Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:43 AM GMT

PDB ID	:	3MV0
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE (R599A) IN COMPLEX WITH D -GALCTOPYRANOSYL-1-ONE
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

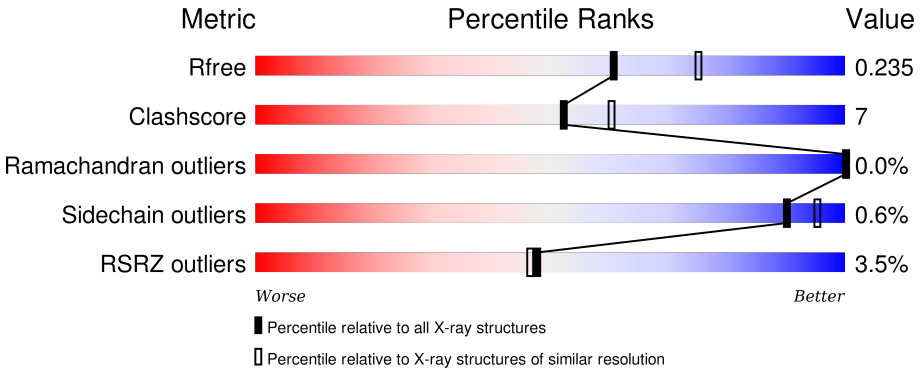
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 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% 80% 16% ·
1	2	1052	3% 82% 14% ·
1	3	1052	3% 81% 15% ·
1	4	1052	4% 79% 17% ·

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	1	5001	-	-	-	X
5	DMS	1	5006	-	-	-	X
5	DMS	1	5007	-	-	-	X
5	DMS	1	5015	-	-	-	X
5	DMS	1	5016	-	-	-	X
5	DMS	1	5029	-	-	X	X
5	DMS	2	1024	-	-	-	X
5	DMS	2	5004	-	-	-	X
5	DMS	2	5006	-	-	-	X
5	DMS	2	5020	-	-	-	X
5	DMS	2	5021	-	-	-	X
5	DMS	2	5023	-	-	-	X
5	DMS	2	5025	-	-	-	X
5	DMS	2	5026	-	-	-	X
5	DMS	2	5033	-	-	-	X
5	DMS	3	1024	-	-	-	X
5	DMS	3	5003	-	-	-	X
5	DMS	3	5004	-	-	-	X
5	DMS	3	5006	-	-	-	X
5	DMS	3	5010	-	-	-	X
5	DMS	3	5016	-	-	-	X
5	DMS	3	5017	-	-	-	X
5	DMS	3	5018	-	-	-	X
5	DMS	3	5020	-	-	-	X
5	DMS	3	5021	-	-	-	X
5	DMS	3	5024	-	-	-	X
5	DMS	3	5028	-	-	-	X
5	DMS	3	5030	-	-	-	X
5	DMS	3	5033	-	-	-	X
5	DMS	3	5034	-	-	-	X
5	DMS	4	5003	-	-	-	X
5	DMS	4	5007	-	-	-	X
5	DMS	4	5020	-	-	-	X
5	DMS	4	5024	-	-	-	X
5	DMS	4	5026	-	-	-	X
5	DMS	4	5028	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 36190 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

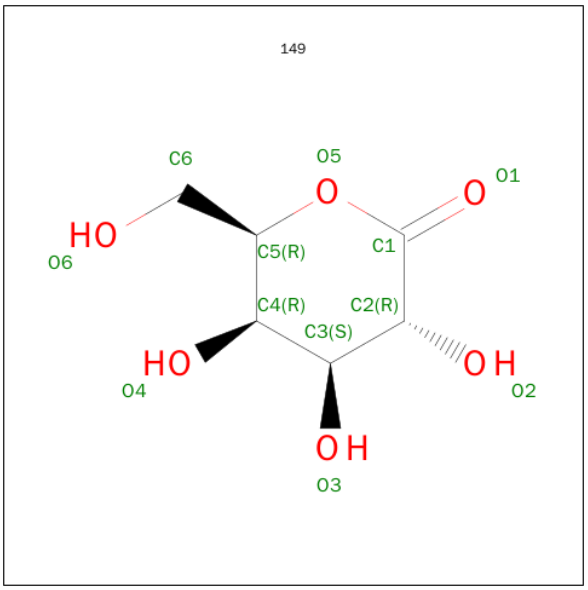
Chain	Residue	Modelled	Actual	Comment	Reference
3	1	ASP	-	EXPRESSION TAG	UNP B8LFD6
3	2	LYS	-	EXPRESSION TAG	UNP B8LFD6
3	3	ASP	-	EXPRESSION TAG	UNP B8LFD6
3	4	PRO	-	EXPRESSION TAG	UNP B8LFD6
3	5	MET	-	EXPRESSION TAG	UNP B8LFD6
3	6	ILE	-	EXPRESSION TAG	UNP B8LFD6
3	7	ASP	-	EXPRESSION TAG	UNP B8LFD6
3	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

Continued on next page...

Continued from previous page...

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 SUGAR (D-GALACTONOLACTONE) (three-letter code: 149) (formula: $C_6H_{10}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	1	1	Total C O 12 6 6	0	0
2	2	1	Total C O 12 6 6	0	0
2	3	1	Total C O 12 6 6	0	0
2	4	1	Total C O 12 6 6	0	0

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

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

Continued on next page...

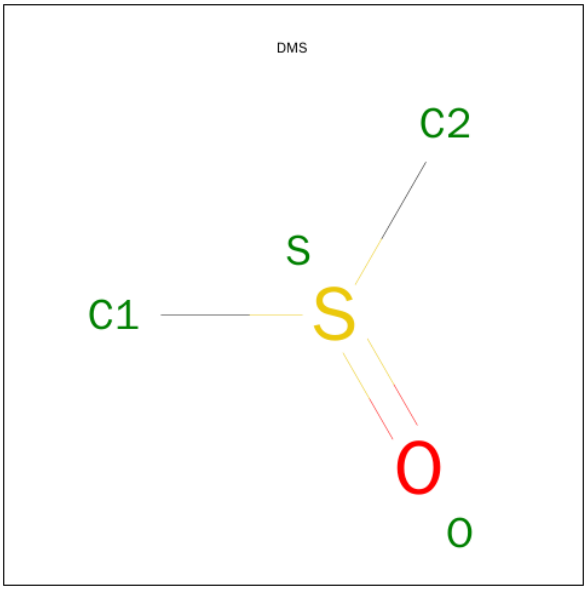
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
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
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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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	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	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

Continued on next page...

