Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:44 AM GMT

PDB ID	:	3MUZ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

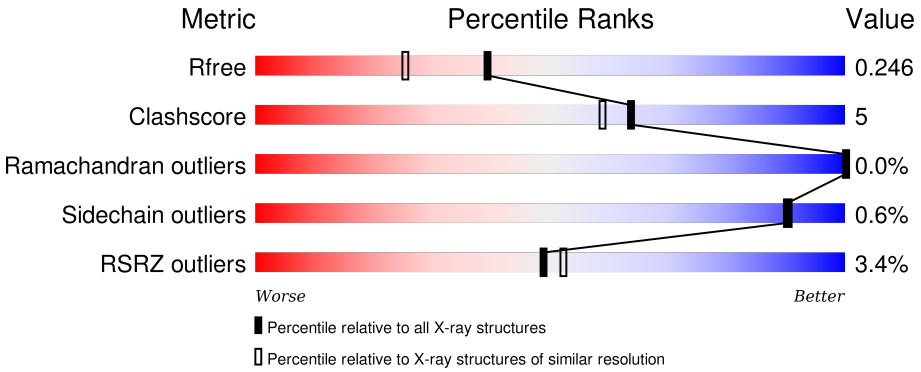
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	4% 82% 15% ·
1	2	1052	2% 85% 11% ·
1	3	1052	3% 85% 11% ·
1	4	1052	4% 82% 14% ·

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
2	IPT	1	2001	-	-	-	X
2	IPT	1	2002	-	-	-	X
2	IPT	2	2002	-	-	-	X
2	IPT	3	2002	-	-	-	X
2	IPT	4	2001	-	-	-	X
5	DMS	1	6001	-	-	-	X
5	DMS	1	6002	-	-	-	X
5	DMS	1	6003	-	-	-	X
5	DMS	1	6006	-	-	-	X
5	DMS	1	6011	-	-	-	X
5	DMS	1	6013	-	-	-	X
5	DMS	1	6018	-	-	-	X
5	DMS	1	6019	-	-	-	X
5	DMS	1	6020	-	-	-	X
5	DMS	1	6023	-	-	-	X
5	DMS	1	6024	-	-	-	X
5	DMS	1	6027	-	-	-	X
5	DMS	1	6030	-	-	-	X
5	DMS	1	6031	-	-	-	X
5	DMS	1	6032	-	-	-	X
5	DMS	2	6000	-	-	-	X
5	DMS	2	6001	-	-	-	X
5	DMS	2	6002	-	-	-	X
5	DMS	2	6003	-	-	-	X
5	DMS	2	6004	-	-	-	X
5	DMS	2	6005	-	-	-	X
5	DMS	2	6012	-	-	-	X
5	DMS	2	6013	-	-	-	X
5	DMS	2	6015	-	-	-	X
5	DMS	2	6016	-	-	-	X
5	DMS	2	6018	-	-	-	X
5	DMS	2	6022	-	-	-	X
5	DMS	2	6023	-	-	-	X
5	DMS	2	6024	-	-	-	X
5	DMS	2	6025	-	-	-	X
5	DMS	2	6028	-	-	-	X
5	DMS	2	6031	-	-	-	X
5	DMS	2	6035	-	-	-	X
5	DMS	2	6038	-	-	-	X
5	DMS	2	6039	-	-	-	X
5	DMS	2	6040	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DMS	3	6001	-	-	-	X
5	DMS	3	6003	-	-	-	X
5	DMS	3	6004	-	-	-	X
5	DMS	3	6005	-	-	-	X
5	DMS	3	6013	-	-	-	X
5	DMS	3	6015	-	-	-	X
5	DMS	3	6017	-	-	-	X
5	DMS	3	6018	-	-	-	X
5	DMS	3	6019	-	-	-	X
5	DMS	3	6020	-	-	-	X
5	DMS	3	6023	-	-	-	X
5	DMS	3	6025	-	-	-	X
5	DMS	3	6026	-	-	-	X
5	DMS	3	6028	-	-	-	X
5	DMS	3	6029	-	-	-	X
5	DMS	3	6031	-	-	-	X
5	DMS	3	6038	-	-	-	X
5	DMS	3	6040	-	-	-	X
5	DMS	4	6000	-	-	-	X
5	DMS	4	6001	-	-	-	X
5	DMS	4	6002	-	-	-	X
5	DMS	4	6003	-	-	-	X
5	DMS	4	6012	-	-	-	X
5	DMS	4	6014	-	-	-	X
5	DMS	4	6015	-	-	-	X
5	DMS	4	6017	-	-	-	X
5	DMS	4	6018	-	-	-	X
5	DMS	4	6021	-	-	-	X
5	DMS	4	6022	-	-	-	X
5	DMS	4	6026	-	-	-	X
5	DMS	4	6027	-	-	-	X
5	DMS	4	6028	-	-	-	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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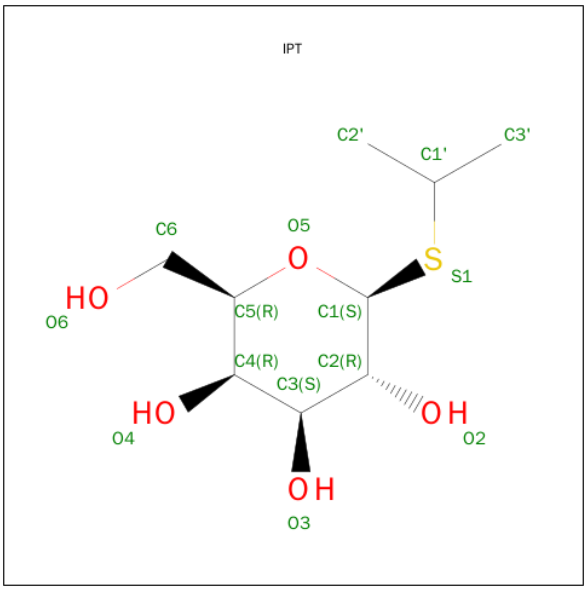
Chain	Residue	Modelled	Actual	Comment	Reference
4	5	MET	-	EXPRESSION TAG	UNP B8LFD6
4	6	ILE	-	EXPRESSION TAG	UNP B8LFD6
4	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
4	8	PRO	-	EXPRESSION TAG	UNP B8LFD6
4	599	ALA	ARG	CONFLICT	UNP B8LFD6

- Molecule 2 is ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).



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

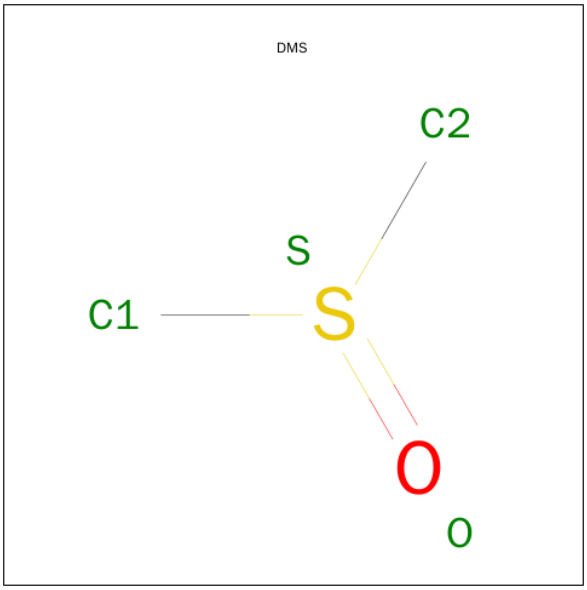
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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

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

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

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

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

- Molecule 6 is water.

