



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:37 AM UTC

PDB ID : 3MV1 / pdb_00003mv1
Title : E.Coli (lacZ) beta-galactosidase (R599A) in complex with Guanidinium
Authors : Dugdale, M.L.; Vance, M.; Driedger, M.L.; Nibber, A.; Tran, A.; Huber, R.E.
Deposited on : 2010-05-03
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

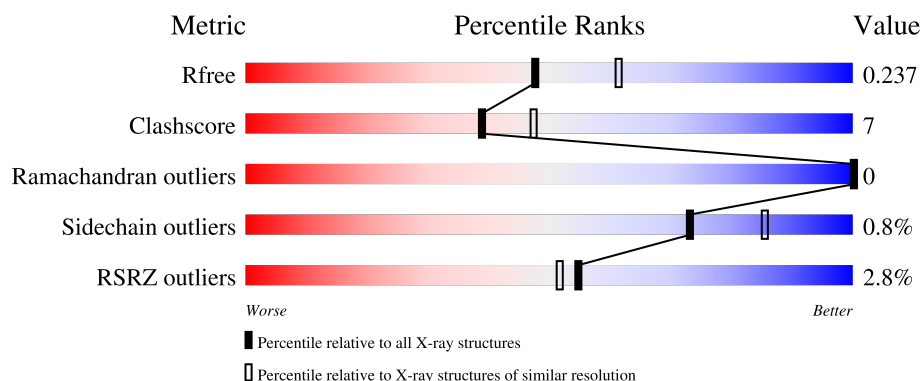
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

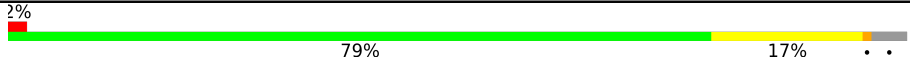
The reported resolution of this entry is 2.20 Å.

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	1	1052	
1	2	1052	
1	3	1052	
1	4	1052	

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	4	7007	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36610 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	engineered mutation	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	engineered mutation	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	engineered mutation	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	engineered mutation	UNP B8LFD6

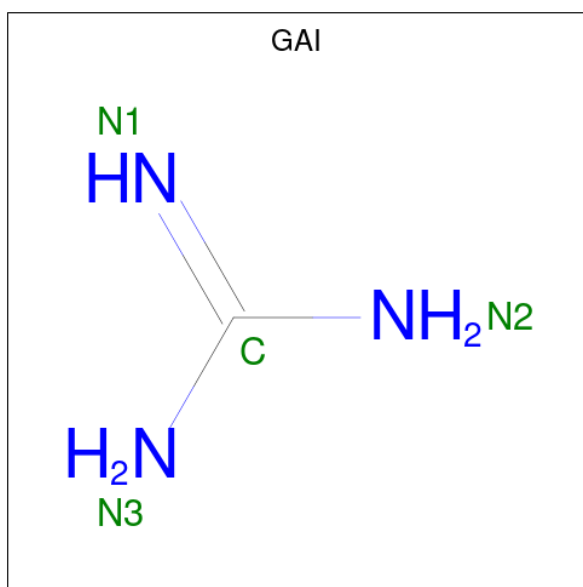
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

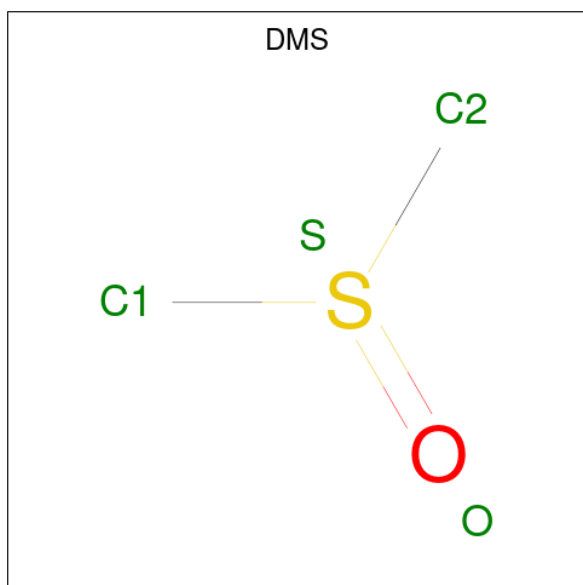
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	4	Total	Na	0	0
			4	4		
3	2	4	Total	Na	0	0
			4	4		
3	3	4	Total	Na	0	0
			4	4		
3	4	4	Total	Na	0	0
			4	4		

- Molecule 4 is GUANIDINE (CCD ID: GAI) (formula: CH₅N₃).



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

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

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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	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

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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		
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	860	Total	O	0	0
			860	860		
6	2	977	Total	O	0	0
			977	977		
6	3	982	Total	O	0	0
			982	982		
6	4	835	Total	O	0	0
			835	835		

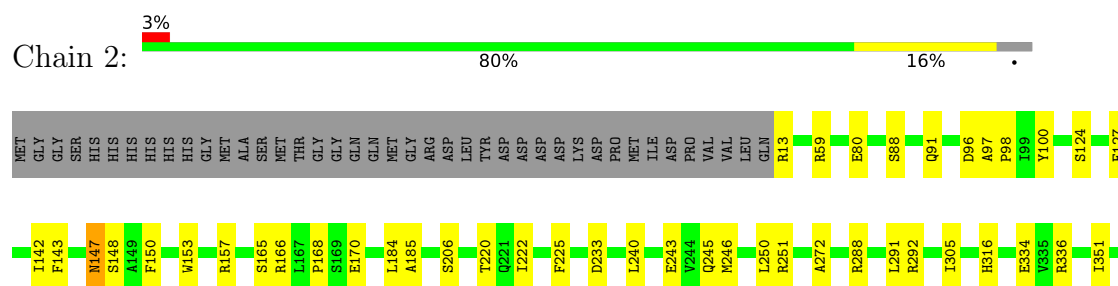
3 Residue-property plots

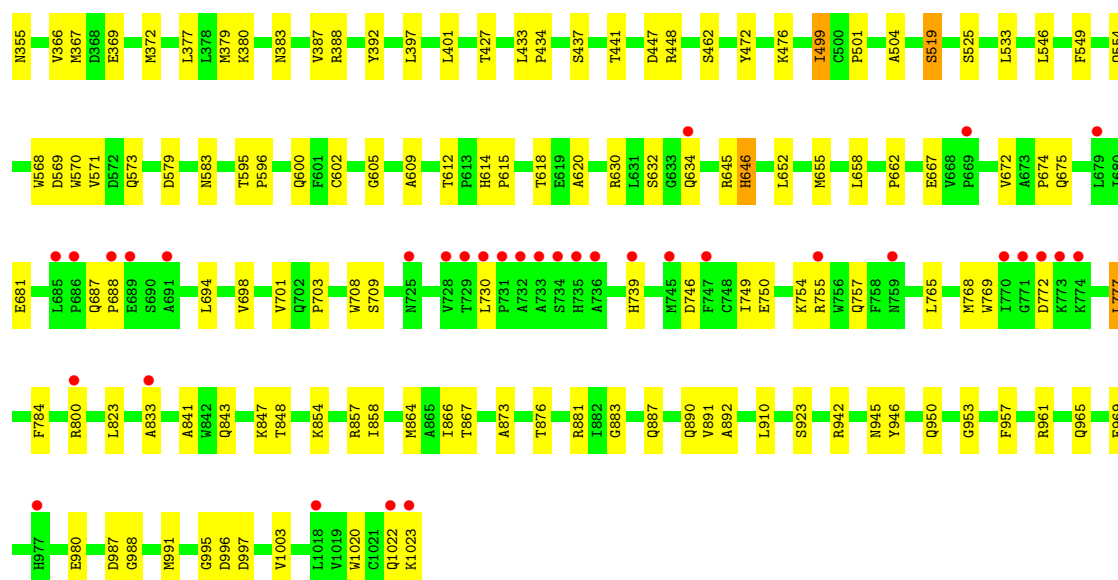
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Beta-galactosidase

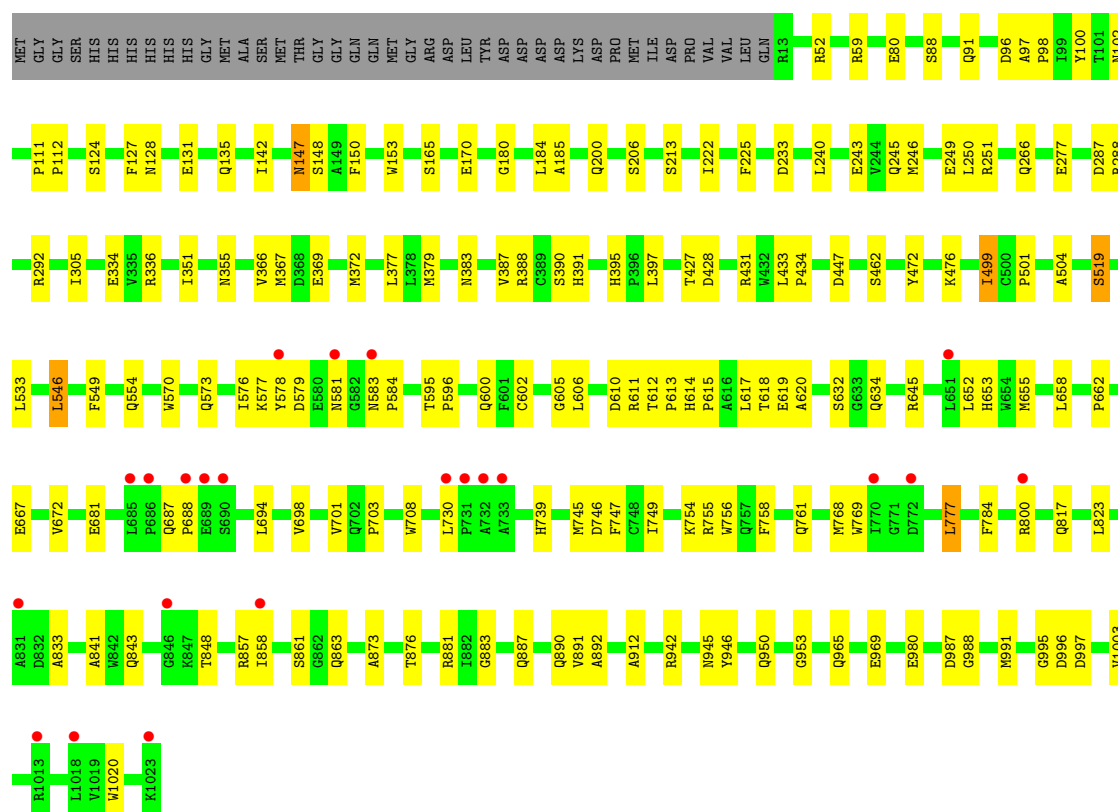
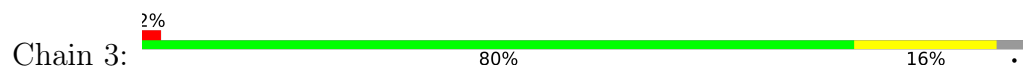