Continued from previous page...

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	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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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	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
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

Continued on next page...

Continued from previous page...

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
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
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

- Molecule 6 is water.

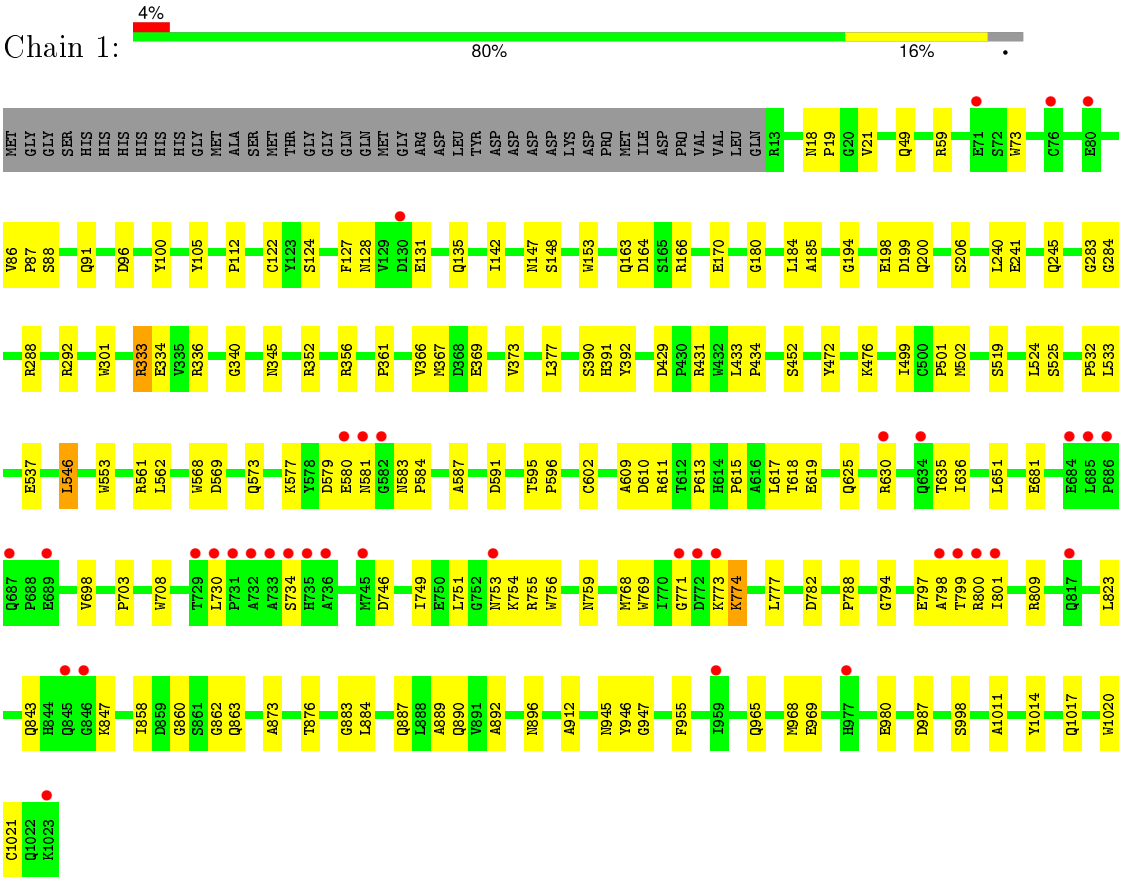
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	1	773	Total O 773 773	0	0
6	2	858	Total O 858 858	0	0
6	3	760	Total O 760 760	0	0
6	4	760	Total O 760 760	0	0

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.

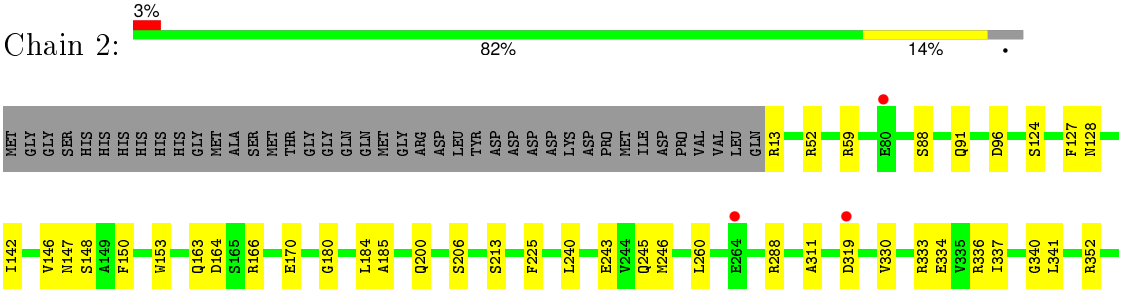
- Molecule 1: Beta-galactosidase

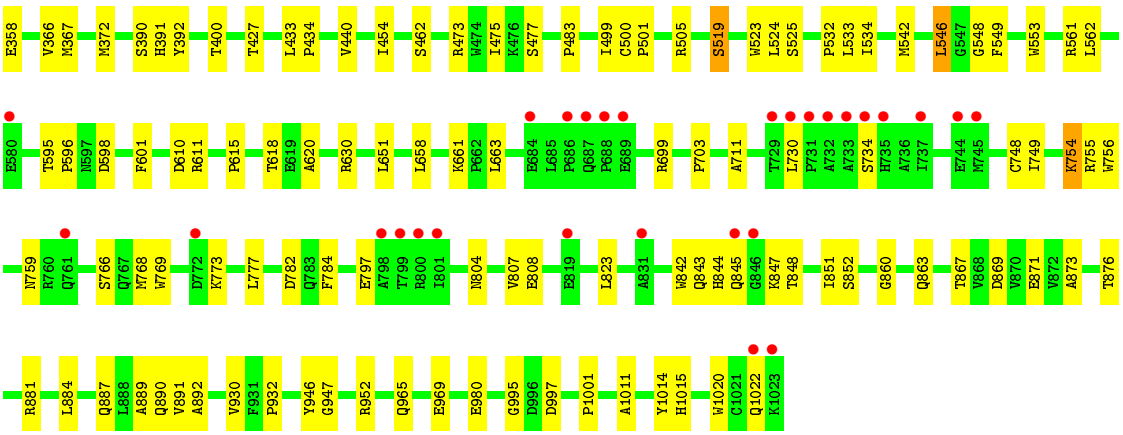
Chain 1:



- Molecule 1: Beta-galactosidase

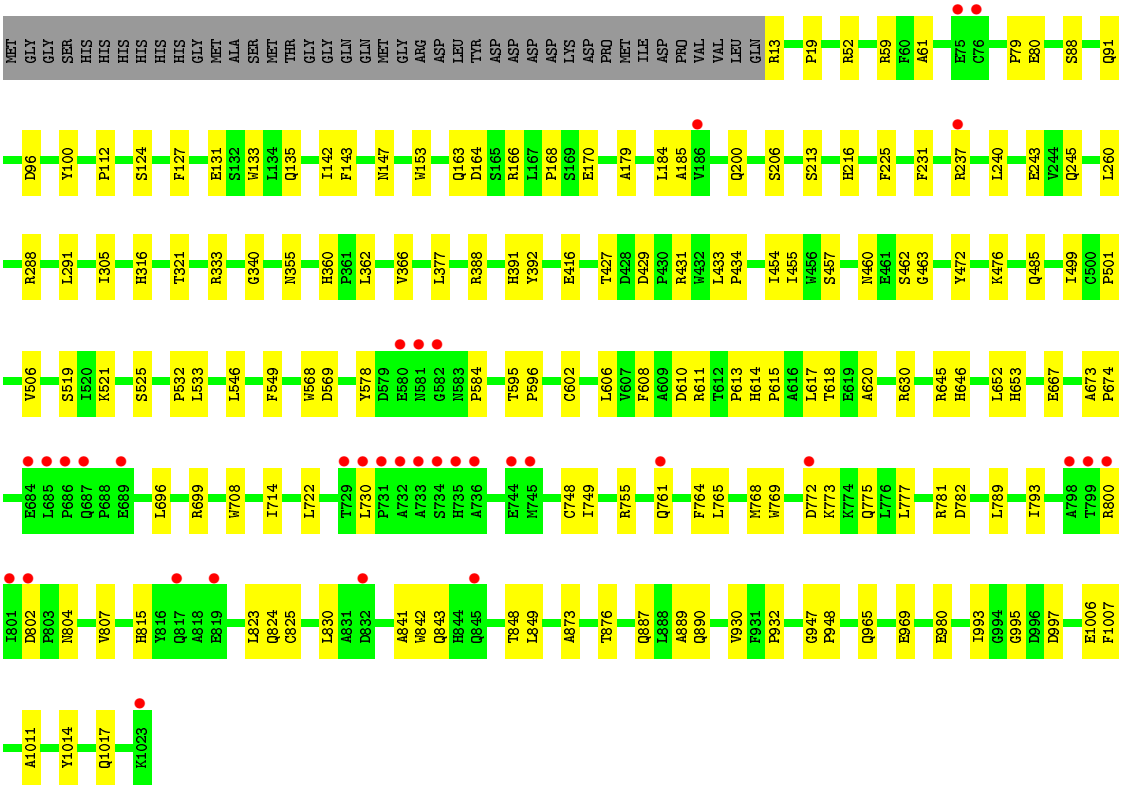
Chain 2:





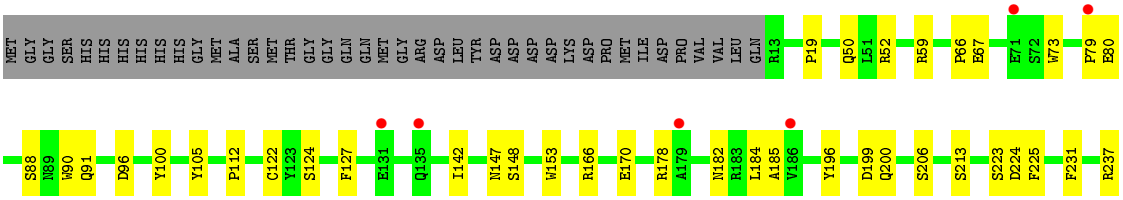
• Molecule 1: Beta-galactosidase

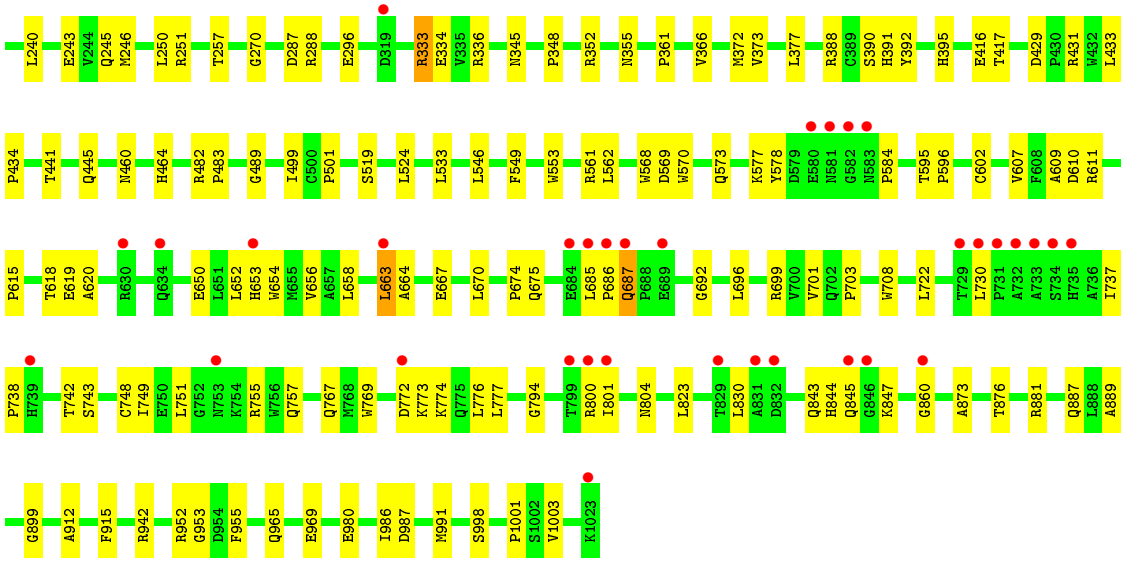
Chain 3:



• Molecule 1: Beta-galactosidase

Chain 4:




L240 E243 V244 Q245 N246 L250 R251 T257 G270 D287 R288 E296 D319 R333 E334 V335 R336 N345 P348 R352 N355 P361 V366 M372 V373 L377 R388 C389 S390 H391 Y392 H395 E416 T417 D429 P430 R431 W432 L433
P434 T441 Q445 N460 H464 R482 P483 G489 I499 C500 P501 S519 L524 L533 L546 F549 W553 R561 L562 W568 D569 W570 Q573 K577 Y578 D579 E580 N581 G582 N583 P584 T595 P596 C602 V607 P608 A609 D610 R611
P615 T618 E619 A620 R630 Q634 E650 L651 L652 H653 W654 M655 V656 A657 L658 L663 A664 E667 L670 P674 Q675 E684 L685 P686 Q687 P688 E689 G692 L696 R699 V700 V701 Q702 P703 W708 L722 T729 L730 P731 A732 A733 S734 H735 A736 I737
P738 H739 T742 S743 C748 I749 E750 L751 G752 M753 K754 R755 W756 Q757 Q767 M768 W769 D772 K773 K774 Q775 L776 L777 G794 I799 R800 I801 N804 L823 T829 L830 A831 D832 Q843 H844 Q845 G846 K847 G860 A873 T876 R881 Q887 L888 A889
G899 A912 F915 R942 R952 G953 D954 F955 Q965 E969 E980 I986 D987 M991 S998 P1001 S1002 V1003 K1023

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.84Å 166.31Å 201.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.23 – 2.20 21.23 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.1 (21.23-2.20) 92.1 (21.23-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.19Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.195 , 0.237 0.192 , 0.235	Depositor DCC
R_{free} test set	3358 reflections (1.44%)	DCC
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.724	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 233822 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	36190	wwPDB-VP
Average B, all atoms (Å^2)	28.0	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 37.12 % 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 4.5024e-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, 149

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	1	0.33	0/8361	0.61	0/11408
1	2	0.33	0/8361	0.62	0/11408
1	3	0.33	0/8361	0.61	0/11408
1	4	0.33	0/8361	0.62	0/11408
All	All	0.33	0/33444	0.62	0/45632

There are no bond length outliers.

There are no bond angle outliers.