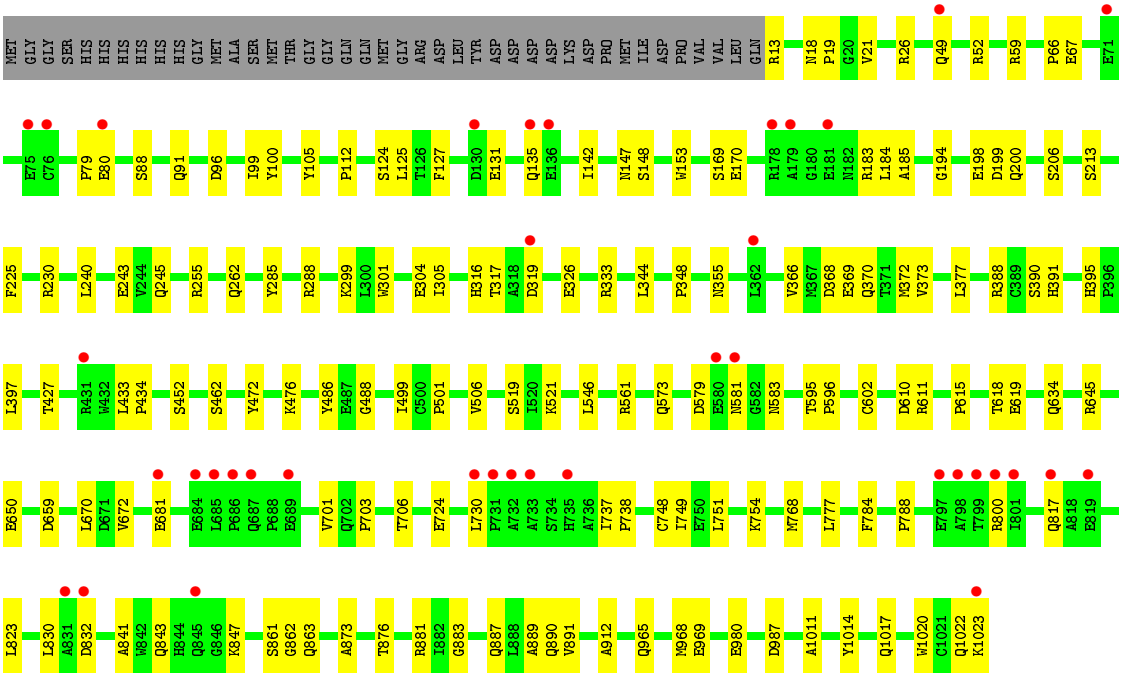
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	1022	Total O 1022 1022	0	0
6	2	1089	Total O 1089 1089	0	0
6	3	1051	Total O 1051 1051	0	0
6	4	946	Total O 946 946	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

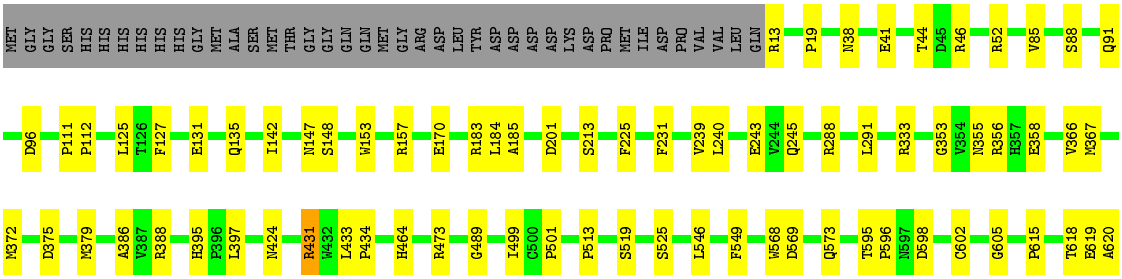
- Molecule 1: Beta-galactosidase

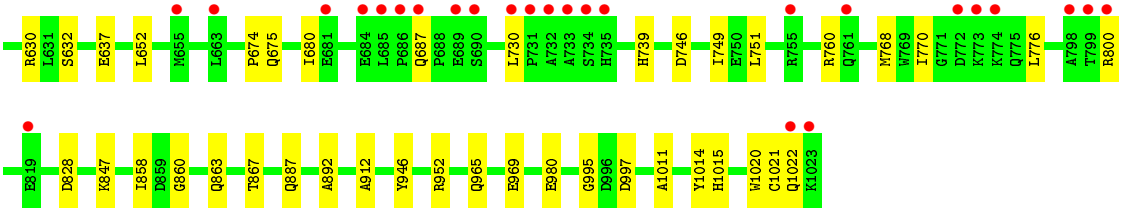
Chain 1:



- Molecule 1: Beta-galactosidase

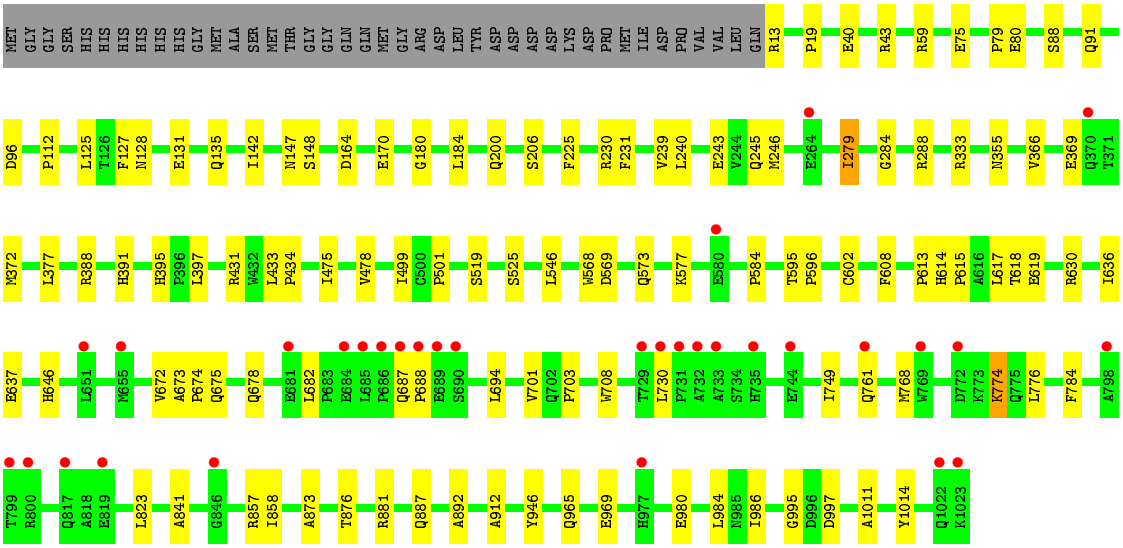
Chain 2:





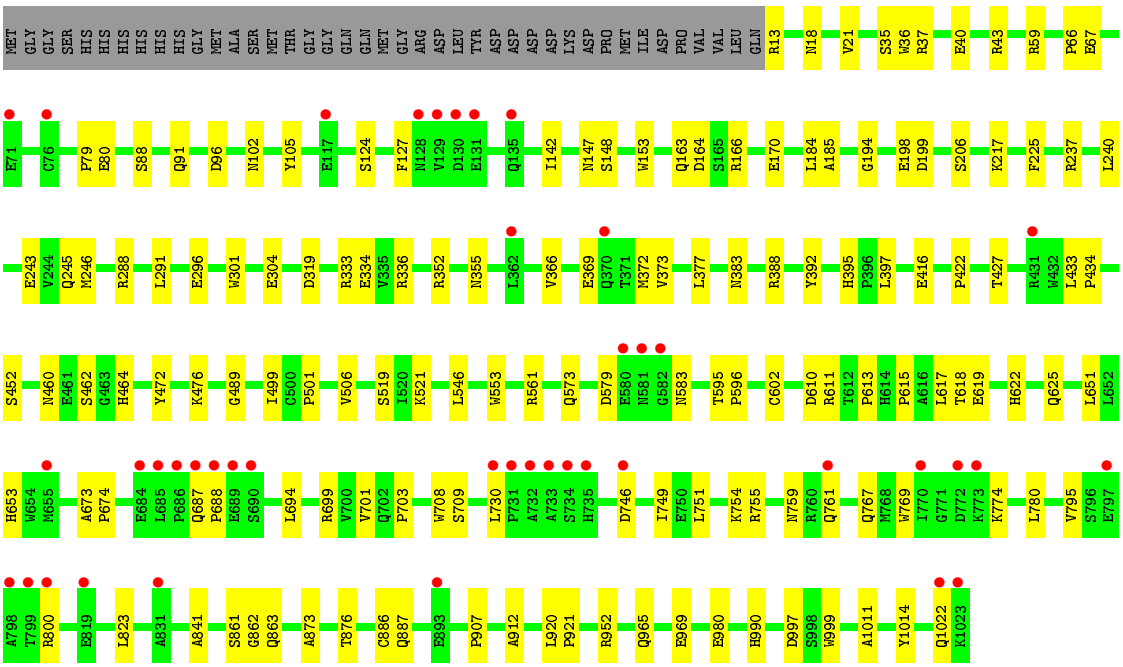
• Molecule 1: Beta-galactosidase

Chain 3:



• Molecule 1: Beta-galactosidase

Chain 4:



4 Data and refinement statistics (i)

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) 94.0 (12.42-1.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 1.90Å)	Xtriage
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%)	DCC
Wilson B-factor (Å^2)	17.0	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 66.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	2 of 370692 reflections (0.001%)	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.30	0/8361	0.61	0/11408
1	2	0.32	0/8361	0.62	0/11408
1	3	0.32	0/8361	0.63	0/11408
1	4	0.30	0/8361	0.60	0/11408
All	All	0.31	0/33444	0.62	0/45632

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.