• Molecule 1: Beta-galactosidase

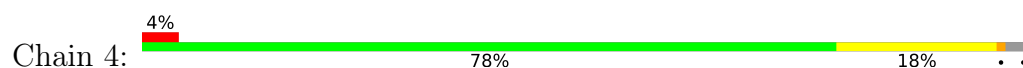


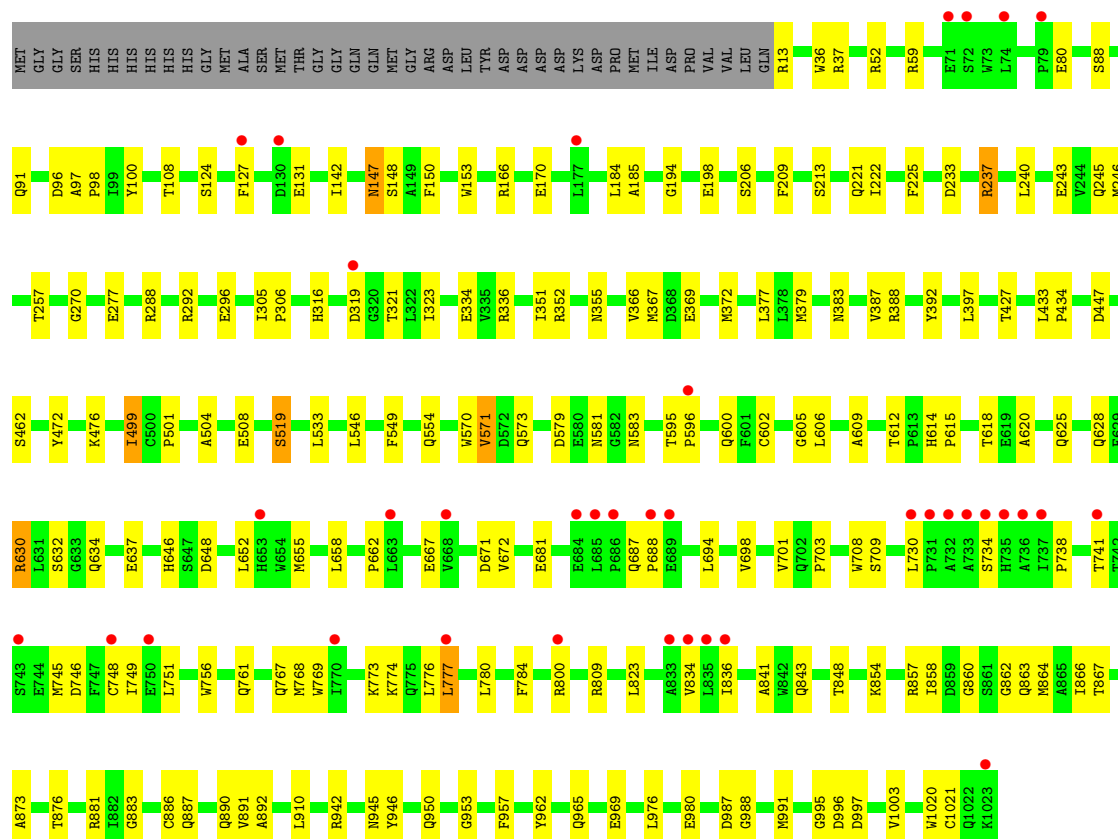


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.73Å 161.52Å 203.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.29 – 2.20 71.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (71.29-2.20) 99.6 (71.29-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.205 , 0.242 0.201 , 0.237	Depositor DCC
R_{free} test set	3595 reflections (1.43%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtrriage
Anisotropy	0.311	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36610	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 38.28 % 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 3.7750e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.35	0/8361	0.88	27/11408 (0.2%)
1	2	0.37	0/8361	0.88	25/11408 (0.2%)
1	3	0.37	0/8361	0.90	26/11408 (0.2%)
1	4	0.36	0/8361	0.95	36/11408 (0.3%)
All	All	0.36	0/33444	0.90	114/45632 (0.2%)

There are no bond length outliers.

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	147	ASN	CA-C-N	17.78	155.50	121.54
1	4	147	ASN	C-N-CA	17.78	155.50	121.54
1	3	431	ARG	NE-CZ-NH2	13.22	131.10	119.20
1	4	630	ARG	NE-CZ-NH2	12.81	130.73	119.20
1	4	630	ARG	NE-CZ-NH1	-12.12	109.38	121.50
1	3	431	ARG	NE-CZ-NH1	-12.07	109.43	121.50
1	4	237	ARG	NE-CZ-NH2	11.52	129.57	119.20
1	4	237	ARG	NE-CZ-NH1	-10.92	110.58	121.50
1	4	147	ASN	O-C-N	10.57	135.61	122.93
1	3	431	ARG	CD-NE-CZ	10.46	139.04	124.40
1	4	630	ARG	CD-NE-CZ	10.16	138.63	124.40
1	4	237	ARG	CD-NE-CZ	8.23	135.93	124.40
1	1	570	TRP	N-CA-C	7.44	119.29	111.03
1	4	570	TRP	N-CA-C	7.41	119.26	111.03
1	2	570	TRP	N-CA-C	7.33	119.17	111.03
1	1	988	GLY	N-CA-C	-7.30	102.91	113.86
1	2	988	GLY	N-CA-C	-7.28	102.94	113.86
1	3	570	TRP	N-CA-C	7.27	119.10	111.03
1	3	97	ALA	N-CA-C	7.25	118.92	109.93
1	1	97	ALA	N-CA-C	7.14	118.79	109.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	988	GLY	N-CA-C	-7.10	103.21	113.86
1	4	988	GLY	N-CA-C	-7.10	103.21	113.86
1	2	97	ALA	N-CA-C	7.01	118.63	109.93
1	4	97	ALA	N-CA-C	6.98	118.58	109.93
1	2	614	HIS	N-CA-C	-6.75	101.32	110.36
1	3	614	HIS	N-CA-C	-6.65	101.45	110.36
1	4	614	HIS	N-CA-C	-6.53	101.61	110.36
1	1	614	HIS	N-CA-C	-6.49	101.67	110.36
1	1	383	ASN	N-CA-C	6.45	120.50	112.24
1	4	777	LEU	N-CA-C	-6.44	105.73	113.97
1	3	383	ASN	N-CA-C	6.38	120.40	112.24
1	2	383	ASN	N-CA-C	6.34	120.35	112.24
1	1	777	LEU	N-CA-C	-6.21	106.02	113.97
1	4	519	SER	N-CA-C	-6.12	101.61	110.24
1	2	147	ASN	CA-C-N	6.11	132.69	121.70
1	2	147	ASN	C-N-CA	6.11	132.69	121.70
1	4	383	ASN	N-CA-C	6.11	120.06	112.24
1	3	147	ASN	CA-C-N	6.09	132.66	121.70
1	3	147	ASN	C-N-CA	6.09	132.66	121.70
1	2	519	SER	N-CA-C	-6.08	101.41	110.23
1	2	605	GLY	N-CA-C	6.06	121.19	112.82
1	3	605	GLY	N-CA-C	6.05	121.17	112.82
1	3	777	LEU	N-CA-C	-6.04	106.25	113.97
1	1	605	GLY	N-CA-C	6.02	121.12	112.82
1	1	147	ASN	CA-C-N	6.00	132.50	121.70
1	1	147	ASN	C-N-CA	6.00	132.50	121.70
1	1	504	ALA	N-CA-C	-6.00	100.72	110.20
1	2	777	LEU	N-CA-C	-5.96	106.34	113.97
1	4	233	ASP	N-CA-C	5.93	118.50	111.33
1	3	519	SER	N-CA-C	-5.92	101.89	110.24
1	1	519	SER	N-CA-C	-5.90	101.68	110.23
1	4	605	GLY	N-CA-C	5.89	120.94	112.82
1	1	746	ASP	N-CA-C	5.84	117.95	109.07
1	3	746	ASP	N-CA-C	5.83	118.04	109.24
1	1	323	ILE	N-CA-C	-5.83	106.14	111.67
1	4	352	ARG	N-CA-C	-5.79	100.89	109.11
1	1	352	ARG	N-CA-C	-5.79	100.89	109.11
1	4	746	ASP	N-CA-C	5.77	117.83	109.07
1	3	612	THR	N-CA-C	-5.75	102.40	109.65
1	4	147	ASN	CA-C-O	5.75	126.73	120.58
1	3	504	ALA	N-CA-C	-5.75	101.12	110.20
1	3	447	ASP	N-CA-C	5.74	120.40	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	504	ALA	N-CA-C	-5.74	101.13	110.20
1	1	646	HIS	N-CA-C	-5.74	102.03	110.52
1	3	233	ASP	N-CA-C	5.70	118.23	111.33
1	2	233	ASP	N-CA-C	5.69	118.21	111.33
1	4	554	GLN	N-CA-C	-5.67	105.18	111.36
1	2	447	ASP	N-CA-C	5.65	120.28	113.17
1	4	612	THR	N-CA-C	-5.63	102.56	109.65
1	2	646	HIS	N-CA-C	-5.62	102.44	110.59
1	1	233	ASP	N-CA-C	5.58	118.08	111.33
1	2	272	ALA	N-CA-C	5.50	113.08	108.13
1	4	323	ILE	N-CA-C	-5.46	106.86	111.56
1	2	504	ALA	N-CA-C	-5.46	101.57	110.20
1	1	612	THR	N-CA-C	-5.41	102.83	109.65
1	2	612	THR	N-CA-C	-5.41	102.83	109.65
1	1	499	ILE	N-CA-C	-5.39	100.90	108.12
1	3	150	PHE	N-CA-C	5.38	116.69	108.52
1	3	222	ILE	N-CA-C	-5.38	100.58	108.54
1	2	351	ILE	N-CA-C	5.36	115.30	108.12
1	4	447	ASP	N-CA-C	5.35	119.91	113.17
1	1	447	ASP	N-CA-C	5.34	119.90	113.17
1	4	150	PHE	N-CA-C	5.33	116.61	108.52
1	1	150	PHE	N-CA-C	5.30	116.58	108.52
1	2	220	THR	N-CA-C	-5.30	99.87	108.41
1	3	554	GLN	N-CA-C	-5.28	105.61	111.36
1	2	98	PRO	N-CA-C	-5.28	102.87	111.68
1	1	351	ILE	N-CA-C	5.26	115.17	108.12
1	1	209	PHE	N-CA-C	5.23	119.64	113.16
1	2	499	ILE	N-CA-C	-5.22	101.13	108.12
1	1	606	LEU	N-CA-C	-5.19	106.45	112.89
1	3	351	ILE	N-CA-C	5.19	115.07	108.12
1	4	98	PRO	N-CA-C	-5.17	103.04	111.68
1	2	746	ASP	N-CA-C	5.16	116.92	109.07
1	4	606	LEU	N-CA-C	-5.15	106.50	112.89
1	1	98	PRO	N-CA-C	-5.15	103.08	111.68
1	2	222	ILE	N-CA-C	-5.15	100.92	108.54
1	1	554	GLN	N-CA-C	-5.14	105.75	111.36
1	3	98	PRO	N-CA-C	-5.14	103.10	111.68
1	4	147	ASN	N-CA-C	5.14	116.68	108.41
1	1	222	ILE	N-CA-C	-5.14	100.94	108.54
1	2	554	GLN	N-CA-C	-5.12	105.78	111.36
1	3	499	ILE	N-CA-C	-5.10	101.29	108.12
1	4	571	VAL	N-CA-C	5.07	116.01	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4	222	ILE	N-CA-C	-5.06	101.05	108.54
1	4	209	PHE	N-CA-C	5.06	119.43	113.16
1	2	150	PHE	N-CA-C	5.05	116.20	108.52
1	4	499	ILE	N-CA-C	-5.03	101.38	108.12
1	3	606	LEU	N-CA-C	-5.02	106.66	112.89
1	2	448	ARG	N-CA-C	5.02	118.51	112.38
1	4	221	GLN	N-CA-C	5.01	116.61	109.14
1	3	395	HIS	N-CA-C	-5.01	103.28	109.64
1	4	351	ILE	N-CA-C	5.01	114.83	108.12
1	1	742	THR	N-CA-C	5.00	117.72	109.72