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	109	0
1	2	8119	0	7708	107	0
1	3	8119	0	7708	110	0
1	4	8119	0	7708	118	0
2	1	12	0	9	0	0
2	2	12	0	9	0	0
2	3	12	0	9	0	0
2	4	12	0	9	0	0
3	1	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	3	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	112	0	168	6	0
5	2	124	0	186	1	0
5	3	136	0	204	1	0
5	4	116	0	174	0	0
6	1	773	0	0	4	0
6	2	858	0	0	5	0
6	3	760	0	0	3	0
6	4	760	0	0	2	0
All	All	36190	0	31600	435	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 (435) 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)
1:3:142:ILE:HG12	1:3:170:GLU:HG2	1.50	0.94
1:1:142:ILE:HG12	1:1:170:GLU:HG2	1.57	0.84
1:4:687:GLN:NE2	1:4:687:GLN:H	1.76	0.83
1:1:823:LEU:O	1:2:730:LEU:HD21	1.80	0.81
1:1:283:GLY:HA3	5:1:5029:DMS:H12	1.63	0.79
1:3:730:LEU:HD11	1:4:823:LEU:HB3	1.66	0.76
1:2:245:GLN:HG2	1:2:288:ARG:HG2	1.69	0.74
1:4:355:ASN:OD1	1:4:388:ARG:HD3	1.89	0.72
1:3:765:LEU:HD21	1:3:768:MET:CE	2.20	0.72
1:4:142:ILE:HG12	1:4:170:GLU:HG2	1.70	0.71
1:2:873:ALA:O	1:2:876:THR:HG22	1.92	0.70
1:1:890:GLN:HE22	1:1:947:GLY:HA3	1.56	0.69
1:2:127:PHE:CE1	1:2:184:LEU:HG	2.30	0.67
1:3:696:LEU:HB2	1:3:722:LEU:HD11	1.75	0.67
1:3:245:GLN:HG2	1:3:288:ARG:HG2	1.76	0.66
1:1:91:GLN:HG3	1:1:96:ASP:OD1	1.96	0.66
1:1:284:GLY:H	5:1:5029:DMS:H12	1.60	0.66
1:4:755:ARG:HB2	1:4:769:TRP:HB2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:166:ARG:HG3	1:1:392:TYR:HB2	1.79	0.65
1:1:863:GLN:HG2	1:1:1021:CYS:HB3	1.79	0.64
1:3:549:PHE:CE2	1:3:620:ALA:HA	2.33	0.64
1:1:245:GLN:HG2	1:1:288:ARG:HG2	1.79	0.64
1:1:892:ALA:HB3	1:1:946:TYR:CE1	2.33	0.64
1:2:142:ILE:HG12	1:2:170:GLU:HG2	1.80	0.64
1:3:237:ARG:NH1	1:3:237:ARG:HB3	2.13	0.64
1:4:153:TRP:HB2	1:4:185:ALA:HB3	1.78	0.63
1:4:237:ARG:HB3	1:4:237:ARG:NH1	2.14	0.63
1:4:615:PRO:O	1:4:618:THR:HG22	1.98	0.63
1:2:91:GLN:HG3	1:2:96:ASP:OD1	1.97	0.63
1:4:88:SER:HA	1:4:366:VAL:HG21	1.80	0.63
1:3:630:ARG:HB3	1:3:630:ARG:HH11	1.63	0.63
1:3:965:GLN:O	1:3:969:GLU:HG3	1.99	0.62
1:3:88:SER:HA	1:3:366:VAL:HG21	1.81	0.62
1:3:237:ARG:HH11	1:3:237:ARG:CB	2.12	0.62
1:4:237:ARG:HB3	1:4:237:ARG:HH11	1.65	0.62
1:1:579:ASP:OD2	1:1:583:ASN:HB2	1.99	0.62
1:3:890:GLN:HE22	1:3:948:PRO:HD3	1.65	0.62
1:2:844:HIS:HE1	1:2:845:GLN:HE21	1.48	0.62
1:4:873:ALA:O	1:4:876:THR:HG22	1.99	0.61
1:1:147:ASN:HB3	1:1:206:SER:HA	1.81	0.61
1:2:890:GLN:HG2	1:2:891:VAL:N	2.15	0.61
1:1:630:ARG:HH21	1:1:630:ARG:HB3	1.66	0.61
1:2:433:LEU:HB3	1:2:434:PRO:HD3	1.83	0.61
1:1:615:PRO:O	1:1:618:THR:HG22	2.01	0.60
1:4:578:TYR:CE1	1:4:584:PRO:HB3	2.36	0.59
1:1:749:ILE:HD12	1:1:749:ILE:N	2.16	0.59
1:1:777:LEU:HG	1:1:889:ALA:HA	1.84	0.59
1:3:506:VAL:HG12	1:3:521:LYS:HE3	1.85	0.59
1:4:573:GLN:HB2	1:4:602:CYS:O	2.03	0.59
1:2:367:MET:HE2	1:2:372:MET:HG3	1.83	0.59
1:1:887:GLN:NE2	1:1:980:GLU:O	2.34	0.58
1:3:777:LEU:HD11	1:3:980:GLU:HG2	1.85	0.58
1:4:147:ASN:HB3	1:4:206:SER:HA	1.84	0.58
1:1:788:PRO:HD2	1:1:968:MET:HG3	1.86	0.58
1:2:965:GLN:O	1:2:969:GLU:HG3	2.04	0.58
1:2:844:HIS:CE1	1:2:845:GLN:HE21	2.22	0.58
1:1:730:LEU:HD21	1:2:823:LEU:O	2.05	0.57
1:4:577:LYS:O	1:4:584:PRO:HA	2.04	0.57
1:4:334:GLU:OE1	1:4:336:ARG:NH1	2.36	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:127:PHE:HE1	1:2:184:LEU:HG	1.67	0.57
1:3:200:GLN:HG2	1:3:391:HIS:HB2	1.87	0.57
1:3:127:PHE:CE1	1:3:184:LEU:HG	2.40	0.57
1:4:245:GLN:HG2	1:4:288:ARG:HG2	1.86	0.56
1:2:887:GLN:NE2	1:2:980:GLU:O	2.37	0.56
1:2:147:ASN:HB3	1:2:206:SER:HA	1.88	0.56
1:3:91:GLN:HG3	1:3:96:ASP:OD1	2.05	0.56
1:1:801:ILE:HD12	1:1:801:ILE:N	2.21	0.56
1:4:237:ARG:HG2	1:4:296:GLU:OE1	2.06	0.56
1:1:651:LEU:HD23	1:1:703:PRO:HG3	1.87	0.56
1:3:777:LEU:HB2	1:3:887:GLN:HG2	1.88	0.55