There are no bond angle outliers.

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	93	0
1	2	8119	0	7707	84	0
1	3	8119	0	7707	76	0
1	4	8119	0	7708	94	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
5	1	132	0	198	0	0
5	2	172	0	258	6	0
5	3	172	0	258	3	0
5	4	124	0	186	2	0
6	1	1022	0	0	12	0
6	2	1089	0	0	4	0
6	3	1051	0	0	6	0
6	4	946	0	0	3	0
All	All	37334	0	31870	336	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 5.

All (336) 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
1:1:153: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
1:2:770:ILE:HG21	1:2:1022:GLN:NE2	2.03	0.73
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:131: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
1:4:372:MET:HE1	1:4:395:HIS:HB3	1.78	0.66
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
1:3:59:ARG:HG2	5:3:6029:DMS:H23	1.78	0.65
1:2:1015:HIS:H	5:2:6026:DMS:H12	1.62	0.65
1:4:754:LYS:HE2	1:4:1022:GLN:HE21	1.60	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
1:4:91: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:CB	1:2:431:ARG:HH21	2.11	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
1:4:88:SER:HA	1:4:366:VAL:HG21	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
1:3:377: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
1:3:984:LEU:HD21	1:3:986:ILE:HD11	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
1:3:127: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)
1:3:768:MET:HE2	1:3:776:LEU:HD11	1.86	0.57
1:1:79:PRO:HG2	1:1:80:GLU:OE2	2.05	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
1:3:372:MET:HE2	6:3:4190:HOH:O	2.04	0.56
1:4:383:ASN:HA	5:4:6002:DMS:H13	1.86	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
1:1:355:ASN:OD1	1:1:388:ARG:HD3	2.05	0.55
1:1:749:ILE:HD12	1:1:749:ILE:N	2.22	0.55
1:1:18:ASN:ND2	1:1:21:VAL:HG23	2.22	0.55
1:3:730:LEU:HD12	1:3:730:LEU:N	2.23	0.55
1:4:952:ARG:HH11	1:4:952:ARG:HB2	1.72	0.54
1:3:431:ARG:HB2	1:3:431:ARG:HH21	1.72	0.54
1:2:375:ASP:O	1:2:379:MET:HG3	2.07	0.54
1:1:372:MET:HE1	1:1:395:HIS:HB3	1.88	0.54
1:4:237:ARG:HD2	1:4:296:GLU:OE1	2.08	0.54
1:4:147:ASN:HB3	1:4:206:SER:HA	1.90	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
1:2:768:MET:HE2	1:2:776:LEU:HD11	1.91	0.53
1:3:749:ILE:CD1	1:3:858:ILE:HD12	2.39	0.53
1:4:767:GLN:HE22	1:4:774:LYS:HE3	1.74	0.53
1:4:613:PRO:HB3	1:4:617:LEU:HD23	1.90	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
1:2:595:THR:HA	1:2:596:PRO:C	2.30	0.53
1:2:615:PRO:O	1:2:618:THR:HG22	2.09	0.53
1:4:651:LEU:HD23	1:4:653:HIS:HE2	1.74	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:887:GLN:NE2	1:3:980:GLU:O	2.42	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:N	1:2:730:LEU:HD12	2.24	0.52
1:3:615:PRO:O	1:3:618:THR:HG22	2.10	0.52
1:4:127:PHE:CE2	1:4:184:LEU:HG	2.45	0.51
1:1:91:GLN:HG3	1:1:96:ASP:OD1	2.10	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
1:4:873:ALA:O	1:4:876:THR:HG22	2.11	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
1:1:768:MET:HE3	1:1:1020:TRP:CZ2	2.45	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
1:2:730:LEU:H	1:2:730:LEU:HD12	1.76	0.50
1:2:201:ASP:OD2	2:2:2001:IPT:H62	2.10	0.50
1:1:368:ASP:OD2	1:1:370:GLN:HB3	2.11	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
1:1:595:THR:HA	1:1:596:PRO:C	2.31	0.50
1:1:13:ARG:NH1	1:4:13:ARG:HG3	2.26	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
1:4:240:LEU:HD23	1:4:240:LEU:C	2.32	0.50
1:1:706:THR:HG22	6:1:4518:HOH:O	2.12	0.49
1:4:625:GLN:HB2	5:4:6001:DMS:H23	1.93	0.49
1:1:348:PRO:HB2	6:1:4921:HOH:O	2.12	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
1:4:36:TRP:O	1:4:37:ARG:HD3	2.13	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
1:2:867:THR:HG23	1:2:1015:HIS:HE1	1.77	0.49
1:4:751:LEU:HD23	1:4:862:GLY:HA2	1.95	0.49
1:3:128:ASN:HA	1:3:180:GLY:O	2.12	0.49
1:4:952:ARG:NH1	1:4:952:ARG:HB2	2.27	0.48
1:3:200:GLN:HG2	1:3:391:HIS:HB2	1.95	0.48
1:4:105:TYR:CE2	1:4:199:ASP:HB2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:739:HIS:HB2	6:2:4974:HOH:O	2.14	0.48
1:2:687:GLN:N	1:2:687:GLN:OE1	2.47	0.48
1:2:1011:ALA:HB3	1:2:1014:TYR:CZ	2.49	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
1:4:887: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
1:4:472:TYR:O	1:4:476:LYS:HG2	2.14	0.47
1:3:372:MET:HE1	1:3:395:HIS:HB3	1.96	0.47
1:2:800:ARG:HG2	1:2:800:ARG:HH11	1.79	0.47
1:3:892:ALA:HB3	1:3:946:TYR:CE1	2.49	0.47
1:2:91:GLN:HG3	1:2:96:ASP:OD1	2.15	0.47
1:1:1017:GLN:HB2	6:1:4900:HOH:O	2.14	0.47
1:1:372:MET:CE	1:1:395:HIS:HB3	2.45	0.47
1:1:1023:LYS:HB3	1:1:1023:LYS:NZ	2.29	0.47
1:3:369:GLU:HG3	1:3:397:LEU:HD21	1.96	0.47
1:1:751:LEU:HD23	1:1:862:GLY:HA2	1.97	0.47
1:4:573:GLN:HB2	1:4:602:CYS:O	2.15	0.47
1:2:619:GLU:HA	1:2:912:ALA:HB2	1.95	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
1:3:688:PRO:HG3	1:3:694:LEU:HD21	1.96	0.47
1:2:240:LEU:C	1:2:240:LEU:HD23	2.35	0.47
1:3:613:PRO:HB3	1:3:617:LEU:HD23	1.96	0.47
1:4:755:ARG:HB2	1:4:769:TRP:HB2	1.96	0.47
1:2:131:GLU:HG3	1:2:135:GLN:HG3	1.97	0.47
1:1:427:THR:HG21	1:1:462:SER:HB3	1.96	0.47
1:2:431:ARG:HB2	1:2:431:ARG:NH2	2.15	0.46
1:1:52:ARG:O	1:1:213:SER:HB2	2.15	0.46
1:2:674:PRO:O	1:2:675:GLN:HB2	2.16	0.46
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.96	0.46
1:2:630:ARG:NH1	1:2:637:GLU:OE1	2.49	0.46
1:3:147:ASN:HA	1:3:148:SER:HA	1.61	0.46
1:2:751:LEU:HD21	1:2:860:GLY:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:4:746:ASP:OD1	1:4:759:ASN:HA	2.16	0.46
1:2:225:PHE:HA	1:2:243:GLU:O	2.16	0.46
1:3:240:LEU:HD23	1:3:240:LEU:C	2.36	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
1:1:701:VAL:O	1:1:703:PRO:HD3	2.15	0.45
1:3:636:ILE:HD11	1:3:682:LEU:HD11	1.99	0.45
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