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	1	8119	0	7708	111	0
1	2	8119	0	7708	105	0
1	3	8119	0	7708	110	0
1	4	8119	0	7707	117	0
2	1	3	0	0	0	0
2	2	3	0	0	0	0
2	3	3	0	0	0	0
2	4	3	0	0	0	0
3	1	4	0	0	0	0
3	2	4	0	0	0	0
3	3	4	0	0	0	0
3	4	4	0	0	0	0
4	1	4	0	4	0	0
4	2	4	0	4	0	0
4	3	4	0	4	0	0
4	4	4	0	4	0	0
5	1	100	0	150	4	0
5	2	120	0	180	10	0
5	3	112	0	168	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	104	0	156	10	0
6	1	860	0	0	9	0
6	2	977	0	0	5	0
6	3	982	0	0	9	0
6	4	835	0	0	5	0
All	All	36610	0	31501	436	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 7.

All (436) 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)
1:3:581:ASN:HB2	1:3:583:ASN:ND2	1.94	0.82
1:4:147:ASN:HB3	1:4:206:SER:HA	1.62	0.81
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.62	0.81
1:1:730:LEU:HD21	1:2:823:LEU:O	1.80	0.81
1:4:767:GLN:NE2	1:4:774:LYS:HG3	1.98	0.79
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.63	0.79
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.64	0.79
1:1:245:GLN:HG2	1:1:288:ARG:HG2	1.64	0.78
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.63	0.78
1:3:245:GLN:HG2	1:3:288:ARG:HG2	1.66	0.78
1:2:245:GLN:HG2	1:2:288:ARG:HG2	1.64	0.77
1:2:754:LYS:HE2	1:2:1022:GLN:HE21	1.51	0.76
1:2:142:ILE:HG12	1:2:170:GLU:HG2	1.67	0.75
1:4:292:ARG:HH12	5:4:7009:DMS:H13	1.52	0.75
1:1:615:PRO:O	1:1:618:THR:HG22	1.87	0.74
1:2:754:LYS:HE2	1:2:1022:GLN:NE2	2.02	0.74
1:3:615:PRO:O	1:3:618:THR:HG22	1.88	0.74
1:4:615:PRO:O	1:4:618:THR:HG22	1.87	0.73
1:2:615:PRO:O	1:2:618:THR:HG22	1.89	0.72
1:3:102:ASN:HD21	5:3:7026:DMS:H12	1.56	0.71
1:3:128:ASN:HA	1:3:180:GLY:O	1.92	0.70
1:2:147:ASN:HB3	1:2:206:SER:HA	1.75	0.69
1:3:581:ASN:HB2	1:3:583:ASN:HD21	1.56	0.69
1:3:749:ILE:HD12	1:3:858:ILE:HD12	1.75	0.69
1:1:147:ASN:HB3	1:1:206:SER:HA	1.74	0.68
1:3:749:ILE:CD1	1:3:858:ILE:HD12	2.24	0.68
1:2:292:ARG:HH12	5:2:7009:DMS:H13	1.59	0.68
1:3:147:ASN:HB3	1:3:206:SER:HA	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:965:GLN:O	1:4:969:GLU:HG3	1.95	0.67
1:2:965:GLN:O	1:2:969:GLU:HG3	1.96	0.66
1:2:750:GLU:HG3	1:2:755:ARG:HG2	1.76	0.66
1:1:737:ILE:HD13	1:1:832:ASP:HA	1.77	0.66
1:4:581:ASN:HB2	1:4:583:ASN:ND2	2.10	0.66
1:1:737:ILE:HD12	1:1:738:PRO:HD2	1.77	0.65
1:1:965:GLN:O	1:1:969:GLU:HG3	1.96	0.65
1:3:131:GLU:O	1:3:135:GLN:HG3	1.97	0.65
1:4:756:TRP:CD2	1:4:858:ILE:HD13	2.32	0.65
1:1:864:MET:HE3	1:1:866:ILE:HD11	1.79	0.64
1:1:579:ASP:OD2	1:1:583:ASN:HB2	1.97	0.64
1:3:88:SER:HA	1:3:366:VAL:HG21	1.80	0.64
1:4:88:SER:HA	1:4:366:VAL:HG21	1.80	0.64
1:2:157:ARG:HD3	6:2:4685:HOH:O	1.99	0.63
1:4:745:MET:HE1	1:4:761:GLN:OE1	1.98	0.63
1:2:991:MET:HE3	1:2:1003:VAL:HG21	1.79	0.63
1:2:88:SER:HA	1:2:366:VAL:HG21	1.79	0.63
1:1:88:SER:HA	1:1:366:VAL:HG21	1.80	0.63
1:3:965:GLN:O	1:3:969:GLU:HG3	1.98	0.62
1:1:377:LEU:HD22	1:1:708:TRP:HA	1.82	0.62
1:3:578:TYR:HA	1:3:583:ASN:O	2.00	0.62
1:3:991:MET:HE3	1:3:1003:VAL:HG21	1.81	0.62
1:4:377:LEU:HD22	1:4:708:TRP:HA	1.81	0.62
1:4:991:MET:HE3	1:4:1003:VAL:HG21	1.81	0.61
1:1:991:MET:HE3	1:1:1003:VAL:HG21	1.83	0.61
1:1:131:GLU:O	1:1:135:GLN:HG3	2.00	0.61
1:1:13:ARG:HG3	1:4:13:ARG:CZ	2.30	0.61
1:1:127:PHE:CE2	1:1:184:LEU:HG	2.36	0.61
1:2:127:PHE:CE2	1:2:184:LEU:HG	2.36	0.61
1:3:377:LEU:HD22	1:3:708:TRP:HA	1.81	0.61
1:4:127:PHE:CE2	1:4:184:LEU:HG	2.36	0.60
1:1:127:PHE:HE2	1:1:184:LEU:HG	1.66	0.60
1:1:13:ARG:CZ	1:4:13:ARG:HG3	2.31	0.60
1:3:833:ALA:HB1	1:3:858:ILE:O	2.02	0.60
1:4:127:PHE:HE2	1:4:184:LEU:HG	1.66	0.60
1:2:864:MET:HE3	1:2:866:ILE:HD11	1.83	0.60
1:2:127:PHE:HE2	1:2:184:LEU:HG	1.66	0.59
1:2:379:MET:HE1	1:2:387:VAL:HB	1.84	0.59
1:2:823:LEU:HD11	1:2:841:ALA:HB2	1.84	0.59
1:3:52:ARG:O	1:3:213:SER:HB2	2.02	0.59
1:3:127:PHE:CE2	1:3:184:LEU:HG	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:127:PHE:HE2	1:3:184:LEU:HG	1.67	0.59
1:1:379:MET:HE1	1:1:387:VAL:HB	1.83	0.59
1:2:377:LEU:HD22	1:2:708:TRP:HA	1.85	0.59
1:4:741:THR:HB	1:4:748:CYS:HB3	1.85	0.59
1:3:577:LYS:O	1:3:584:PRO:HA	2.02	0.59
1:4:379:MET:HE1	1:4:387:VAL:HB	1.83	0.58
1:4:823:LEU:HD11	1:4:841:ALA:HB2	1.85	0.58
1:1:823:LEU:HD11	1:1:841:ALA:HB2	1.84	0.58
1:3:379:MET:HE1	1:3:387:VAL:HB	1.85	0.58
1:4:734:SER:OG	1:4:860:GLY:HA3	2.04	0.57
1:3:292:ARG:HH12	5:3:7009:DMS:H13	1.69	0.57
1:2:579:ASP:OD2	1:2:583:ASN:HB2	2.05	0.57
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.85	0.57
1:4:508:GLU:OE2	5:4:7024:DMS:H21	2.04	0.57
1:1:749:ILE:N	1:1:749:ILE:HD12	2.20	0.57
1:4:749:ILE:N	1:4:749:ILE:HD12	2.19	0.57
1:1:873:ALA:O	1:1:876:THR:HG22	2.05	0.56
1:4:237:ARG:HD2	1:4:296:GLU:OE1	2.04	0.56
1:4:767:GLN:NE2	1:4:774:LYS:HE3	2.20	0.56
1:4:863:GLN:HG2	1:4:1021:CYS:HB3	1.85	0.56
1:2:945:ASN:OD1	1:2:950:GLN:HG3	2.05	0.56
1:3:890:GLN:HB2	6:3:4427:HOH:O	2.03	0.56
1:1:262:GLN:HG2	6:1:4836:HOH:O	2.04	0.56
1:1:204:ARG:HB3	6:1:4190:HOH:O	2.05	0.56
1:2:292:ARG:HH12	5:2:7009:DMS:C1	2.19	0.56
1:3:942:ARG:HA	1:3:953:GLY:O	2.06	0.56
1:2:334:GLU:OE1	1:2:336:ARG:NH1	2.38	0.55
1:3:653:HIS:HB3	6:3:4967:HOH:O	2.06	0.55
1:1:768:MET:HE1	1:1:1020:TRP:CZ2	2.41	0.55
1:3:334:GLU:OE1	1:3:336:ARG:NH1	2.40	0.55
1:4:334:GLU:OE1	1:4:336:ARG:NH1	2.39	0.55
1:3:873:ALA:O	1:3:876:THR:HG22	2.07	0.55
1:2:630:ARG:HH21	5:2:7024:DMS:H21	1.71	0.55
1:4:945:ASN:OD1	1:4:950:GLN:HG3	2.07	0.55
1:3:576:ILE:HG12	5:3:7008:DMS:H23	1.89	0.55
1:2:675:GLN:HG3	6:2:5019:HOH:O	2.07	0.55
1:2:942:ARG:HA	1:2:953:GLY:O	2.06	0.55
1:3:277:GLU:HG2	6:3:4755:HOH:O	2.07	0.55
1:3:632:SER:HB3	5:3:7020:DMS:H12	1.89	0.55
1:4:768:MET:HE1	1:4:1020:TRP:CZ2	2.42	0.55
1:2:873:ALA:O	1:2:876:THR:HG22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:945:ASN:OD1	1:3:950:GLN:HG3	2.07	0.54
1:4:942:ARG:HA	1:4:953:GLY:O	2.08	0.54
1:1:738:PRO:HB2	1:1:834:VAL:HG23	1.90	0.54
1:4:748:CYS:C	1:4:749:ILE:HD12	2.32	0.54
1:2:1023:LYS:HA	6:2:4992:HOH:O	2.08	0.54
1:1:573:GLN:HB2	1:1:602:CYS:O	2.08	0.54
1:3:768:MET:HE1	1:3:1020:TRP:CZ2	2.43	0.54
1:4:91:GLN:HG3	1:4:96:ASP:OD1	2.08	0.53
1:4:573:GLN:HB2	1:4:602:CYS:O	2.08	0.53
1:4:873:ALA:O	1:4:876:THR:HG22	2.08	0.53
1:3:91:GLN:HG3	1:3:96:ASP:OD1	2.08	0.53
1:4:628:GLN:HE22	5:4:7001:DMS:C2	2.22	0.53
1:1:334:GLU:OE1	1:1:336:ARG:NH1	2.40	0.53
1:1:942:ARG:HA	1:1:953:GLY:O	2.09	0.53
1:2:91:GLN:HG3	1:2:96:ASP:OD1	2.07	0.53
1:2:749:ILE:HD12	1:2:858:ILE:HD12	1.91	0.53
1:2:768:MET:HE1	1:2:1020:TRP:CZ2	2.43	0.53
1:1:91:GLN:HG3	1:1:96:ASP:OD1	2.08	0.53
1:2:749:ILE:CD1	1:2:858:ILE:HD12	2.38	0.53
1:3:573:GLN:HB2	1:3:602:CYS:O	2.09	0.53
1:2:632:SER:HB2	5:2:7024:DMS:H23	1.90	0.53
1:2:730:LEU:HD12	1:2:730:LEU:N	2.24	0.52
1:1:260:LEU:HD11	1:1:309:TYR:HB3	1.91	0.52
1:1:52:ARG:O	1:1:213:SER:HB2	2.10	0.52
1:2:573:GLN:HB2	1:2:602:CYS:O	2.10	0.52
1:3:369:GLU:HG3	1:3:397:LEU:HD21	1.91	0.52
1:3:533:LEU:C	1:3:533:LEU:HD23	2.34	0.52