1:3:79:PRO:HD2	1:3:80:GLU:OE2	2.06	0.55
1:3:873:ALA:O	1:3:876:THR:HG22	2.05	0.55
1:1:292:ARG:HH12	5:1:5012:DMS:C1	2.19	0.55
1:2:777:LEU:HD11	1:2:980:GLU:HG2	1.89	0.55
1:4:200:GLN:HG2	1:4:391:HIS:HB2	1.89	0.55
1:2:473:ARG:HH12	1:2:477:SER:HB2	1.71	0.55
1:4:656:VAL:HG21	1:4:685:LEU:CD1	2.37	0.55
1:4:757:GLN:HE21	1:4:767:GLN:HB3	1.72	0.55
1:3:765:LEU:HD21	1:3:768:MET:HE1	1.87	0.55
1:3:610:ASP:O	1:3:611:ARG:HB2	2.07	0.55
1:2:892:ALA:HB3	1:2:946:TYR:CE1	2.43	0.54
1:2:524:LEU:HD11	1:2:562:LEU:HG	1.89	0.54
1:4:429:ASP:OD1	1:4:431:ARG:HG3	2.07	0.54
1:3:1017:GLN:HB2	6:3:4736:HOH:O	2.07	0.54
1:3:305:ILE:HD11	1:3:645:ARG:HB3	1.88	0.54
1:3:355:ASN:OD1	1:3:388:ARG:HD3	2.07	0.54
1:3:237:ARG:HH11	1:3:237:ARG:HB3	1.73	0.54
1:2:595:THR:HA	1:2:596:PRO:C	2.29	0.53
1:2:153:TRP:HB2	1:2:185:ALA:HB3	1.90	0.53
1:4:794:GLY:HA2	1:4:998:SER:O	2.07	0.53
1:2:630:ARG:HB3	5:2:5033:DMS:H22	1.89	0.53
1:1:284:GLY:N	5:1:5029:DMS:H12	2.23	0.53
1:4:804:ASN:ND2	1:4:1001:PRO:HG2	2.24	0.53
1:3:765:LEU:HD21	1:3:768:MET:HE2	1.90	0.53
1:3:240:LEU:HD23	1:3:240:LEU:C	2.29	0.53
1:2:615:PRO:O	1:2:618:THR:HG22	2.09	0.53
1:3:823:LEU:HD11	1:3:841:ALA:HB2	1.90	0.52
1:3:245:GLN:HG2	1:3:288:ARG:CD	2.39	0.52
1:1:896:ASN:HB3	1:1:945:ASN:HB2	1.90	0.52
1:2:166:ARG:HG3	1:2:392:TYR:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:250:LEU:O	1:4:251:ARG:HD3	2.09	0.52
1:1:166:ARG:HG3	1:1:392:TYR:CB	2.40	0.52
1:2:843:GLN:HA	1:2:847:LYS:O	2.08	0.52
1:1:595:THR:HA	1:1:596:PRO:C	2.30	0.52
1:2:59:ARG:HB2	1:2:124:SER:OG	2.09	0.52
1:2:777:LEU:CD1	1:2:980:GLU:HG2	2.40	0.52
1:4:654:TRP:CH2	1:4:685:LEU:HD21	2.45	0.52
1:4:361:PRO:HB3	1:4:609:ALA:HB1	1.91	0.52
1:1:352:ARG:HG2	1:1:553:TRP:CH2	2.44	0.52
1:4:777:LEU:HB2	1:4:887:GLN:HG2	1.91	0.52
1:1:630:ARG:NH2	1:1:630:ARG:HB3	2.25	0.52
1:4:887:GLN:NE2	1:4:980:GLU:O	2.40	0.52
1:1:751:LEU:HD23	1:1:862:GLY:HA2	1.91	0.52
1:1:127:PHE:CE1	1:1:184:LEU:HG	2.44	0.52
1:4:100:TYR:CE1	1:4:602:CYS:HB3	2.45	0.52
1:1:573:GLN:HB2	1:1:602:CYS:O	2.11	0.51
1:3:131:GLU:O	1:3:135:GLN:HG3	2.10	0.51
1:4:166:ARG:HG3	1:4:392:TYR:HB2	1.92	0.51
1:4:91:GLN:HG3	1:4:96:ASP:OD1	2.10	0.51
1:4:730:LEU:N	1:4:730:LEU:HD12	2.25	0.51
1:1:292:ARG:HH12	5:1:5012:DMS:H12	1.75	0.51
1:3:653:HIS:CD2	1:3:667:GLU:HB3	2.46	0.51
1:3:499:ILE:HG22	1:3:501:PRO:HD3	1.93	0.51
1:3:800:ARG:HG2	1:3:800:ARG:HH11	1.75	0.51
1:1:890:GLN:HG2	6:1:4394:HOH:O	2.11	0.51
1:3:1011:ALA:HB3	1:3:1014:TYR:CZ	2.45	0.51
1:1:105:TYR:CE1	1:1:199:ASP:HB2	2.46	0.51
1:1:194:GLY:O	1:1:198:GLU:HG3	2.11	0.51
1:3:245:GLN:HG2	1:3:288:ARG:CG	2.41	0.50
1:2:759:ASN:HB2	1:2:766:SER:OG	2.11	0.50
1:4:570:TRP:O	1:4:607:VAL:HG22	2.11	0.50
1:4:610:ASP:O	1:4:611:ARG:HB2	2.11	0.50
1:3:608:PHE:CE2	1:3:614:HIS:HD2	2.30	0.50
1:2:651:LEU:C	1:2:651:LEU:HD12	2.32	0.50
1:1:18:ASN:ND2	1:1:21:VAL:HG23	2.26	0.50
1:4:749:ILE:N	1:4:749:ILE:HD12	2.26	0.50
1:3:133:TRP:CE3	1:3:216:HIS:HB2	2.46	0.50
1:3:131:GLU:OE1	1:3:179:ALA:HB2	2.12	0.50
1:4:773:LYS:NZ	1:4:774:LYS:HG2	2.27	0.50
1:1:369:GLU:O	1:1:373:VAL:HG23	2.12	0.50
1:2:128:ASN:HA	1:2:180:GLY:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:3:887:GLN:NE2	1:3:980:GLU:O	2.45	0.49
1:3:749:ILE:N	1:3:749:ILE:HD12	2.27	0.49
1:2:52:ARG:O	1:2:213:SER:HB2	2.11	0.49
1:3:578:TYR:CE1	1:3:584:PRO:HB3	2.48	0.49
1:1:625:GLN:NE2	6:1:4833:HOH:O	2.46	0.49
1:1:88:SER:HA	1:1:366:VAL:HG21	1.94	0.49
1:2:549:PHE:CE2	1:2:620:ALA:HA	2.48	0.49
1:3:506:VAL:CG1	1:3:521:LYS:HE3	2.42	0.49
1:4:777:LEU:HG	1:4:889:ALA:HA	1.94	0.49
1:4:843:GLN:HA	1:4:847:LYS:O	2.12	0.49
1:3:699:ARG:HD2	1:3:714:ILE:HD13	1.94	0.49
1:4:433:LEU:HB3	1:4:434:PRO:HD3	1.95	0.49
1:2:1011:ALA:HB3	1:2:1014:TYR:CZ	2.48	0.49
1:4:751:LEU:HD21	1:4:860:GLY:O	2.13	0.49