1:2:1015:HIS:H	5:2:6026:DMS:C1	2.29	0.45
1:1:887:GLN:NE2	1:1:980:GLU:O	2.49	0.45
1:3:674:PRO:O	1:3:675:GLN:HB2	2.16	0.45
1:3:372:MET:CE	1:3:395:HIS:HB3	2.46	0.45
1:1:240:LEU:C	1:1:240:LEU:HD23	2.36	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
1:4:952:ARG:HH11	1:4:952:ARG:CB	2.30	0.45
1:3:19:PRO:HD3	1:3:112:PRO:CB	2.47	0.45
1:2:568:TRP:CD2	1:2:569:ASP:HB3	2.52	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
1:3:279:ILE:HG23	1:3:284:GLY:HA2	1.99	0.45
1:2:111:PRO:HA	1:2:112:PRO:HA	1.83	0.45
1:1:317:THR:OG1	1:1:319:ASP:OD1	2.32	0.45
1:3:431:ARG:NH2	6:3:4869:HOH:O	2.50	0.44
1:1:634:GLN:HB2	1:1:681:GLU:OE2	2.17	0.44
1:1:200:GLN:HG2	1:1:391:HIS:HB2	1.99	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
1:4:595:THR:HA	1:4:596:PRO:C	2.38	0.44
1:1:131:GLU:HG3	1:1:135:GLN:HG3	2.00	0.44
1:3:246:MET:SD	1:3:246:MET:C	2.96	0.44
1:4:246:MET:SD	1:4:246:MET:C	2.96	0.44
1:3:40:GLU:OE2	1:3:43:ARG:NH2	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.99	0.44
1:4:861:SER:OG	1:4:863:GLN:HG3	2.18	0.44
1:3:595:THR:HA	1:3:596:PRO:C	2.37	0.44
1:1:1011:ALA:HB3	1:1:1014:TYR:CZ	2.53	0.44
1:4:40:GLU:OE2	1:4:43:ARG:NH2	2.51	0.44
1:1:777:LEU:HG	1:1:889:ALA:HA	1.99	0.44
1:2:372:MET:CE	1:2:395:HIS:HB3	2.48	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
1:1:49:GLN:HG2	6:1:4584:HOH:O	2.17	0.44
1:3:125:LEU:HA	5:3:6029:DMS:C2	2.48	0.43
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
1:3:125:LEU:HA	5:3:6029:DMS:H21	2.00	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
1:4:416:GLU:HG3	1:4:460:ASN:O	2.17	0.43
1:1:823:LEU:HD11	1:1:841:ALA:HB2	2.01	0.43
1:1:486:TYR:CE2	1:1:488:GLY:HA3	2.53	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
1:2:800:ARG:HG3	6:2:4921:HOH:O	2.17	0.43
1:4:1011:ALA:HB3	1:4:1014:TYR:CZ	2.54	0.43
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.54	0.43
1:2:13:ARG:HG3	1:3:13:ARG:CZ	2.48	0.43
1:4:673:ALA:HB1	1:4:674:PRO:HD2	2.00	0.43
1:2:770:ILE:HG22	1:2:770:ILE:O	2.19	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
1:1:369: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
1:2:867:THR:HG23	1:2:1015:HIS:CE1	2.54	0.43
1:1:131:GLU:HG3	1:1:135:GLN:CG	2.49	0.43
1:3:239:VAL:HG23	2:3:2002:IPT:H2'1	2.01	0.43
1:4:163:GLN:O	1:4:164:ASP:HB3	2.19	0.43
1:3:577:LYS:O	1:3:584:PRO:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:147:ASN:HA	1:2:148:SER:HA	1.58	0.42
1:3:231:PHE:N	1:3:231:PHE:CD1	2.88	0.42
1:4:651:LEU:CD2	1:4:653:HIS:HE2	2.31	0.42
1:2:19:PRO:HD3	1:2:112:PRO:CB	2.49	0.42
1:1:19:PRO:HD3	1:1:112:PRO:HB3	2.01	0.42
1:4:433:LEU:HB3	1:4:434:PRO:HD3	2.00	0.42
1:2:353:GLY:HA2	1:2:386:ALA:O	2.20	0.42
1:1:748:CYS:C	1:1:749:ILE:HD12	2.39	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
1:4:352:ARG:HG2	1:4:553:TRP:CH2	2.55	0.42
1:4:780:LEU:HA	1:4:886:CYS:HB3	2.01	0.42
1:2:464:HIS:HB2	1:2:489:GLY:HA3	2.02	0.42
1:4:653:HIS:ND1	1:4:699:ARG:NH2	2.68	0.42
1:2:632:SER:HB2	5:2:6022:DMS:H22	2.01	0.42
1:3:475:ILE:HA	1:3:478:VAL:HG22	2.02	0.42
1:4:18:ASN:ND2	1:4:21:VAL:HG23	2.34	0.42
1:4:800:ARG:HH11	1:4:800:ARG:HG2	1.85	0.42
1:1:754:LYS:HE2	1:1:1022:GLN:HE21	1.84	0.42
1:4:759:ASN:OD1	1:4:761:GLN:HB3	2.18	0.42
1:1:784:PHE:HA	1:1:881:ARG:O	2.20	0.41
1:1:373:VAL:O	1:1:377:LEU:HG	2.20	0.41
1:2:358:GLU:HB3	1:2:367:MET:CG	2.50	0.41
1:2:397:LEU:HD11	5:2:6018:DMS:H12	2.01	0.41
1:1:326:GLU:OE1	1:1:326:GLU:HA	2.20	0.41
1:2:231:PHE:N	1:2:231:PHE:CD1	2.88	0.41
1:1:285:TYR:CE1	1:4:422:PRO:HG3	2.54	0.41
1:4:147:ASN:HA	1:4:148:SER:HA	1.63	0.41
1:1:883:GLY:HA3	1:1:987:ASP:HA	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
1:1:66:PRO:HG2	1:1:67:GLU:OE1	2.21	0.41
1:4:708:TRP:CE3	1:4:709:SER:HB3	2.54	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
1:1:788:PRO:HD2	1:1:968:MET:HG3	2.03	0.41
1:1:301:TRP:CH2	1:1:452:SER:HA	2.55	0.41
1:4:622:HIS:O	1:4:625:GLN:HG3	2.20	0.41
1:1:390:SER:HA	1:1:391:HIS:HA	1.83	0.41
1:2:291:LEU:HD22	1:2:291:LEU:N	2.35	0.41
1:3:995:GLY:C	1:3:997:ASP:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:44:THR:OG1	1:2:46:ARG:HG3	2.21	0.41
1:4:373:VAL:O	1:4:377:LEU:HG	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
1:1:581: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
1:4:907:PRO:HG2	1:4:990:HIS:O	2.20	0.41
1:4:301:TRP:CH2	1:4:452:SER:HA	2.56	0.41
1:4:35:SER:HB2	1:4:217:LYS:HG2	2.01	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
1:4:610:ASP:O	1:4:611:ARG:HB2	2.21	0.41
1:3:701:VAL:O	1:3:703:PRO:HD3	2.21	0.41
1:3:79:PRO:HG2	1:3:80:GLU:OE2	2.21	0.41
1:3:784:PHE:HA	1:3:881:ARG:O	2.21	0.41
1:3:608:PHE:CD1	1:3:614:HIS:HD2	2.39	0.41
1:3:225:PHE:HA	1:3:243:GLU:O	2.21	0.40
1:2:473:ARG:HD2	1:2:473:ARG:HA	1.92	0.40
1:4:506:VAL:HG12	1:4:521:LYS:HE3	2.03	0.40
1:2:652:LEU:HD23	1:2:680:ILE:HD12	2.03	0.40
1:2:1020:TRP:HD1	1:2:1021:CYS:N	2.18	0.40
1:2:38:ASN:CG	1:2:41:GLU:HG3	2.42	0.40
1:2:424:ASN:CG	1:3:279:ILE:HD11	2.40	0.40
1:2:995:GLY:C	1:2:997:ASP:N	2.75	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
1:2:356:ARG:HD2	1:2:379:MET:HE3	2.02	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
1:1:99: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
1:4:701:VAL:O	1:4:703:PRO:HD3	2.21	0.40
1:4:730:LEU:CD1	1:4:730:LEU:H	2.34	0.40
1:3:431:ARG:HB2	1:3:431:ARG:NH2	2.36	0.40
1:3:230:ARG:HG3	2:3:2002:IPT:H2'3	2.03	0.40
1:2:598:ASP:HB3	5:2:6032:DMS:H12	2.03	0.40
1:2:355:ASN:OD1	1:2:388:ARG:HD3	2.21	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%)	56 46
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%)	857 (99%)	6 (1%)	88 88
1	2	863/897 (96%)	859 (100%)	4 (0%)	92 92
1	3	863/897 (96%)	856 (99%)	7 (1%)	86 86
1	4	863/897 (96%)	859 (100%)	4 (0%)	92 92
All	All	3452/3588 (96%)	3431 (99%)	21 (1%)	90 90