1:3:266:GLN:O	5:3:7018:DMS:H22	2.10	0.52
1:3:730:LEU:N	1:3:730:LEU:HD12	2.24	0.52
1:2:950:GLN:HB2	1:2:1023:LYS:HB2	1.92	0.52
1:4:369:GLU:HG3	1:4:397:LEU:HD21	1.91	0.52
1:1:756:TRP:CD2	1:1:858:ILE:HD13	2.45	0.51
1:3:249:GLU:CD	1:3:251:ARG:HD3	2.34	0.51
1:4:892:ALA:HB3	1:4:946:TYR:CE1	2.45	0.51
1:1:748:CYS:C	1:1:749:ILE:HD12	2.35	0.51
1:2:316:HIS:CD2	5:2:7005:DMS:H23	2.45	0.51
1:1:730:LEU:N	1:1:730:LEU:HD12	2.25	0.51
1:2:595:THR:HA	1:2:596:PRO:C	2.36	0.51
1:3:800:ARG:HH11	1:3:800:ARG:HG2	1.75	0.51
1:1:892:ALA:HB3	1:1:946:TYR:CE1	2.45	0.51
1:3:745:MET:HE1	1:3:761:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:945:ASN:OD1	1:1:950:GLN:HG3	2.10	0.51
1:3:730:LEU:HD21	1:4:823:LEU:O	2.10	0.51
1:4:976:LEU:HD12	5:4:7014:DMS:H22	1.92	0.51
1:2:533:LEU:C	1:2:533:LEU:HD23	2.36	0.51
1:4:277:GLU:HG2	6:4:4549:HOH:O	2.09	0.51
1:4:751:LEU:HD21	1:4:860:GLY:O	2.11	0.50
1:2:730:LEU:HD12	1:2:730:LEU:H	1.77	0.50
1:4:533:LEU:C	1:4:533:LEU:HD23	2.36	0.50
1:1:148:SER:HA	1:1:165:SER:OG	2.11	0.50
1:1:653:HIS:HB3	6:1:4865:HOH:O	2.11	0.50
1:2:369:GLU:HG3	1:2:397:LEU:HD21	1.93	0.50
1:3:579:ASP:OD2	1:3:583:ASN:HB2	2.11	0.50
1:4:316:HIS:HB2	1:4:321:THR:O	2.11	0.50
1:1:800:ARG:HG2	1:1:800:ARG:HH11	1.77	0.50
1:4:730:LEU:N	1:4:730:LEU:HD12	2.25	0.50
1:1:292:ARG:HH12	5:1:7009:DMS:H13	1.77	0.50
1:3:749:ILE:HB	1:3:756:TRP:HB2	1.92	0.50
1:3:892:ALA:HB3	1:3:946:TYR:CE1	2.46	0.50
1:2:433:LEU:HB3	1:2:434:PRO:HD3	1.94	0.50
1:3:433:LEU:HB3	1:3:434:PRO:HD3	1.94	0.50
1:1:260:LEU:HD11	1:1:309:TYR:CB	2.41	0.50
1:1:595:THR:HA	1:1:596:PRO:C	2.37	0.50
1:4:800:ARG:HG2	1:4:800:ARG:HH11	1.76	0.50
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.47	0.50
1:4:579:ASP:OD2	1:4:583:ASN:HB2	2.12	0.50
1:4:767:GLN:HE22	1:4:774:LYS:HE3	1.77	0.50
1:2:800:ARG:HG2	1:2:800:ARG:HH11	1.76	0.49
1:1:240:LEU:C	1:1:240:LEU:HD23	2.37	0.49
1:2:634:GLN:HB2	1:2:681:GLU:OE2	2.12	0.49
1:3:240:LEU:HD23	1:3:240:LEU:C	2.36	0.49
1:3:730:LEU:HD12	1:3:730:LEU:H	1.77	0.49
1:1:369:GLU:HG3	1:1:397:LEU:HD21	1.92	0.49
1:1:533:LEU:HD23	1:1:533:LEU:C	2.37	0.49
1:2:655:MET:HE1	1:2:662:PRO:HB3	1.95	0.49
1:4:595:THR:HA	1:4:596:PRO:C	2.37	0.49
1:1:634:GLN:HB2	1:1:681:GLU:OE2	2.13	0.49
1:1:655:MET:HE1	1:1:662:PRO:HB3	1.95	0.49
1:1:646:HIS:CE1	1:1:671:ASP:OD1	2.65	0.49
1:4:738:PRO:HB2	1:4:834:VAL:HG23	1.94	0.49
1:4:864:MET:HE3	1:4:866:ILE:HD11	1.92	0.49
1:4:634:GLN:HB2	1:4:681:GLU:OE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:730:LEU:HD12	1:4:730:LEU:H	1.77	0.49
1:1:632:SER:HB3	5:1:7019:DMS:H12	1.94	0.49
1:1:823:LEU:O	1:2:730:LEU:HD21	2.12	0.49
1:3:688:PRO:HD3	1:3:694:LEU:HD11	1.95	0.49
1:4:240:LEU:C	1:4:240:LEU:HD23	2.37	0.49
1:4:246:MET:SD	1:4:246:MET:C	2.95	0.49
1:4:433:LEU:HB3	1:4:434:PRO:HD3	1.95	0.49
1:4:549:PHE:CE2	1:4:620:ALA:HA	2.48	0.49
1:1:887:GLN:NE2	1:1:980:GLU:O	2.46	0.48
1:2:240:LEU:C	1:2:240:LEU:HD23	2.38	0.48
1:3:595:THR:HA	1:3:596:PRO:C	2.37	0.48
1:3:148:SER:HA	1:3:165:SER:OG	2.13	0.48
1:1:246:MET:C	1:1:246:MET:SD	2.97	0.48
1:2:401:LEU:HD21	5:2:7020:DMS:H23	1.95	0.48
1:2:658:LEU:HD22	1:2:688:PRO:HB2	1.95	0.48
1:3:887:GLN:NE2	1:3:980:GLU:O	2.46	0.48
1:1:737:ILE:HD12	1:1:738:PRO:CD	2.43	0.48
1:4:769:TRP:HA	1:4:773:LYS:O	2.14	0.48
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.95	0.48
1:2:688:PRO:HD3	1:2:694:LEU:HD11	1.96	0.48
1:3:658:LEU:HD22	1:3:688:PRO:HB2	1.95	0.48
1:1:724:GLU:O	1:2:847:LYS:NZ	2.47	0.48
1:3:655:MET:HE1	1:3:662:PRO:HB3	1.96	0.48
1:4:809:ARG:HD2	6:4:4569:HOH:O	2.14	0.48
1:3:634:GLN:HB2	1:3:681:GLU:OE2	2.13	0.48
1:1:561:ARG:HD3	1:2:525:SER:O	2.14	0.48
1:4:887:GLN:NE2	1:4:980:GLU:O	2.47	0.48
1:3:701:VAL:O	1:3:703:PRO:HD3	2.14	0.47
1:4:632:SER:HB3	5:4:7021:DMS:H12	1.95	0.47
1:4:655:MET:HE1	1:4:662:PRO:HB3	1.96	0.47
1:1:688:PRO:HD3	1:1:694:LEU:HD11	1.95	0.47
1:2:476:LYS:HD2	6:2:4199:HOH:O	2.14	0.47
1:4:36:TRP:O	1:4:37:ARG:HD3	2.13	0.47
1:4:646:HIS:NE2	1:4:671:ASP:OD1	2.47	0.47
1:4:688:PRO:HD3	1:4:694:LEU:HD11	1.95	0.47
1:2:148:SER:HA	1:2:165:SER:OG	2.13	0.47
1:3:355:ASN:OD1	1:3:388:ARG:HD3	2.14	0.47
1:4:658:LEU:HD22	1:4:688:PRO:HB2	1.96	0.47
1:4:701:VAL:O	1:4:703:PRO:HD3	2.15	0.47
1:1:658:LEU:HD22	1:1:688:PRO:HB2	1.96	0.47
1:1:730:LEU:HD12	1:1:730:LEU:H	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:755:ARG:HB2	1:1:769:TRP:HB2	1.97	0.47
1:4:751:LEU:HD23	1:4:862:GLY:HA2	1.96	0.47
1:4:774:LYS:HE2	1:4:776:LEU:O	2.15	0.47
1:3:476:LYS:HD2	6:3:4199:HOH:O	2.15	0.47
1:3:823:LEU:O	1:4:730:LEU:HD21	2.15	0.47
1:4:355:ASN:OD1	1:4:388:ARG:HD3	2.15	0.47
1:3:546:LEU:HA	6:3:4128:HOH:O	2.14	0.47
1:4:749:ILE:HD11	1:4:836:ILE:HD11	1.97	0.47
1:4:306:PRO:HD2	6:4:4751:HOH:O	2.14	0.47
1:1:600:GLN:CD	1:1:600:GLN:H	2.24	0.46
1:3:754:LYS:HA	1:3:769:TRP:O	2.16	0.46
1:4:427:THR:HG21	1:4:462:SER:HB3	1.97	0.46
1:4:499:ILE:HG22	1:4:501:PRO:HD3	1.98	0.46
1:3:153:TRP:HB2	1:3:185:ALA:HB3	1.97	0.46
1:1:37:ARG:HG2	1:1:50:GLN:NE2	2.31	0.46
1:2:427:THR:HG21	1:2:462:SER:HB3	1.98	0.46
1:2:549:PHE:CE2	1:2:620:ALA:HA	2.49	0.46
1:1:549:PHE:CE2	1:1:620:ALA:HA	2.50	0.46
1:2:250:LEU:O	1:2:251:ARG:HD2	2.15	0.46
1:2:887:GLN:NE2	1:2:980:GLU:O	2.49	0.46
1:1:153:TRP:HB2	1:1:185:ALA:HB3	1.97	0.46
1:4:131:GLU:HG3	6:4:4732:HOH:O	2.15	0.46
1:3:861:SER:OG	1:3:863:GLN:HG3	2.16	0.46
1:2:890:GLN:HG3	1:2:891:VAL:N	2.31	0.46
1:3:245:GLN:HG2	1:3:288:ARG:CG	2.42	0.46
1:3:749:ILE:HD13	1:3:858:ILE:HD12	1.97	0.46
1:4:962:TYR:OH	5:4:7014:DMS:H21	2.16	0.46
1:1:648:ASP:HB3	6:1:4828:HOH:O	2.14	0.45
1:2:355:ASN:OD1	1:2:388:ARG:HD3	2.16	0.45
1:4:245:GLN:HG2	1:4:288:ARG:CG	2.39	0.45
1:1:49:GLN:HG2	6:1:4609:HOH:O	2.15	0.45
1:3:427:THR:HG21	1:3:462:SER:HB3	1.99	0.45
1:1:255:ARG:HG3	1:1:318:ALA:HA	1.97	0.45
1:1:701:VAL:O	1:1:703:PRO:HD3	2.17	0.45
1:2:153:TRP:HB2	1:2:185:ALA:HB3	1.98	0.45
1:2:499:ILE:HG22	1:2:501:PRO:HD3	1.99	0.45
1:2:923:SER:HA	5:2:7018:DMS:H22	1.99	0.45
1:3:600:GLN:CD	1:3:600:GLN:H	2.25	0.45
1:1:499:ILE:HG22	1:1:501:PRO:HD3	1.98	0.45
1:2:739:HIS:O	1:2:749:ILE:HA	2.16	0.45
1:4:153:TRP:HB2	1:4:185:ALA:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:742:THR:HG22	1:1:743:SER:N	2.32	0.45
1:3:549:PHE:CE2	1:3:620:ALA:HA	2.51	0.45
1:4:890:GLN:HG3	1:4:891:VAL:N	2.31	0.45
1:1:28:ALA:HB1	6:1:4889:HOH:O	2.16	0.45
1:2:367:MET:HB3	1:2:372:MET:HE2	1.99	0.45
1:3:499:ILE:HG22	1:3:501:PRO:HD3	1.99	0.45
1:4:600:GLN:H	1:4:600:GLN:CD	2.24	0.45
1:1:473:ARG:NH1	6:1:4608:HOH:O	2.50	0.45
1:4:367:MET:HB3	1:4:372:MET:HE2	2.00	0.44
1:1:355:ASN:OD1	1:1:388:ARG:HD3	2.17	0.44
1:2:600:GLN:H	1:2:600:GLN:CD	2.26	0.44
1:2:754:LYS:HA	1:2:769:TRP:O	2.18	0.44
1:3:246:MET:SD	1:3:246:MET:C	3.00	0.44
1:4:52:ARG:O	1:4:213:SER:HB2	2.17	0.44
1:2:380:LYS:O	5:2:7002:DMS:H21	2.17	0.44
1:2:701:VAL:O	1:2:703:PRO:HD3	2.18	0.44
1:4:194:GLY:O	1:4:198:GLU:HG3	2.18	0.44