1:2:730:LEU:N	1:2:730:LEU:HD12	2.27	0.49
1:4:687:GLN:NE2	1:4:687:GLN:N	2.55	0.49
1:4:66:PRO:HG2	1:4:67:GLU:OE1	2.13	0.49
1:3:225:PHE:HA	1:3:243:GLU:O	2.13	0.49
1:1:153:TRP:HB2	1:1:185:ALA:HB3	1.95	0.49
1:2:334:GLU:OE1	1:2:336:ARG:NH1	2.45	0.49
1:4:730:LEU:HD12	1:4:730:LEU:H	1.77	0.48
1:4:377:LEU:HD22	1:4:708:TRP:HA	1.94	0.48
1:3:777:LEU:CD1	1:3:980:GLU:HG2	2.43	0.48
1:2:473:ARG:NH1	1:2:477:SER:HB2	2.27	0.48
1:4:942:ARG:HA	1:4:953:GLY:O	2.14	0.48
1:2:499:ILE:HG22	1:2:501:PRO:HD3	1.95	0.48
1:4:100:TYR:CZ	1:4:602:CYS:HB3	2.48	0.48
1:4:801:ILE:HD12	1:4:801:ILE:N	2.28	0.48
1:1:636:ILE:HD13	1:1:698:VAL:HG11	1.95	0.48
1:2:863:GLN:OE1	1:2:952:ARG:NH2	2.47	0.48
1:1:241:GLU:HG2	1:1:292:ARG:HG2	1.95	0.48
1:4:656:VAL:HG21	1:4:685:LEU:HD13	1.94	0.48
1:3:533:LEU:HD23	1:3:533:LEU:C	2.34	0.48
1:2:754:LYS:HZ1	1:2:1022:GLN:NE2	2.12	0.48
1:3:630:ARG:HB3	1:3:630:ARG:NH1	2.28	0.48
1:3:930:VAL:O	1:3:932:PRO:HD3	2.12	0.48
1:4:225:PHE:HA	1:4:243:GLU:O	2.14	0.48
1:2:890:GLN:OE1	1:2:947:GLY:HA3	2.13	0.48
1:2:651:LEU:HD12	1:2:651:LEU:O	2.14	0.48
1:1:361:PRO:HB3	1:1:609:ALA:HB1	1.96	0.48
1:2:768:MET:HE1	1:2:1020:TRP:CZ2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:105:TYR:CE1	1:4:199:ASP:HB2	2.49	0.47
1:3:52:ARG:O	1:3:213:SER:HB2	2.14	0.47
1:2:734:SER:HB2	1:2:860:GLY:HA3	1.95	0.47
1:4:952:ARG:NH1	1:4:952:ARG:HB2	2.29	0.47
1:2:610:ASP:O	1:2:611:ARG:HB2	2.14	0.47
1:4:50:GLN:HG2	6:4:4738:HOH:O	2.13	0.47
1:2:754:LYS:NZ	1:2:1022:GLN:NE2	2.62	0.47
1:4:240:LEU:HD23	1:4:240:LEU:C	2.34	0.47
1:4:800:ARG:C	1:4:801:ILE:HD12	2.34	0.47
1:1:773:LYS:HG2	1:1:774:LYS:N	2.29	0.47
1:1:734:SER:HB2	1:1:860:GLY:HA3	1.97	0.47
1:4:52:ARG:O	1:4:213:SER:HB2	2.15	0.47
1:3:730:LEU:HD12	1:3:730:LEU:N	2.30	0.47
1:3:730:LEU:HD21	1:4:823:LEU:O	2.15	0.47
1:3:890:GLN:OE1	1:3:947:GLY:HA3	2.15	0.47
1:3:606:LEU:O	1:3:614:HIS:HB2	2.14	0.47
1:3:646:HIS:CE1	1:3:673:ALA:HB2	2.50	0.47
1:2:311:ALA:HB2	1:2:330:VAL:HG21	1.95	0.47
1:2:661:LYS:O	1:2:663:LEU:HD22	2.15	0.47
1:3:755:ARG:HB3	1:3:769:TRP:HB2	1.97	0.47
1:4:147:ASN:HA	1:4:148:SER:HA	1.62	0.47
1:2:851:ILE:HB	1:2:871:GLU:HB2	1.97	0.47
1:2:358:GLU:HB3	1:2:367:MET:HG2	1.97	0.47
1:4:742:THR:HG22	1:4:743:SER:N	2.30	0.47
1:3:789:LEU:HD11	1:3:993:ILE:HG22	1.97	0.47
1:4:952:ARG:HH11	1:4:952:ARG:CB	2.28	0.47
1:1:499:ILE:HG22	1:1:501:PRO:HD3	1.97	0.47
1:2:782:ASP:HA	1:2:884:LEU:HD23	1.97	0.46
1:1:433:LEU:HB3	1:1:434:PRO:HD3	1.97	0.46
1:3:427:THR:HG21	1:3:462:SER:HB3	1.98	0.46
1:4:257:THR:HA	1:4:270:GLY:O	2.16	0.46
1:2:225:PHE:HA	1:2:243:GLU:O	2.15	0.46
1:1:340:GLY:O	1:1:532:PRO:HB3	2.16	0.46
1:4:881:ARG:HE	1:4:987:ASP:CG	2.18	0.46
1:3:433:LEU:HB3	1:3:434:PRO:HD3	1.96	0.46
1:2:352:ARG:HG2	1:2:553:TRP:CH2	2.50	0.46
1:3:237:ARG:NH1	1:3:237:ARG:CB	2.75	0.46
1:1:59:ARG:HB2	1:1:124:SER:OG	2.15	0.46
1:2:804:ASN:ND2	1:2:1001:PRO:HG2	2.30	0.46
1:3:100:TYR:CZ	1:3:602:CYS:HB3	2.51	0.46
1:1:147:ASN:HA	1:1:148:SER:HA	1.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:373:VAL:O	1:4:377:LEU:HG	2.16	0.46
1:3:100:TYR:CE1	1:3:602:CYS:HB3	2.50	0.46
1:4:844:HIS:ND1	1:4:845:GLN:HG2	2.31	0.46
1:4:674:PRO:O	1:4:675:GLN:HB2	2.16	0.46
1:3:340:GLY:O	1:3:532:PRO:HB3	2.15	0.46
1:3:153:TRP:HB2	1:3:185:ALA:HB3	1.97	0.46
1:2:245:GLN:HG2	1:2:288:ARG:CG	2.42	0.46
1:3:61:ALA:HA	5:3:5030:DMS:H11	1.96	0.46
1:1:472:TYR:O	1:1:476:LYS:HG2	2.16	0.46
1:3:653:HIS:HB3	6:3:4793:HOH:O	2.15	0.46
1:4:773:LYS:HZ3	1:4:774:LYS:HG2	1.81	0.46
1:4:464:HIS:HB2	1:4:489:GLY:HA3	1.98	0.46
1:4:390:SER:HA	1:4:391:HIS:HA	1.70	0.46
1:1:756:TRP:CD2	1:1:858:ILE:HD13	2.51	0.46
1:3:147:ASN:HB3	1:3:206:SER:HA	1.97	0.46
1:4:90:TRP:NE1	1:4:96:ASP:OD2	2.36	0.45
1:3:416:GLU:HA	1:3:460:ASN:O	2.16	0.45