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	333	ARG
1	1	344	LEU
1	1	519	SER
1	1	546	LEU
1	1	659	ASP
1	1	672	VAL
1	2	333	ARG
1	2	431	ARG
1	2	519	SER
1	2	546	LEU
1	3	279	ILE
1	3	333	ARG
1	3	519	SER
1	3	546	LEU
1	3	687	GLN
1	3	761	GLN
1	3	774	LYS
1	4	333	ARG
1	4	519	SER
1	4	546	LEU
1	4	687	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	163	GLN
1	1	583	ASN
1	1	653	HIS
1	1	775	GLN
1	1	804	ASN
1	1	1022	GLN
1	2	863	GLN
1	2	1022	GLN
1	3	653	HIS
1	4	583	ASN
1	4	704	ASN
1	4	1022	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
2	IPT	1	2001	4	15,15,15	0.79	0	19,21,21	0.66	0
2	IPT	1	2002	-	15,15,15	0.93	1 (6%)	19,21,21	0.70	0
5	DMS	1	6000	-	3,3,3	0.25	0	3,3,3	0.56	0
5	DMS	1	6001	-	3,3,3	0.18	0	3,3,3	0.53	0
5	DMS	1	6002	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	1	6003	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	1	6004	-	3,3,3	0.21	0	3,3,3	0.54	0
5	DMS	1	6005	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	6006	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	1	6007	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	1	6008	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	1	6009	-	3,3,3	0.23	0	3,3,3	0.55	0
5	DMS	1	6010	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	1	6011	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	1	6012	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	1	6013	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	1	6014	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	6015	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	6016	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	6017	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	6018	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	1	6019	-	3,3,3	0.23	0	3,3,3	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	1	6020	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	1	6021	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	1	6022	-	3,3,3	0.24	0	3,3,3	0.61	0
5	DMS	1	6023	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	1	6024	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	1	6025	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	1	6026	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	1	6027	-	3,3,3	0.26	0	3,3,3	0.59	0
5	DMS	1	6028	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	6029	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	1	6030	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	6031	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	1	6032	-	3,3,3	0.20	0	3,3,3	0.57	0
2	IPT	2	2001	4	15,15,15	0.85	1 (6%)	19,21,21	0.68	0
2	IPT	2	2002	-	15,15,15	0.83	1 (6%)	19,21,21	0.68	0
5	DMS	2	6000	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	2	6001	-	3,3,3	0.17	0	3,3,3	0.54	0
5	DMS	2	6002	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	2	6003	-	3,3,3	0.24	0	3,3,3	0.63	0
5	DMS	2	6004	-	3,3,3	0.23	0	3,3,3	0.53	0
5	DMS	2	6005	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6006	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	2	6007	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	2	6008	-	3,3,3	0.21	0	3,3,3	0.53	0
5	DMS	2	6009	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	6010	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	2	6011	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	6012	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6013	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	2	6014	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6015	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	2	6016	4	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6017	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	6018	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6019	-	3,3,3	0.19	0	3,3,3	0.57	0
5	DMS	2	6020	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	2	6021	-	3,3,3	0.20	0	3,3,3	0.55	0
5	DMS	2	6022	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	2	6023	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	2	6024	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	2	6025	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	6026	-	3,3,3	0.32	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	6027	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	2	6028	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	2	6029	-	3,3,3	0.21	0	3,3,3	0.56	0
5	DMS	2	6030	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	2	6031	-	3,3,3	0.20	0	3,3,3	0.59	0
5	DMS	2	6032	-	3,3,3	0.23	0	3,3,3	0.55	0
5	DMS	2	6033	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	6034	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	2	6035	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	6036	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6037	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	6038	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	6039	-	3,3,3	0.20	0	3,3,3	0.62	0
5	DMS	2	6040	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	6042	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	6043	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	3	1024	-	3,3,3	0.13	0	3,3,3	0.59	0
2	IPT	3	2001	4	15,15,15	0.84	1 (6%)	19,21,21	0.67	0
2	IPT	3	2002	-	15,15,15	0.86	1 (6%)	19,21,21	0.68	0
5	DMS	3	6000	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	3	6001	-	3,3,3	0.18	0	3,3,3	0.55	0
5	DMS	3	6002	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6003	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	3	6004	-	3,3,3	0.23	0	3,3,3	0.54	0
5	DMS	3	6005	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	6006	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	3	6007	-	3,3,3	0.27	0	3,3,3	0.58	0
5	DMS	3	6008	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	3	6009	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	6010	-	3,3,3	0.25	0	3,3,3	0.57	0
5	DMS	3	6011	-	3,3,3	0.21	0	3,3,3	0.56	0
5	DMS	3	6012	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	3	6013	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6014	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	6015	-	3,3,3	0.20	0	3,3,3	0.55	0
5	DMS	3	6016	4	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	3	6017	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	3	6018	-	3,3,3	0.19	0	3,3,3	0.56	0
5	DMS	3	6019	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	6020	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	3	6021	-	3,3,3	0.25	0	3,3,3	0.60	0
5	DMS	3	6022	-	3,3,3	0.20	0	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	3	6023	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	3	6024	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	6025	-	3,3,3	0.25	0	3,3,3	0.57	0
5	DMS	3	6026	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6027	-	3,3,3	0.18	0	3,3,3	0.60	0
5	DMS	3	6028	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6029	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	3	6030	-	3,3,3	0.26	0	3,3,3	0.56	0
5	DMS	3	6031	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6032	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	6033	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	6034	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	6035	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6036	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	3	6037	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	3	6038	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	3	6039	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	6040	-	3,3,3	0.20	0	3,3,3	0.61	0
5	DMS	3	6041	-	3,3,3	0.22	0	3,3,3	0.60	0
2	IPT	4	2001	4	15,15,15	0.83	1 (6%)	19,21,21	0.69	0
2	IPT	4	2002	-	15,15,15	0.86	1 (6%)	19,21,21	0.68	0
5	DMS	4	6000	-	3,3,3	0.21	0	3,3,3	0.56	0
5	DMS	4	6001	-	3,3,3	0.15	0	3,3,3	0.55	0
5	DMS	4	6002	-	3,3,3	0.27	0	3,3,3	0.57	0
5	DMS	4	6003	-	3,3,3	0.20	0	3,3,3	0.56	0
5	DMS	4	6004	-	3,3,3	0.22	0	3,3,3	0.55	0
5	DMS	4	6005	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	4	6006	-	3,3,3	0.21	0	3,3,3	0.56	0
5	DMS	4	6007	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	4	6008	-	3,3,3	0.27	0	3,3,3	0.57	0
5	DMS	4	6009	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	4	6010	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	4	6011	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	4	6012	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	4	6013	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	4	6014	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	4	6015	-	3,3,3	0.21	0	3,3,3	0.56	0
5	DMS	4	6016	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	4	6017	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	4	6018	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	4	6019	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	4	6020	-	3,3,3	0.21	0	3,3,3	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	4	6021	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	4	6022	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	4	6023	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	4	6024	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	4	6025	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	4	6026	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	4	6027	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	4	6028	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	4	6029	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	4	6030	-	3,3,3	0.22	0	3,3,3	0.58	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	1	2001	4	-	0/6/26/26	0/1/1/1
2	IPT	1	2002	-	-	0/6/26/26	0/1/1/1
5	DMS	1	6000	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6001	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6002	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6003	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6004	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6005	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6006	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6007	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6008	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6009	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6010	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6011	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6012	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6013	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6014	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6015	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6016	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6017	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6018	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6019	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6020	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6021	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6022	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6023	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	1	6024	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6025	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6026	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6027	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6028	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6029	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6030	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6031	-	-	0/0/0/0	0/0/0/0
5	DMS	1	6032	-	-	0/0/0/0	0/0/0/0
2	IPT	2	2001	4	-	0/6/26/26	0/1/1/1
2	IPT	2	2002	-	-	0/6/26/26	0/1/1/1
5	DMS	2	6000	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6001	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6002	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6003	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6004	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6005	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6006	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6007	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6008	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6009	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6010	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6011	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6012	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6013	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6014	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6015	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6016	4	-	0/0/0/0	0/0/0/0
5	DMS	2	6017	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6018	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6019	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6020	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6021	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6022	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6023	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6024	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6025	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6026	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6027	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6028	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6029	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6030	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	2	6031	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6032	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6033	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6034	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6035	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6036	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6037	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6038	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6039	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6040	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6042	-	-	0/0/0/0	0/0/0/0
5	DMS	2	6043	-	-	0/0/0/0	0/0/0/0
5	DMS	3	1024	-	-	0/0/0/0	0/0/0/0
2	IPT	3	2001	4	-	0/6/26/26	0/1/1/1
2	IPT	3	2002	-	-	0/6/26/26	0/1/1/1
5	DMS	3	6000	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6001	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6002	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6003	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6004	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6005	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6006	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6007	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6008	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6009	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6010	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6011	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6012	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6013	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6014	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6015	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6016	4	-	0/0/0/0	0/0/0/0
5	DMS	3	6017	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6018	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6019	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6020	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6021	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6022	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6023	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6024	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6025	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6026	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	3	6027	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6028	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6029	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6030	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6031	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6032	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6033	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6034	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6035	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6036	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6037	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6038	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6039	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6040	-	-	0/0/0/0	0/0/0/0
5	DMS	3	6041	-	-	0/0/0/0	0/0/0/0
2	IPT	4	2001	4	-	0/6/26/26	0/1/1/1
2	IPT	4	2002	-	-	0/6/26/26	0/1/1/1
5	DMS	4	6000	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6001	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6002	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6003	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6004	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6005	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6006	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6007	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6008	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6009	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6010	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6011	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6012	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6013	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6014	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6015	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6016	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6017	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6018	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6019	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6020	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6021	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6022	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6023	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6024	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	4	6025	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6026	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6027	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6028	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6029	-	-	0/0/0/0	0/0/0/0
5	DMS	4	6030	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	2001	IPT	O5-C1	2.08	1.46	1.42
2	2	2002	IPT	O5-C1	2.15	1.46	1.42
2	4	2002	IPT	O5-C1	2.16	1.46	1.42
2	4	2001	IPT	O5-C1	2.20	1.46	1.42
2	3	2002	IPT	O5-C1	2.33	1.46	1.42
2	2	2001	IPT	O5-C1	2.43	1.46	1.42
2	1	2002	IPT	O5-C1	2.46	1.46	1.42