1:4:995:GLY:O	1:4:996:ASP:C	2.61	0.44
1:3:857:ARG:HH11	1:3:857:ARG:HG2	1.82	0.44
1:4:124:SER:HA	1:4:184:LEU:O	2.17	0.44
1:1:367:MET:HB3	1:1:372:MET:HE2	2.00	0.44
1:1:472:TYR:O	1:1:476:LYS:HG2	2.18	0.44
1:3:367:MET:HB3	1:3:372:MET:HE2	2.00	0.44
1:1:883:GLY:HA3	1:1:987:ASP:HA	2.00	0.44
1:1:890:GLN:HG3	1:1:891:VAL:N	2.32	0.44
1:3:250:LEU:O	1:3:251:ARG:HD2	2.17	0.43
1:3:390:SER:HA	1:3:391:HIS:HA	1.74	0.43
1:4:472:TYR:O	1:4:476:LYS:HG2	2.18	0.43
1:4:749:ILE:HG13	1:4:834:VAL:HG11	2.00	0.43
1:1:251:ARG:HG3	1:1:253:TYR:CZ	2.53	0.43
1:2:784:PHE:HA	1:2:881:ARG:O	2.18	0.43
1:3:755:ARG:HB2	1:3:769:TRP:HB2	2.00	0.43
1:4:59:ARG:HB2	1:4:124:SER:OG	2.19	0.43
1:4:305:ILE:HA	6:4:4751:HOH:O	2.19	0.43
1:1:777:LEU:HB2	1:1:887:GLN:HG2	2.00	0.43
1:3:890:GLN:HG3	1:3:891:VAL:N	2.32	0.43
1:4:883:GLY:HA3	1:4:987:ASP:HA	1.99	0.43
1:1:59:ARG:HB2	1:1:124:SER:OG	2.19	0.43
1:1:124:SER:HA	1:1:184:LEU:O	2.18	0.43
1:1:784:PHE:HA	1:1:881:ARG:O	2.19	0.43
1:3:472:TYR:O	1:3:476:LYS:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:784:PHE:HA	1:3:881:ARG:O	2.18	0.43
1:4:863:GLN:HG2	1:4:1021:CYS:CB	2.48	0.43
1:2:369:GLU:OE2	5:2:7020:DMS:H21	2.19	0.43
5:3:7011:DMS:H21	5:3:7025:DMS:H11	2.00	0.43
1:4:100:TYR:CE1	1:4:602:CYS:HB3	2.54	0.43
1:4:957:PHE:CD1	1:4:957:PHE:C	2.97	0.43
1:1:133:TRP:CE3	1:1:216:HIS:HB2	2.54	0.43
1:1:854:LYS:HA	1:1:867:THR:O	2.19	0.43
1:4:857:ARG:HG2	1:4:857:ARG:HH11	1.83	0.43
1:2:883:GLY:HA3	1:2:987:ASP:HA	1.99	0.43
1:2:961:ARG:HG3	5:2:7018:DMS:H12	2.01	0.43
1:2:833:ALA:HB1	1:2:858:ILE:O	2.19	0.43
1:3:817:GLN:HG2	6:3:4333:HOH:O	2.19	0.43
1:4:628:GLN:HE22	5:4:7001:DMS:H22	1.84	0.42
1:4:854:LYS:HA	1:4:867:THR:O	2.19	0.42
1:1:245:GLN:HG2	1:1:288:ARG:CG	2.41	0.42
1:3:881:ARG:HE	1:3:987:ASP:CG	2.27	0.42
1:4:625:GLN:HB2	5:4:7001:DMS:H21	2.00	0.42
1:1:131:GLU:HG3	1:1:135:GLN:CD	2.45	0.42
1:1:857:ARG:HG2	1:1:857:ARG:HH11	1.83	0.42
1:2:881:ARG:HE	1:2:987:ASP:CG	2.26	0.42
1:3:59:ARG:HB2	1:3:124:SER:OG	2.19	0.42
1:1:427:THR:HG21	1:1:462:SER:HB3	2.00	0.42
1:3:124:SER:HA	1:3:184:LEU:O	2.19	0.42
1:1:131:GLU:HG3	1:1:135:GLN:CG	2.50	0.42
1:1:521:LYS:HE2	6:1:4411:HOH:O	2.19	0.42
1:2:245:GLN:HG2	1:2:288:ARG:CG	2.41	0.42
1:2:472:TYR:O	1:2:476:LYS:HG2	2.20	0.42
1:2:843:GLN:HG2	1:2:848:THR:HA	2.02	0.42
1:2:857:ARG:HG2	1:2:857:ARG:HH11	1.84	0.42
1:3:652:LEU:HD11	1:3:698:VAL:HB	2.01	0.42
1:2:124:SER:HA	1:2:184:LEU:O	2.19	0.42
1:3:428:ASP:O	5:3:7013:DMS:H11	2.20	0.42
1:3:576:ILE:HD11	6:3:4216:HOH:O	2.18	0.42
1:3:843:GLN:HG2	1:3:848:THR:HA	2.02	0.42
1:4:751:LEU:HD23	1:4:862:GLY:CA	2.50	0.42
1:4:843:GLN:HG2	1:4:848:THR:HA	2.02	0.42
1:4:910:LEU:C	1:4:910:LEU:HD12	2.45	0.42
1:1:100:TYR:CE1	1:1:602:CYS:HB3	2.54	0.42
1:1:652:LEU:HD11	1:1:698:VAL:HB	2.01	0.42
1:4:777:LEU:HB2	1:4:887:GLN:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:708:TRP:CE3	1:2:709:SER:HB3	2.55	0.42
1:2:777:LEU:HB2	1:2:887:GLN:HG2	2.02	0.42
1:4:225:PHE:HA	1:4:243:GLU:O	2.20	0.42
1:1:131:GLU:HG3	1:1:135:GLN:HG3	2.01	0.42
1:1:737:ILE:O	1:1:737:ILE:HG23	2.20	0.42
1:3:883:GLY:HA3	1:3:987:ASP:HA	2.01	0.42
1:4:257:THR:HA	1:4:270:GLY:O	2.19	0.42
1:1:50:GLN:N	1:1:50:GLN:CD	2.78	0.41
1:2:246:MET:SD	1:2:246:MET:C	3.02	0.41
1:3:100:TYR:CE1	1:3:602:CYS:HB3	2.55	0.41
1:3:305:ILE:HD11	1:3:645:ARG:HB3	2.01	0.41
1:3:777:LEU:HB2	1:3:887:GLN:HG2	2.01	0.41
1:3:200:GLN:HG2	1:3:391:HIS:HB2	2.02	0.41
1:4:377:LEU:CD2	1:4:708:TRP:HA	2.49	0.41
1:1:239:VAL:HG23	5:1:7017:DMS:H21	2.01	0.41
1:1:619:GLU:HA	1:1:912:ALA:HB2	2.03	0.41
1:1:881:ARG:HE	1:1:987:ASP:CG	2.28	0.41
1:2:225:PHE:HA	1:2:243:GLU:O	2.20	0.41
1:1:437:SER:O	1:1:441:THR:HG23	2.21	0.41
1:3:578:TYR:CE2	1:3:584:PRO:HB3	2.55	0.41
1:4:652:LEU:HD11	1:4:698:VAL:HB	2.02	0.41
1:2:750:GLU:N	1:2:750:GLU:CD	2.79	0.41
1:3:52:ARG:HD2	6:3:4818:HOH:O	2.20	0.41
1:4:708:TRP:CE3	1:4:709:SER:HB3	2.55	0.41
1:1:250:LEU:HD11	1:1:287:ASP:HA	2.01	0.41
1:3:596:PRO:HG2	6:3:4456:HOH:O	2.21	0.41
1:4:108:THR:HA	5:4:7012:DMS:H23	2.03	0.41
1:4:166:ARG:HG3	1:4:392:TYR:HB2	2.02	0.41
1:4:652:LEU:O	1:4:667:GLU:HA	2.21	0.41
1:1:780:LEU:HA	1:1:886:CYS:HB3	2.02	0.41
1:1:818:ALA:HB3	6:1:4943:HOH:O	2.19	0.41
1:2:652:LEU:HD11	1:2:698:VAL:HB	2.02	0.41
1:3:995:GLY:O	1:3:996:ASP:C	2.61	0.41
1:2:59:ARG:HB2	1:2:124:SER:OG	2.21	0.41
1:2:571:VAL:CG2	1:2:609:ALA:HA	2.51	0.41
1:2:674:PRO:O	1:2:675:GLN:HB2	2.20	0.41
1:2:957:PHE:CD1	1:2:957:PHE:C	2.98	0.41
1:3:613:PRO:HB3	1:3:617:LEU:HD23	2.03	0.41
1:1:166:ARG:HG3	1:1:392:TYR:HB2	2.03	0.41
1:1:637:GLU:HB2	5:1:7019:DMS:H11	2.03	0.41
1:1:652:LEU:O	1:1:667:GLU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:143:PHE:O	1:2:168:PRO:HA	2.21	0.41
1:2:568:TRP:HA	1:2:569:ASP:HA	1.84	0.41
1:2:652:LEU:O	1:2:667:GLU:HA	2.21	0.41
1:2:757:GLN:O	1:2:765:LEU:HD12	2.21	0.41
1:2:995:GLY:C	1:2:997:ASP:N	2.78	0.41
1:2:995:GLY:O	1:2:996:ASP:C	2.63	0.41
1:3:111:PRO:HA	1:3:112:PRO:HA	1.88	0.41
1:3:225:PHE:HA	1:3:243:GLU:O	2.21	0.41
1:3:619:GLU:HA	1:3:912:ALA:HB2	2.03	0.41
1:3:652:LEU:O	1:3:667:GLU:HA	2.21	0.41
1:4:637:GLU:HB2	5:4:7021:DMS:S	2.60	0.41
1:4:995:GLY:C	1:4:997:ASP:N	2.78	0.41
1:1:579:ASP:OD1	1:1:579:ASP:C	2.64	0.41
1:2:305:ILE:HD11	1:2:645:ARG:HB3	2.02	0.41
1:2:910:LEU:C	1:2:910:LEU:HD12	2.46	0.41
1:4:780:LEU:HA	1:4:886:CYS:HB3	2.02	0.41
1:2:854:LYS:HA	1:2:867:THR:O	2.21	0.40
1:4:571:VAL:CG2	1:4:609:ALA:HA	2.51	0.40
1:2:166:ARG:HG3	1:2:392:TYR:HB2	2.03	0.40
1:2:437:SER:O	1:2:441:THR:HG23	2.20	0.40
1:3:433:LEU:N	1:3:434:PRO:CD	2.84	0.40
1:3:747:PHE:HB2	1:3:758:PHE:HB2	2.04	0.40
1:4:767:GLN:HE22	1:4:774:LYS:HG3	1.80	0.40
1:1:225:PHE:HA	1:1:243:GLU:O	2.22	0.40
1:1:708:TRP:CE3	1:1:709:SER:HB3	2.56	0.40
1:1:843:GLN:HG2	1:1:848:THR:HA	2.02	0.40
1:2:291:LEU:N	1:2:291:LEU:HD22	2.36	0.40
1:3:377:LEU:CD2	1:3:708:TRP:HA	2.50	0.40
1:4:784:PHE:HA	1:4:881:ARG:O	2.21	0.40
1:4:881:ARG:HE	1:4:987:ASP:CG	2.28	0.40
1:1:194:GLY:O	1:1:198:GLU:HG3	2.21	0.40
1:3:287:ASP:OD1	1:3:287:ASP:N	2.51	0.40
1:3:610:ASP:O	1:3:611:ARG:HB2	2.21	0.40
1:3:739:HIS:O	1:3:749:ILE:HA	2.21	0.40
1:3:995:GLY:C	1:3:997:ASP:N	2.78	0.40
1:2:13:ARG:N	6:2:5013:HOH:O	2.54	0.40
1:2:100:TYR:CE1	1:2:602:CYS:HB3	2.57	0.40
1:3:292:ARG:HH12	5:3:7009:DMS:C1	2.33	0.40
1:4:800:ARG:HG2	1:4:800:ARG:NH1	2.37	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	1	1009/1052 (96%)	964 (96%)	45 (4%)	0	100	100
1	2	1009/1052 (96%)	961 (95%)	48 (5%)	0	100	100
1	3	1009/1052 (96%)	960 (95%)	49 (5%)	0	100	100
1	4	1009/1052 (96%)	963 (95%)	46 (5%)	0	100	100
All	All	4036/4208 (96%)	3848 (95%)	188 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	1	863/897 (96%)	857 (99%)	6 (1%)	76	87
1	2	863/897 (96%)	856 (99%)	7 (1%)	73	85
1	3	863/897 (96%)	858 (99%)	5 (1%)	78	89
1	4	863/897 (96%)	854 (99%)	9 (1%)	68	81
All	All	3452/3588 (96%)	3425 (99%)	27 (1%)	73	85

