	6003	4/4	0.94	0.11	26,26,27,30	0
5	DMS	3	6009	4/4	0.94	0.11	38,38,39,39	0
5	DMS	3	6028	4/4	0.94	0.10	42,42,42,43	0
5	DMS	2	6024	4/4	0.94	0.09	31,32,33,35	0
5	DMS	4	6003	4/4	0.94	0.13	34,35,36,37	0
5	DMS	2	6009	4/4	0.95	0.12	34,35,36,37	0
5	DMS	1	6005	4/4	0.95	0.09	52,53,53,53	0
3	MG	2	3001	1/1	0.95	0.03	13,13,13,13	0
3	MG	1	3001	1/1	0.95	0.03	16,16,16,16	0
3	MG	2	3004	1/1	0.95	0.04	34,34,34,34	0
5	DMS	2	6002	4/4	0.96	0.09	31,32,32,34	0
4	NA	1	3103	1/1	0.96	0.05	29,29,29,29	0
4	NA	1	3104	1/1	0.96	0.05	32,32,32,32	0
5	DMS	4	6000	4/4	0.96	0.10	23,25,25,27	0
3	MG	4	3001	1/1	0.96	0.04	17,17,17,17	0
5	DMS	2	6000	4/4	0.96	0.10	16,21,23,23	0
5	DMS	2	6021	4/4	0.96	0.08	39,40,40,40	0
3	MG	1	3004	1/1	0.96	0.04	43,43,43,43	0
4	NA	4	3101	1/1	0.97	0.04	19,19,19,19	0
5	DMS	3	6002	4/4	0.97	0.07	30,31,32,32	0
5	DMS	2	6004	4/4	0.97	0.09	27,28,29,29	0
5	DMS	3	6004	4/4	0.97	0.10	25,25,26,26	0
3	MG	4	3002	1/1	0.97	0.07	23,23,23,23	0
5	DMS	4	6008	4/4	0.97	0.09	36,37,38,39	0
5	DMS	1	6008	4/4	0.97	0.07	36,36,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NA	1	3101	1/1	0.98	0.05	18,18,18,18	0
4	NA	1	3102	1/1	0.98	0.02	12,12,12,12	0
5	DMS	3	6000	4/4	0.98	0.07	14,19,19,21	0
5	DMS	2	6008	4/4	0.98	0.07	24,25,27,27	0
5	DMS	1	6000	4/4	0.98	0.06	18,23,23,25	0
5	DMS	4	6004	4/4	0.98	0.06	28,29,30,30	0
3	MG	2	3002	1/1	0.98	0.07	15,15,15,15	0
4	NA	3	3101	1/1	0.98	0.02	13,13,13,13	0
4	NA	2	3101	1/1	0.99	0.05	15,15,15,15	0
4	NA	3	3102	1/1	0.99	0.02	14,14,14,14	0
5	DMS	1	6004	4/4	0.99	0.05	26,27,28,29	0
4	NA	2	3102	1/1	0.99	0.03	13,13,13,13	0
3	MG	3	3001	1/1	0.99	0.02	13,13,13,13	0
5	DMS	3	6008	4/4	0.99	0.05	20,22,22,22	0
3	MG	3	3002	1/1	0.99	0.04	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.