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	2001	IPT	1	0
2	2	2002	IPT	1	0
5	2	6010	DMS	1	0
5	2	6018	DMS	1	0
5	2	6022	DMS	1	0
5	2	6026	DMS	2	0
5	2	6032	DMS	1	0
2	3	2002	IPT	2	0
5	3	6029	DMS	3	0
2	4	2001	IPT	1	0
5	4	6001	DMS	1	0
5	4	6002	DMS	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.00	38 (3%) 44 48	10, 20, 40, 66	0
1	2	1011/1052 (96%)	-0.17	26 (2%) 59 63	8, 16, 36, 68	0
1	3	1011/1052 (96%)	-0.19	32 (3%) 51 54	9, 16, 33, 67	0
1	4	1011/1052 (96%)	0.01	42 (4%) 40 44	10, 21, 39, 70	0
All	All	4044/4208 (96%)	-0.09	138 (3%) 49 52	8, 19, 37, 70	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	2	731	PRO	10.2
1	2	732	ALA	9.7
1	1	735	HIS	8.7
1	4	735	HIS	8.7
1	2	730	LEU	7.0
1	3	689	GLU	6.8
1	4	687	GLN	6.6
1	2	689	GLU	6.5
1	3	1023	LYS	6.3
1	1	800	ARG	6.2
1	4	689	GLU	6.1
1	3	731	PRO	6.1
1	1	731	PRO	6.0
1	2	686	PRO	5.9
1	4	730	LEU	5.8
1	3	800	ARG	5.8
1	1	687	GLN	5.7
1	2	733	ALA	5.7
1	2	800	ARG	5.7
1	2	1023	LYS	5.6
1	1	689	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	1	798	ALA	5.4
1	3	799	THR	5.3
1	3	798	ALA	5.3
1	4	580	GLU	5.2
1	4	798	ALA	5.2
1	4	800	ARG	5.1
1	1	730	LEU	5.0
1	1	1023	LYS	5.0
1	1	684	GLU	5.0
1	3	684	GLU	4.9
1	1	733	ALA	4.8
1	1	685	LEU	4.8
1	3	733	ALA	4.8
1	3	687	GLN	4.6
1	3	732	ALA	4.6
1	3	735	HIS	4.5
1	4	797	GLU	4.5
1	4	732	ALA	4.4
1	2	687	GLN	4.3
1	1	686	PRO	4.3
1	1	799	THR	4.2
1	2	735	HIS	4.2
1	4	799	THR	4.2
1	2	685	LEU	4.1
1	3	730	LEU	4.1
1	2	684	GLU	3.9
1	4	581	ASN	3.9
1	4	684	GLU	3.8
1	3	686	PRO	3.6
1	2	799	THR	3.6
1	2	1022	GLN	3.6
1	4	731	PRO	3.5
1	1	580	GLU	3.5
1	4	733	ALA	3.4
1	3	690	SER	3.4
1	2	772	ASP	3.3
1	4	1022	GLN	3.3
1	4	772	ASP	3.3
1	1	76	CYS	3.2
1	3	580	GLU	3.2
1	1	71	GLU	3.1
1	1	80	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	2	798	ALA	3.1
1	4	685	LEU	3.1
1	2	734	SER	3.1
1	1	732	ALA	3.0
1	1	75	GLU	3.0
1	3	772	ASP	3.0
1	4	819	GLU	3.0
1	4	686	PRO	3.0
1	3	1022	GLN	2.9
1	1	801	ILE	2.9
1	1	135	GLN	2.8
1	4	1023	LYS	2.8
1	2	773	LYS	2.8
1	1	130	ASP	2.8
1	4	76	CYS	2.8
1	1	831	ALA	2.8
1	4	71	GLU	2.8
1	4	688	PRO	2.8
1	1	178	ARG	2.7
1	4	734	SER	2.7
1	4	761	GLN	2.7
1	1	819	GLU	2.7
1	2	819	GLU	2.7
1	3	681	GLU	2.6
1	1	832	ASP	2.6
1	3	846	GLY	2.6
1	2	690	SER	2.6
1	4	128	ASN	2.5
1	1	49	GLN	2.5
1	4	131	GLU	2.5
1	4	690	SER	2.5
1	4	362	LEU	2.5
1	4	582	GLY	2.5
1	1	362	LEU	2.4
1	1	581	ASN	2.4
1	2	755	ARG	2.3
1	4	130	ASP	2.3
1	1	181	GLU	2.3
1	3	264	GLU	2.3
1	3	819	GLU	2.3
1	3	688	PRO	2.3
1	1	179	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	3	685	LEU	2.3
1	1	319	ASP	2.3
1	4	746	ASP	2.3
1	1	845	GLN	2.3
1	2	774	LYS	2.2
1	4	135	GLN	2.2
1	4	655	MET	2.2
1	4	831	ALA	2.2
1	3	655	MET	2.2
1	3	370	GLN	2.2
1	3	817	GLN	2.2
1	1	431	ARG	2.2
1	4	773	LYS	2.2
1	2	663	LEU	2.1
1	1	681	GLU	2.1
1	3	729	THR	2.1
1	4	129	VAL	2.1
1	4	117	GLU	2.1
1	4	431	ARG	2.1
1	4	770	ILE	2.1
1	3	769	TRP	2.1
1	3	651	LEU	2.1
1	3	761	GLN	2.1
1	1	136	GLU	2.1
1	1	797	GLU	2.1
1	2	681	GLU	2.0
1	3	977	HIS	2.0
1	1	817	GLN	2.0
1	4	370	GLN	2.0
1	4	893	GLU	2.0
1	2	655	MET	2.0
1	3	744	GLU	2.0
1	2	761	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	1	6006	4/4	0.83	0.22	19.05	61,61,61,62	0
5	DMS	3	6031	4/4	0.75	0.29	18.51	84,84,84,85	0
5	DMS	2	6012	4/4	0.64	0.39	18.50	77,78,79,79	0
5	DMS	3	6015	4/4	0.78	0.26	18.27	70,71,71,71	0
5	DMS	3	6040	4/4	0.35	0.37	16.39	51,53,55,56	0
5	DMS	3	6005	4/4	0.80	0.20	13.27	53,53,53,54	0
5	DMS	1	6024	4/4	0.73	0.28	13.23	80,81,81,81	0
5	DMS	3	6038	4/4	0.76	0.18	11.81	68,68,69,70	0
5	DMS	2	6039	4/4	0.83	0.28	11.64	47,48,48,48	0
5	DMS	2	6040	4/4	0.41	0.38	11.30	92,92,93,93	0
5	DMS	1	6011	4/4	0.78	0.23	10.99	84,84,84,84	0
5	DMS	2	6015	4/4	0.66	0.27	10.30	85,85,85,85	0
5	DMS	1	6019	4/4	0.11	0.62	10.23	99,99,100,100	0
5	DMS	4	6026	4/4	0.88	0.21	9.96	67,68,68,68	0
5	DMS	4	6002	4/4	0.87	0.22	9.41	43,45,45,46	0
5	DMS	1	6027	4/4	0.85	0.24	9.33	49,49,49,51	0
5	DMS	1	6032	4/4	0.61	0.36	9.14	75,76,76,76	0
5	DMS	3	6029	4/4	0.89	0.22	8.96	55,55,56,57	0
5	DMS	4	6003	4/4	0.96	0.18	8.94	34,35,36,37	0