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	80	GLU
1	1	319	ASP

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Mol	Chain	Res	Type
1	1	519	SER
1	1	546	LEU
1	1	672	VAL
1	1	687	GLN
1	2	80	GLU
1	2	519	SER
1	2	546	LEU
1	2	646	HIS
1	2	672	VAL
1	2	687	GLN
1	2	772	ASP
1	3	80	GLU
1	3	519	SER
1	3	546	LEU
1	3	672	VAL
1	3	687	GLN
1	4	80	GLU
1	4	148	SER
1	4	319	ASP
1	4	519	SER
1	4	546	LEU
1	4	630	ARG
1	4	648	ASP
1	4	672	VAL
1	4	687	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	262	GLN
1	1	365	GLN
1	1	374	GLN
1	1	445	GLN
1	1	485	GLN
1	1	510	GLN
1	1	583	ASN
1	1	628	GLN
1	1	634	GLN
1	1	653	HIS
1	1	804	ASN
1	1	843	GLN
1	1	844	HIS

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Mol	Chain	Res	Type
1	1	885	ASN
1	1	903	GLN
1	2	50	GLN
1	2	374	GLN
1	2	445	GLN
1	2	485	GLN
1	2	628	GLN
1	2	634	GLN
1	2	653	HIS
1	2	739	HIS
1	2	804	ASN
1	2	843	GLN
1	2	885	ASN
1	2	1022	GLN
1	3	262	GLN
1	3	374	GLN
1	3	445	GLN
1	3	485	GLN
1	3	583	ASN
1	3	634	GLN
1	3	646	HIS
1	3	653	HIS
1	3	739	HIS
1	3	757	GLN
1	3	804	ASN
1	3	843	GLN
1	4	50	GLN
1	4	307	ASN
1	4	363	HIS
1	4	445	GLN
1	4	485	GLN
1	4	583	ASN
1	4	628	GLN
1	4	634	GLN
1	4	653	HIS
1	4	804	ASN
1	4	843	GLN
1	4	844	HIS
1	4	863	GLN
1	4	885	ASN

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 141 ligands modelled in this entry, 28 are monoatomic - leaving 113 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	1	7014	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	3	7011	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	1	7013	-	3,3,3	0.20	0	3,3,3	0.63	0
5	DMS	1	7007	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	2	7011	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	3	7022	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	1	7011	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	7020	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	7000	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	7002	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	4	7010	-	3,3,3	0.26	0	3,3,3	0.64	0
4	GAI	2	2001	-	3,3,3	0.68	0	3,3,3	1.14	0
5	DMS	3	7000	-	3,3,3	0.19	0	3,3,3	0.63	0
5	DMS	4	7003	-	3,3,3	0.29	0	3,3,3	0.67	0
5	DMS	3	7005	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	1	7008	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	2	7028	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	7024	-	3,3,3	0.22	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	3	7021	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	2	7016	3	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	2	7013	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	7024	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	3	7019	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	7023	-	3,3,3	0.27	0	3,3,3	0.63	0
5	DMS	1	7005	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	7021	-	3,3,3	0.20	0	3,3,3	0.62	0
5	DMS	2	7007	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	7015	-	3,3,3	0.21	0	3,3,3	0.61	0
4	GAI	1	2001	-	3,3,3	0.73	0	3,3,3	1.13	0
5	DMS	1	7023	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	2	7004	-	3,3,3	0.28	0	3,3,3	0.63	0
5	DMS	3	7017	-	3,3,3	0.22	0	3,3,3	0.61	0
4	GAI	4	2001	-	3,3,3	0.68	0	3,3,3	1.09	0
5	DMS	1	7004	-	3,3,3	0.19	0	3,3,3	0.63	0
5	DMS	1	7002	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	7001	-	3,3,3	0.17	0	3,3,3	0.62	0
5	DMS	4	7000	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	2	7017	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	3	7025	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	7012	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	1	7016	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	2	7006	-	3,3,3	0.19	0	3,3,3	0.62	0
5	DMS	2	7002	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	1	7010	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	4	7009	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	7024	-	3,3,3	0.22	0	3,3,3	0.62	0
5	DMS	4	7016	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	1	7017	-	3,3,3	0.26	0	3,3,3	0.65	0
5	DMS	4	7013	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	3	7006	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	4	7025	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	3	7003	-	3,3,3	0.20	0	3,3,3	0.68	0
5	DMS	4	7007	-	3,3,3	0.24	0	3,3,3	0.64	0
5	DMS	4	7014	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	7005	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	4	7004	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	4	7011	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	3	7010	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	7015	-	3,3,3	0.20	0	3,3,3	0.65	0
5	DMS	4	7002	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	3	1024	-	3,3,3	0.28	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	2	7019	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	4	7017	-	3,3,3	0.23	0	3,3,3	0.65	0
5	DMS	2	7012	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	7006	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	4	7001	-	3,3,3	0.18	0	3,3,3	0.64	0
5	DMS	1	7022	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	4	7021	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	7015	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	2	7009	-	3,3,3	0.26	0	3,3,3	0.59	0
5	DMS	2	7022	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	2	7027	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	4	7005	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	3	7007	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	1	7012	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	1	7001	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	7009	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	3	7004	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	2	7008	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	7009	-	3,3,3	0.27	0	3,3,3	0.62	0
5	DMS	4	7019	-	3,3,3	0.29	0	3,3,3	0.64	0
5	DMS	2	7010	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	4	7023	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	7018	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	3	7012	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	1	7003	-	3,3,3	0.20	0	3,3,3	0.68	0
5	DMS	4	7006	-	3,3,3	0.21	0	3,3,3	0.62	0
5	DMS	2	7023	-	3,3,3	0.25	0	3,3,3	0.63	0
5	DMS	4	7022	-	3,3,3	0.24	0	3,3,3	0.62	0
5	DMS	2	7020	-	3,3,3	0.19	0	3,3,3	0.62	0
5	DMS	1	7018	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	3	7018	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	3	7026	-	3,3,3	0.25	0	3,3,3	0.65	0
4	GAI	3	2001	-	3,3,3	0.70	0	3,3,3	1.12	0
5	DMS	3	7014	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	7024	-	3,3,3	0.24	0	3,3,3	0.65	0
5	DMS	2	7029	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	7001	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	7026	-	3,3,3	0.28	0	3,3,3	0.59	0
5	DMS	2	7025	-	3,3,3	0.25	0	3,3,3	0.65	0
5	DMS	3	7020	-	3,3,3	0.25	0	3,3,3	0.64	0
5	DMS	2	7014	-	3,3,3	0.23	0	3,3,3	0.63	0
5	DMS	1	7019	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	4	7018	-	3,3,3	0.23	0	3,3,3	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMS	2	7015	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	7000	-	3,3,3	0.21	0	3,3,3	0.67	0
5	DMS	1	7021	-	3,3,3	0.26	0	3,3,3	0.64	0
5	DMS	3	7008	-	3,3,3	0.25	0	3,3,3	0.62	0
5	DMS	4	7020	-	3,3,3	0.27	0	3,3,3	0.65	0
5	DMS	3	7016	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	3	7013	-	3,3,3	0.23	0	3,3,3	0.64	0
5	DMS	2	7003	-	3,3,3	0.24	0	3,3,3	0.69	0
5	DMS	4	7008	-	3,3,3	0.25	0	3,3,3	0.61	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