5	DMS	1	6018	4/4	0.90	0.15	8.91	64,64,65,65	0
5	DMS	2	6031	4/4	0.66	0.25	8.83	75,76,76,77	0
5	DMS	2	6016	4/4	0.67	0.35	8.39	91,92,92,92	0
5	DMS	2	6001	4/4	0.93	0.20	8.02	27,29,29,30	0
5	DMS	2	6018	4/4	0.87	0.22	7.37	65,65,66,66	0
2	IPT	2	2002	15/15	0.80	0.26	7.21	32,37,39,39	0
5	DMS	4	6017	4/4	0.58	0.33	7.01	75,76,76,76	0
5	DMS	2	6024	4/4	0.94	0.12	6.32	31,32,33,35	0
5	DMS	2	6002	4/4	0.96	0.12	6.21	31,32,32,34	0
5	DMS	3	6019	4/4	0.85	0.21	6.08	77,77,77,77	0
5	DMS	2	6038	4/4	0.74	0.21	6.06	55,55,55,57	0
2	IPT	3	2002	15/15	0.82	0.24	5.91	32,36,38,39	0
5	DMS	3	6018	4/4	0.83	0.25	5.88	59,59,60,61	0
5	DMS	1	6002	4/4	0.94	0.15	5.82	39,40,40,41	0
5	DMS	3	6001	4/4	0.90	0.19	5.60	29,31,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	1	6001	4/4	0.94	0.17	5.57	28,31,31,31	0
5	DMS	3	6023	4/4	0.90	0.18	5.44	51,52,52,53	0
5	DMS	4	6001	4/4	0.92	0.19	5.18	35,36,36,37	0
5	DMS	2	6022	4/4	0.64	0.32	5.17	81,81,82,82	0
5	DMS	1	6030	4/4	0.88	0.20	5.06	66,66,66,67	0
5	DMS	1	6013	4/4	0.89	0.19	5.06	55,55,56,56	0
5	DMS	2	6005	4/4	0.92	0.22	4.94	50,51,51,51	0
5	DMS	4	6027	4/4	0.76	0.24	4.38	60,60,60,61	0
5	DMS	1	6003	4/4	0.90	0.15	4.24	55,56,57,57	0
5	DMS	2	6003	4/4	0.95	0.12	4.24	26,26,27,30	0
5	DMS	2	6028	4/4	0.75	0.26	4.05	44,45,46,49	0
5	DMS	3	6003	4/4	0.95	0.13	4.01	37,37,38,39	0
2	IPT	4	2001	15/15	0.86	0.17	3.96	20,25,32,34	0
5	DMS	4	6014	4/4	0.83	0.21	3.93	91,91,91,91	0
5	DMS	2	6035	4/4	0.60	0.30	3.92	75,75,76,76	0
5	DMS	3	6020	4/4	0.77	0.32	3.84	64,65,65,65	0
5	DMS	4	6015	4/4	0.90	0.15	3.82	63,63,63,64	0
5	DMS	4	6000	4/4	0.97	0.11	3.78	23,25,25,27	0
5	DMS	2	6004	4/4	0.98	0.14	3.73	27,28,29,29	0
5	DMS	4	6021	4/4	0.69	0.31	3.59	82,82,82,82	0
5	DMS	3	6017	4/4	0.86	0.18	3.58	57,57,57,58	0
5	DMS	2	6023	4/4	0.90	0.16	3.54	72,72,72,73	0
5	DMS	2	6000	4/4	0.96	0.11	3.46	16,21,23,23	0
2	IPT	1	2002	15/15	0.74	0.21	3.36	27,31,34,35	15
5	DMS	2	6025	4/4	0.82	0.24	3.22	66,67,67,67	0
5	DMS	3	6026	4/4	0.42	0.32	3.17	97,97,98,98	0
5	DMS	4	6018	4/4	0.76	0.33	3.15	80,81,81,81	0
2	IPT	1	2001	15/15	0.87	0.15	2.99	17,21,28,30	0
5	DMS	4	6022	4/4	0.82	0.29	2.88	54,55,55,56	0
5	DMS	3	6004	4/4	0.98	0.14	2.84	25,25,26,26	0
5	DMS	4	6012	4/4	0.88	0.16	2.79	79,79,79,80	0
5	DMS	1	6023	4/4	0.84	0.25	2.72	59,60,61,61	0
5	DMS	3	6013	4/4	0.93	0.13	2.68	54,54,55,55	0
5	DMS	1	6020	4/4	0.87	0.22	2.67	63,63,63,63	0
5	DMS	4	6028	4/4	0.80	0.34	2.66	89,89,90,90	0
5	DMS	3	6028	4/4	0.95	0.13	2.66	42,42,42,43	0
5	DMS	2	6013	4/4	0.97	0.12	2.61	43,43,44,44	0
5	DMS	3	6025	4/4	0.80	0.21	2.52	60,60,61,61	0
5	DMS	1	6031	4/4	0.79	0.24	2.02	73,74,74,74	0
2	IPT	4	2002	15/15	0.82	0.17	1.91	27,30,32,32	0
5	DMS	1	6022	4/4	0.90	0.19	1.84	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	3	6016	4/4	0.91	0.18	1.83	65,65,65,65	0
2	IPT	3	2001	15/15	0.93	0.12	1.81	12,18,23,26	0
5	DMS	1	6005	4/4	0.94	0.13	1.67	52,53,53,53	0
5	DMS	1	6017	4/4	0.85	0.20	1.45	38,41,42,46	0
5	DMS	4	6009	4/4	0.91	0.19	1.41	45,46,46,47	0
5	DMS	3	6021	4/4	0.94	0.14	1.38	44,45,45,46	0
5	DMS	1	6009	4/4	0.91	0.20	1.30	57,57,57,58	0
5	DMS	3	6030	4/4	0.88	0.20	1.28	51,51,52,52	0
5	DMS	3	6000	4/4	0.98	0.09	1.24	14,19,19,21	0
5	DMS	2	6009	4/4	0.96	0.15	1.20	34,35,36,37	0
5	DMS	4	6007	4/4	0.85	0.21	1.19	74,74,74,74	0
2	IPT	2	2001	15/15	0.94	0.11	1.13	10,16,21,21	0
4	NA	3	3104	1/1	0.95	0.16	0.96	28,28,28,28	0
5	DMS	4	6019	4/4	0.86	0.18	0.93	63,64,64,64	0
5	DMS	4	6023	4/4	0.97	0.14	0.92	41,41,42,42	0
5	DMS	3	6009	4/4	0.96	0.14	0.89	38,38,39,39	0
5	DMS	4	6005	4/4	0.91	0.18	0.74	50,50,51,52	0
4	NA	2	3101	1/1	0.99	0.09	0.61	15,15,15,15	0
5	DMS	3	6024	4/4	0.94	0.14	0.56	60,60,60,60	0
5	DMS	1	6021	4/4	0.93	0.13	0.50	59,59,59,60	0
5	DMS	3	6002	4/4	0.98	0.09	0.49	30,31,32,32	0
5	DMS	2	6027	4/4	0.97	0.11	0.47	44,44,44,45	0
5	DMS	1	6004	4/4	0.99	0.10	0.42	26,27,28,29	0
3	MG	2	3002	1/1	1.00	0.09	0.35	15,15,15,15	0
5	DMS	2	6021	4/4	0.95	0.12	0.29	39,40,40,40	0
3	MG	4	3001	1/1	0.96	0.08	0.25	17,17,17,17	0
5	DMS	2	6017	4/4	0.96	0.11	0.09	61,61,62,62	0