23 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	7011	DMS	1	0
5	2	7024	DMS	2	0
5	3	7025	DMS	1	0
5	4	7012	DMS	1	0
5	2	7002	DMS	1	0
5	4	7009	DMS	1	0
5	4	7024	DMS	1	0
5	1	7017	DMS	1	0
5	4	7014	DMS	2	0
5	2	7005	DMS	1	0
5	4	7001	DMS	3	0
5	4	7021	DMS	2	0
5	2	7009	DMS	2	0
5	1	7009	DMS	1	0
5	3	7009	DMS	2	0
5	2	7018	DMS	2	0
5	2	7020	DMS	2	0
5	3	7018	DMS	1	0
5	3	7026	DMS	1	0
5	3	7020	DMS	1	0
5	1	7019	DMS	2	0
5	3	7008	DMS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	3	7013	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%)	-0.04	19 (1%) 66 63	9, 25, 47, 75	0
1	2	1011/1052 (96%)	-0.10	34 (3%) 48 45	8, 20, 47, 78	0
1	3	1011/1052 (96%)	-0.17	22 (2%) 62 59	7, 20, 44, 78	0
1	4	1011/1052 (96%)	0.14	37 (3%) 45 42	10, 27, 50, 77	0
All	All	4044/4208 (96%)	-0.04	112 (2%) 55 52	7, 23, 47, 78	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	731	PRO	4.4
1	2	733	ALA	4.1
1	1	730	LEU	4.0
1	1	686	PRO	4.0
1	4	688	PRO	4.0
1	3	688	PRO	3.9
1	1	732	ALA	3.8
1	2	685	LEU	3.8
1	2	689	GLU	3.6
1	1	737	ILE	3.6
1	4	730	LEU	3.6
1	2	1023	LYS	3.5
1	3	686	PRO	3.5
1	3	733	ALA	3.5
1	3	731	PRO	3.5
1	1	685	LEU	3.4
1	4	685	LEU	3.4
1	4	79	PRO	3.3
1	1	689	GLU	3.3
1	2	1022	GLN	3.3
1	2	728	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	3	689	GLU	3.2
1	3	772	ASP	3.2
1	4	686	PRO	3.1
1	4	736	ALA	3.0
1	1	735	HIS	3.0
1	4	735	HIS	3.0
1	4	127	PHE	2.9
1	4	833	ALA	2.9
1	2	686	PRO	2.9
1	2	747	PHE	2.9
1	2	739	HIS	2.9
1	3	800	ARG	2.9
1	1	733	ALA	2.9
1	2	688	PRO	2.8
1	3	578	TYR	2.8
1	2	772	ASP	2.8
1	2	729	THR	2.7
1	2	732	ALA	2.7
1	1	800	ARG	2.7
1	4	71	GLU	2.7
1	4	733	ALA	2.7
1	2	735	HIS	2.6
1	2	774	LYS	2.6
1	3	685	LEU	2.6
1	4	1023	LYS	2.6
1	2	691	ALA	2.6
1	2	669	PRO	2.6
1	4	689	GLU	2.5
1	4	800	ARG	2.5
1	3	583	ASN	2.5
1	4	743	SER	2.5
1	2	755	ARG	2.5
1	2	1018	LEU	2.5
1	4	130	ASP	2.4
1	4	319	ASP	2.4
1	4	750	GLU	2.4
1	4	737	ILE	2.4
1	1	773	LYS	2.4
1	3	730	LEU	2.4
1	2	771	GLY	2.4
1	3	831	ALA	2.4
1	3	690	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	1	748	CYS	2.4
1	4	668	VAL	2.4
1	4	177	LEU	2.4
1	3	846	GLY	2.3
1	4	734	SER	2.3
1	2	679	LEU	2.3
1	1	801	ILE	2.3
1	3	1023	LYS	2.3
1	2	734	SER	2.3
1	4	684	GLU	2.3
1	4	731	PRO	2.3
1	2	833	ALA	2.2
1	4	836	ILE	2.2
1	2	730	LEU	2.2
1	4	74	LEU	2.2
1	1	79	PRO	2.2
1	1	687	GLN	2.2
1	1	729	THR	2.2
1	4	741	THR	2.2
1	4	72	SER	2.2
1	2	770	ILE	2.2
1	4	835	LEU	2.2
1	4	834	VAL	2.2
1	2	800	ARG	2.2
1	2	736	ALA	2.2
1	1	731	PRO	2.2
1	4	653	HIS	2.2
1	4	770	ILE	2.1
1	3	770	ILE	2.1
1	4	663	LEU	2.1
1	1	71	GLU	2.1
1	4	596	PRO	2.1
1	4	748	CYS	2.1
1	2	759	ASN	2.1
1	3	581	ASN	2.1
1	2	634	GLN	2.1
1	3	732	ALA	2.1
1	4	777	LEU	2.1
1	2	725	ASN	2.1
1	1	688	PRO	2.1
1	2	745	MET	2.0
1	2	977	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	3	651	LEU	2.0
1	3	858	ILE	2.0
1	3	1013	ARG	2.0
1	1	1023	LYS	2.0
1	4	732	ALA	2.0
1	3	1018	LEU	2.0
1	2	773	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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(Å ²)	Q<0.9
5	DMS	4	7007	4/4	0.55	0.40	89,89,90,90	0
5	DMS	3	7013	4/4	0.65	0.37	70,70,72,72	0
5	DMS	2	7019	4/4	0.66	0.30	104,104,104,104	0
5	DMS	2	7013	4/4	0.67	0.36	76,76,77,78	0
5	DMS	2	7027	4/4	0.70	0.36	96,96,96,97	0
5	DMS	4	7016	4/4	0.72	0.34	95,95,95,96	0
5	DMS	3	7026	4/4	0.73	0.35	98,98,99,99	0
5	DMS	1	7020	4/4	0.74	0.27	91,91,91,91	0
5	DMS	4	7010	4/4	0.76	0.29	87,87,87,87	0
5	DMS	4	7021	4/4	0.76	0.28	99,99,99,100	0
5	DMS	4	7019	4/4	0.77	0.21	69,70,70,70	0
5	DMS	3	7005	4/4	0.78	0.28	72,73,73,74	0
5	DMS	1	7022	4/4	0.78	0.36	107,107,107,108	0
5	DMS	4	7023	4/4	0.78	0.28	89,89,90,90	0
5	DMS	2	7018	4/4	0.79	0.31	96,96,96,96	0
5	DMS	2	7024	4/4	0.79	0.22	79,80,80,80	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	1	7019	4/4	0.80	0.23	69,69,69,70	0
5	DMS	3	7007	4/4	0.80	0.27	86,86,86,87	0
5	DMS	1	7014	4/4	0.80	0.29	86,86,86,87	0
5	DMS	4	7013	4/4	0.80	0.21	82,82,82,82	0
5	DMS	4	7024	4/4	0.80	0.24	66,67,67,67	0
5	DMS	3	7019	4/4	0.81	0.26	91,91,91,91	0
4	GAI	1	2001	4/4	0.82	0.18	63,63,63,64	0
5	DMS	2	7007	4/4	0.82	0.28	96,97,97,97	0
5	DMS	2	7011	4/4	0.83	0.21	82,82,82,83	0
5	DMS	1	7015	4/4	0.83	0.28	93,93,94,94	0
5	DMS	1	7016	4/4	0.83	0.20	67,67,67,67	0
5	DMS	4	7020	4/4	0.83	0.20	68,69,69,70	0
4	GAI	2	2001	4/4	0.83	0.15	54,55,55,56	0
5	DMS	3	7012	4/4	0.83	0.19	69,69,69,69	0
5	DMS	4	7012	4/4	0.83	0.23	86,86,87,87	0
5	DMS	3	7011	4/4	0.84	0.24	76,76,77,77	0
5	DMS	3	7020	4/4	0.84	0.24	79,80,80,80	0
5	DMS	1	7012	4/4	0.84	0.18	68,69,69,69	0
3	NA	3	3104	1/1	0.84	0.09	32,32,32,32	0
5	DMS	4	7017	4/4	0.84	0.20	66,67,67,67	0
5	DMS	4	7005	4/4	0.85	0.20	72,72,72,72	0
5	DMS	2	7012	4/4	0.85	0.21	73,73,73,73	0
5	DMS	1	7006	4/4	0.85	0.24	78,78,78,78	0
5	DMS	2	7016	4/4	0.85	0.19	69,70,70,70	0
2	MG	2	3004	1/1	0.86	0.10	61,61,61,61	0
5	DMS	4	7025	4/4	0.86	0.22	67,67,67,67	0
2	MG	4	3004	1/1	0.87	0.12	51,51,51,51	0
5	DMS	2	7005	4/4	0.87	0.20	63,64,65,65	0
5	DMS	1	7007	4/4	0.87	0.19	63,64,64,64	0
2	MG	3	3004	1/1	0.87	0.06	53,53,53,53	0
5	DMS	2	7020	4/4	0.87	0.19	61,61,62,63	0
4	GAI	3	2001	4/4	0.87	0.15	60,61,61,61	0
5	DMS	2	7025	4/4	0.87	0.21	70,70,71,71	0
5	DMS	4	7014	4/4	0.87	0.20	82,83,83,83	0
5	DMS	1	7011	4/4	0.88	0.22	86,86,86,86	0
5	DMS	3	7021	4/4	0.88	0.18	63,63,63,64	0
5	DMS	4	7022	4/4	0.88	0.17	65,65,65,66	0
4	GAI	4	2001	4/4	0.88	0.13	55,56,56,57	0
5	DMS	4	7018	4/4	0.88	0.18	54,55,55,55	0
5	DMS	2	7017	4/4	0.88	0.21	75,76,76,76	0
5	DMS	3	7016	4/4	0.89	0.21	52,54,54,55	0
5	DMS	2	7021	4/4	0.89	0.16	59,59,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	4	7006	4/4	0.89	0.18	65,65,66,66	0
5	DMS	1	7017	4/4	0.89	0.21	74,74,74,75	0
5	DMS	3	7008	4/4	0.89	0.15	52,52,53,53	0
5	DMS	3	7022	4/4	0.89	0.19	72,72,72,72	0
3	NA	1	3103	1/1	0.90	0.08	40,40,40,40	0
5	DMS	3	1024	4/4	0.90	0.18	45,47,48,48	0
5	DMS	1	7010	4/4	0.90	0.17	60,61,61,62	0
5	DMS	4	7015	4/4	0.90	0.16	52,53,54,54	0
5	DMS	1	7021	4/4	0.90	0.19	72,72,72,73	0
5	DMS	3	7003	4/4	0.90	0.17	38,39,41,44	0
5	DMS	2	7023	4/4	0.90	0.15	54,54,54,54	0
5	DMS	1	7024	4/4	0.91	0.15	47,47,48,49	0
5	DMS	2	7010	4/4	0.91	0.16	46,46,47,47	0
5	DMS	4	7003	4/4	0.91	0.18	36,38,39,40	0
5	DMS	2	7015	4/4	0.91	0.18	69,69,69,69	0
5	DMS	1	7003	4/4	0.91	0.14	31,32,36,38	0
5	DMS	3	7014	4/4	0.91	0.17	70,70,70,70	0
5	DMS	3	7023	4/4	0.91	0.18	67,67,68,68	0
5	DMS	2	7003	4/4	0.92	0.13	32,33,35,38	0
3	NA	3	3103	1/1	0.92	0.10	42,42,42,42	0
5	DMS	3	7025	4/4	0.92	0.15	53,53,53,54	0
5	DMS	2	7028	4/4	0.92	0.15	58,58,58,59	0
5	DMS	4	7008	4/4	0.93	0.13	50,51,52,52	0
3	NA	2	3104	1/1	0.93	0.06	30,30,30,30	0
5	DMS	3	7018	4/4	0.93	0.15	53,53,54,54	0
5	DMS	1	7005	4/4	0.93	0.13	60,60,60,60	0
3	NA	3	3101	1/1	0.93	0.04	22,22,22,22	0
5	DMS	2	7006	4/4	0.93	0.12	40,41,41,43	0
5	DMS	1	7023	4/4	0.93	0.15	53,54,54,54	0
5	DMS	2	7008	4/4	0.93	0.14	59,60,60,60	0
5	DMS	2	7022	4/4	0.94	0.14	60,60,60,61	0
5	DMS	4	7009	4/4	0.94	0.14	52,53,53,54	0
5	DMS	1	7009	4/4	0.94	0.12	43,44,45,45	0
5	DMS	4	7011	4/4	0.94	0.12	71,71,72,72	0
3	NA	4	3104	1/1	0.94	0.07	45,45,45,45	0
3	NA	2	3103	1/1	0.94	0.07	39,39,39,39	0
3	NA	4	3103	1/1	0.94	0.09	37,37,37,37	0
5	DMS	2	7014	4/4	0.94	0.13	56,56,56,56	0
5	DMS	1	7013	4/4	0.94	0.12	48,49,50,50	0
2	MG	1	3004	1/1	0.95	0.11	49,49,49,49	0
3	NA	4	3101	1/1	0.95	0.05	22,22,22,22	0
5	DMS	3	7015	4/4	0.95	0.12	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	2	7004	4/4	0.95	0.11	29,31,31,33	0
5	DMS	3	7017	4/4	0.95	0.14	50,50,51,51	0
5	DMS	1	7001	4/4	0.95	0.12	26,26,27,29	0
3	NA	1	3104	1/1	0.95	0.06	40,40,40,40	0
5	DMS	2	7026	4/4	0.95	0.12	47,47,48,48	0
5	DMS	1	7018	4/4	0.95	0.12	52,53,54,54	0
5	DMS	1	7004	4/4	0.96	0.10	36,36,38,39	0
5	DMS	3	7024	4/4	0.96	0.11	57,57,57,57	0
3	NA	4	3102	1/1	0.96	0.04	15,15,15,15	0
5	DMS	3	7001	4/4	0.96	0.09	23,23,24,28	0
2	MG	1	3002	1/1	0.96	0.05	24,24,24,24	0
5	DMS	4	7001	4/4	0.96	0.11	32,33,33,35	0
5	DMS	4	7002	4/4	0.96	0.11	34,35,35,37	0
5	DMS	3	7004	4/4	0.96	0.10	30,31,32,32	0
5	DMS	4	7004	4/4	0.96	0.10	32,33,34,35	0
5	DMS	2	7009	4/4	0.96	0.10	42,42,43,44	0
5	DMS	3	7006	4/4	0.96	0.10	45,45,46,46	0
5	DMS	1	7002	4/4	0.96	0.09	32,32,35,35	0
5	DMS	1	7008	4/4	0.96	0.10	44,44,44,45	0
5	DMS	3	7009	4/4	0.96	0.10	40,41,42,42	0
3	NA	1	3101	1/1	0.96	0.06	30,30,30,30	0
5	DMS	2	7029	4/4	0.97	0.08	43,43,44,44	0
2	MG	1	3001	1/1	0.97	0.03	25,25,25,25	0
5	DMS	3	7002	4/4	0.97	0.08	31,31,32,33	0
2	MG	4	3002	1/1	0.97	0.04	25,25,25,25	0
3	NA	2	3101	1/1	0.97	0.03	16,16,16,16	0
5	DMS	3	7010	4/4	0.97	0.10	41,42,43,43	0
2	MG	2	3001	1/1	0.98	0.03	20,20,20,20	0
5	DMS	1	7000	4/4	0.98	0.06	19,21,21,25	0
5	DMS	2	7000	4/4	0.98	0.06	22,23,24,24	0
5	DMS	2	7001	4/4	0.98	0.07	25,25,25,29	0
5	DMS	4	7000	4/4	0.98	0.06	24,26,27,27	0
5	DMS	2	7002	4/4	0.98	0.07	30,30,30,31	0
2	MG	3	3001	1/1	0.99	0.02	16,16,16,16	0
2	MG	3	3002	1/1	0.99	0.05	12,12,12,12	0
5	DMS	3	7000	4/4	0.99	0.04	17,18,18,21	0
3	NA	2	3102	1/1	0.99	0.03	18,18,18,18	0
2	MG	2	3002	1/1	0.99	0.07	15,15,15,15	0
3	NA	1	3102	1/1	0.99	0.03	15,15,15,15	0
2	MG	4	3001	1/1	0.99	0.02	23,23,23,23	0
3	NA	3	3102	1/1	0.99	0.02	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.