3	MG	1	3004	1/1	0.94	0.11	-0.02	43,43,43,43	0
4	NA	2	3103	1/1	0.95	0.11	-0.05	36,36,36,36	0
4	NA	3	3103	1/1	0.94	0.11	-0.06	34,34,34,34	0
5	DMS	2	6008	4/4	0.98	0.10	-0.18	24,25,27,27	0
5	DMS	1	6015	4/4	0.94	0.13	-0.19	70,70,70,70	0
4	NA	4	3102	1/1	0.97	0.08	-0.36	16,16,16,16	0
4	NA	2	3104	1/1	0.94	0.10	-0.53	31,31,31,31	0
3	MG	4	3002	1/1	0.99	0.09	-0.56	23,23,23,23	0
5	DMS	1	6000	4/4	0.98	0.08	-0.74	18,23,23,25	0
5	DMS	4	6004	4/4	0.99	0.08	-0.88	28,29,30,30	0
4	NA	1	3104	1/1	0.95	0.08	-1.01	32,32,32,32	0
4	NA	4	3103	1/1	0.92	0.09	-1.23	37,37,37,37	0
4	NA	4	3104	1/1	0.90	0.09	-1.32	35,35,35,35	0
4	NA	4	3101	1/1	0.98	0.06	-1.35	19,19,19,19	0
3	MG	1	3002	1/1	0.94	0.08	-1.44	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NA	1	3103	1/1	0.95	0.07	-1.54	29,29,29,29	0
4	NA	3	3101	1/1	0.98	0.05	-1.74	13,13,13,13	0
4	NA	1	3101	1/1	0.98	0.05	-1.94	18,18,18,18	0
3	MG	2	3001	1/1	0.98	0.05	-2.50	13,13,13,13	0
4	NA	1	3102	1/1	0.98	0.05	-2.87	12,12,12,12	0
3	MG	1	3001	1/1	0.98	0.05	-3.55	16,16,16,16	0
4	NA	2	3102	1/1	0.99	0.05	-3.81	13,13,13,13	0
3	MG	3	3001	1/1	0.99	0.03	-3.95	13,13,13,13	0
5	DMS	3	6008	4/4	0.99	0.07	-4.13	20,22,22,22	0
3	MG	3	3002	1/1	1.00	0.02	-4.41	16,16,16,16	0
4	NA	3	3102	1/1	1.00	0.02	-4.84	14,14,14,14	0
3	MG	1	3003	1/1	0.81	0.26	-	59,59,59,59	0
5	DMS	1	6028	4/4	0.74	0.22	-	70,71,71,71	0
5	DMS	1	6016	4/4	0.95	0.18	-	66,66,66,66	0
5	DMS	3	6011	4/4	0.91	0.17	-	39,41,41,43	0
5	DMS	2	6029	4/4	0.57	0.45	-	80,81,81,82	0
3	MG	2	3004	1/1	0.97	0.09	-	34,34,34,34	0
3	MG	2	3003	1/1	0.89	0.16	-	52,52,52,52	0
5	DMS	4	6029	4/4	0.77	0.21	-	73,73,74,75	0
5	DMS	2	6010	4/4	0.91	0.24	-	40,40,42,43	0
5	DMS	4	6030	4/4	0.80	0.28	-	81,82,82,82	0
5	DMS	3	6014	4/4	0.79	0.21	-	60,60,60,61	0
5	DMS	1	6007	4/4	0.87	0.22	-	51,51,51,51	0
5	DMS	3	6041	4/4	0.67	0.26	-	77,78,78,79	0
5	DMS	4	6013	4/4	0.84	0.20	-	66,66,66,67	0
5	DMS	1	6029	4/4	0.80	0.19	-	67,68,69,69	0
5	DMS	2	6030	4/4	0.87	0.17	-	64,64,65,65	0
5	DMS	1	6008	4/4	0.97	0.10	-	36,36,37,37	0
5	DMS	4	6008	4/4	0.96	0.14	-	36,37,38,39	0
5	DMS	2	6032	4/4	0.90	0.17	-	42,46,47,48	0
5	DMS	1	6010	4/4	0.86	0.18	-	58,58,58,59	0
5	DMS	1	6026	4/4	0.86	0.17	-	76,76,76,77	0
5	DMS	2	6007	4/4	0.91	0.17	-	43,44,45,46	0
5	DMS	4	6024	4/4	0.76	0.26	-	67,68,68,68	0
5	DMS	2	6043	4/4	0.89	0.22	-	56,56,57,57	0
5	DMS	3	6037	4/4	0.76	0.22	-	74,75,75,75	0
5	DMS	2	6019	4/4	0.89	0.14	-	63,63,64,64	0
5	DMS	2	6034	4/4	0.75	0.25	-	67,68,69,69	0
5	DMS	3	6036	4/4	0.58	0.35	-	97,97,98,98	0
5	DMS	4	6020	4/4	0.93	0.15	-	36,38,39,41	0
3	MG	3	3003	1/1	0.72	0.22	-	74,74,74,74	0
5	DMS	3	6035	4/4	0.48	0.36	-	88,88,88,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	2	6036	4/4	0.89	0.22	-	52,52,53,54	0
5	DMS	4	6016	4/4	0.62	0.43	-	93,94,94,94	0
5	DMS	2	6014	4/4	0.96	0.11	-	55,56,56,56	0
5	DMS	3	6010	4/4	0.95	0.17	-	33,35,36,37	0
5	DMS	3	6032	4/4	0.50	0.43	-	85,86,86,86	0
5	DMS	2	6020	4/4	0.90	0.13	-	60,60,60,61	0
5	DMS	3	6022	4/4	0.81	0.22	-	74,75,75,75	0
5	DMS	4	6025	4/4	0.82	0.22	-	68,69,69,69	0
5	DMS	3	6034	4/4	0.85	0.18	-	57,57,58,59	0
5	DMS	4	6006	4/4	0.93	0.15	-	45,46,46,46	0
5	DMS	3	1024	4/4	0.94	0.13	-	58,58,58,60	0
5	DMS	3	6027	4/4	0.89	0.15	-	41,41,42,44	0
5	DMS	2	6011	4/4	0.93	0.18	-	59,59,60,60	0
5	DMS	1	6014	4/4	0.63	0.36	-	94,94,94,94	0
3	MG	4	3003	1/1	0.82	0.20	-	65,65,65,65	0
5	DMS	1	6012	4/4	0.88	0.26	-	69,69,70,70	0
5	DMS	3	6033	4/4	0.87	0.24	-	66,67,67,67	0
5	DMS	3	6007	4/4	0.89	0.13	-	49,50,50,51	0
5	DMS	1	6025	4/4	0.66	0.32	-	82,83,83,83	0
5	DMS	3	6012	4/4	0.88	0.18	-	57,57,57,57	0
5	DMS	2	6042	4/4	0.47	0.40	-	95,96,96,96	0
5	DMS	4	6010	4/4	0.96	0.19	-	55,55,55,55	0
5	DMS	3	6006	4/4	0.93	0.12	-	46,47,47,47	0
5	DMS	2	6037	4/4	0.85	0.20	-	74,74,75,75	0
5	DMS	3	6039	4/4	0.85	0.20	-	59,59,60,61	0
5	DMS	4	6011	4/4	0.84	0.23	-	56,57,57,58	0
5	DMS	2	6026	4/4	0.72	0.27	-	40,42,45,45	0
5	DMS	2	6006	4/4	0.89	0.17	-	43,44,44,45	0
5	DMS	2	6033	4/4	0.79	0.29	-	92,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.