1:3:890:GLN:NE2	1:3:948:PRO:HD3	2.30	0.45
1:4:952:ARG:HB2	1:4:952:ARG:HH11	1.81	0.45
1:1:334:GLU:OE1	1:1:336:ARG:NH1	2.43	0.45
1:4:19:PRO:HD3	1:4:112:PRO:CB	2.46	0.45
1:2:533:LEU:C	1:2:533:LEU:HD23	2.36	0.45
1:2:147:ASN:HA	1:2:148:SER:HA	1.60	0.45
1:3:525:SER:O	1:4:561:ARG:HD3	2.16	0.45
1:4:687:GLN:HE21	1:4:687:GLN:H	1.59	0.45
1:2:367:MET:CE	1:2:372:MET:HG3	2.47	0.45
1:3:463:GLY:HA2	6:3:4559:HOH:O	2.16	0.45
1:4:223:SER:O	1:4:224:ASP:HB2	2.17	0.45
1:3:748:CYS:C	1:3:749:ILE:HD12	2.37	0.45
1:4:658:LEU:HD11	1:4:692:GLY:HA3	1.99	0.45
1:4:178:ARG:HG2	1:4:182:ASN:OD1	2.17	0.45
1:1:635:THR:OG1	1:1:681:GLU:HG3	2.17	0.45
1:3:143:PHE:O	1:3:168:PRO:HA	2.16	0.45
1:4:246:MET:SD	1:4:246:MET:C	2.95	0.45
1:3:377:LEU:HD22	1:3:708:TRP:HA	1.99	0.45
1:3:19:PRO:HD3	1:3:112:PRO:CB	2.46	0.45
1:4:524:LEU:HD11	1:4:562:LEU:HG	1.99	0.45
1:2:773:LYS:HD3	6:2:4925:HOH:O	2.16	0.45
1:4:231:PHE:CD1	1:4:231:PHE:N	2.85	0.45
1:2:246:MET:C	1:2:246:MET:SD	2.95	0.45
1:3:768:MET:O	1:3:775:GLN:HG2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:651:LEU:C	1:1:651:LEU:HD12	2.37	0.45
1:2:88:SER:HA	1:2:366:VAL:HG21	1.98	0.45
1:4:568:TRP:CD2	1:4:569:ASP:HB3	2.52	0.45
1:3:764:PHE:CE2	1:3:781:ARG:NH1	2.85	0.45
1:1:610:ASP:O	1:1:611:ARG:HB2	2.17	0.45
1:3:777:LEU:HG	1:3:889:ALA:HA	1.99	0.44
1:2:843:GLN:HG2	1:2:848:THR:HA	1.98	0.44
1:1:577:LYS:O	1:1:584:PRO:HA	2.18	0.44
1:3:568:TRP:CD2	1:3:569:ASP:HB3	2.51	0.44
1:1:533:LEU:HD23	1:1:533:LEU:C	2.37	0.44
1:3:673:ALA:HB1	1:3:674:PRO:HD2	1.99	0.44
1:4:965:GLN:O	1:4:969:GLU:HG3	2.17	0.44
1:2:390:SER:HA	1:2:391:HIS:HA	1.81	0.44
1:1:782:ASP:HA	1:1:884:LEU:HD23	1.98	0.44
1:4:372:MET:HE1	1:4:395:HIS:HB3	1.98	0.44
1:4:390:SER:HB2	1:4:391:HIS:CE1	2.53	0.44
1:1:377:LEU:HD22	1:1:708:TRP:HA	1.99	0.44
1:1:100:TYR:CE1	1:1:602:CYS:HB3	2.53	0.44
1:4:653:HIS:HB3	1:4:699:ARG:NH1	2.32	0.44
1:2:930:VAL:O	1:2:932:PRO:HD3	2.17	0.44
1:2:548:GLY:HA2	6:2:4069:HOH:O	2.18	0.44
1:4:619:GLU:HA	1:4:912:ALA:HB2	2.00	0.44
1:3:472:TYR:O	1:3:476:LYS:HG2	2.17	0.44
1:4:663:LEU:CD1	1:4:686:PRO:HG2	2.48	0.44
1:3:131:GLU:HG3	1:3:135:GLN:HG3	1.98	0.44
1:1:965:GLN:O	1:1:969:GLU:HG3	2.17	0.44
1:2:427:THR:HG21	1:2:462:SER:HB3	2.00	0.44
1:1:49:GLN:HA	1:1:49:GLN:OE1	2.17	0.44
1:4:166:ARG:HG3	1:4:392:TYR:CB	2.47	0.44
1:2:749:ILE:N	1:2:749:ILE:HD12	2.33	0.44
1:3:615:PRO:O	1:3:618:THR:HG22	2.18	0.43
1:1:561:ARG:HD3	1:2:525:SER:O	2.18	0.43
1:1:100:TYR:CZ	1:1:602:CYS:HB3	2.53	0.43
1:2:651:LEU:HD23	1:2:703:PRO:HG3	1.99	0.43
1:1:73:TRP:CE2	1:1:122:CYS:HB3	2.53	0.43
1:1:797:GLU:C	1:1:799:THR:H	2.22	0.43
1:1:613:PRO:HB3	1:1:617:LEU:HD23	2.00	0.43
1:2:755:ARG:HD3	1:2:769:TRP:CE3	2.53	0.43
1:3:843:GLN:HG2	1:3:848:THR:HA	1.99	0.43
1:2:400:THR:HA	6:2:4148:HOH:O	2.18	0.43
1:1:525:SER:O	1:2:561:ARG:HD3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:240:LEU:CD1	1:2:260:LEU:HD13	2.48	0.43
1:4:196:TYR:O	1:4:417:THR:HG22	2.19	0.43
1:4:199:ASP:C	1:4:416:GLU:HG2	2.39	0.43
1:1:873:ALA:O	1:1:876:THR:HG22	2.18	0.43
1:1:809:ARG:HD2	6:1:4886:HOH:O	2.19	0.43
1:4:595:THR:HA	1:4:596:PRO:C	2.39	0.43
1:3:166:ARG:HG3	1:3:392:TYR:HB2	2.00	0.43
1:2:546:LEU:HA	6:2:4129:HOH:O	2.18	0.43
1:1:546:LEU:HA	6:1:4128:HOH:O	2.18	0.43
1:4:348:PRO:HG2	6:4:4309:HOH:O	2.19	0.43
1:3:457:SER:HA	1:3:485:GLN:O	2.19	0.43
1:4:237:ARG:CB	1:4:237:ARG:HH11	2.30	0.43
1:1:131:GLU:O	1:1:135:GLN:HG3	2.19	0.43
1:1:429:ASP:OD1	1:1:431:ARG:HG3	2.19	0.43
1:1:356:ARG:HH22	1:1:367:MET:CE	2.32	0.43
1:2:748:CYS:C	1:2:749:ILE:HD12	2.39	0.43
1:2:163:GLN:O	1:2:164:ASP:HB3	2.19	0.43
1:2:784:PHE:HA	1:2:881:ARG:O	2.18	0.43
1:3:291:LEU:N	1:3:291:LEU:HD22	2.34	0.43
1:3:802:ASP:OD2	1:3:804:ASN:HB3	2.18	0.43
1:1:301:TRP:CH2	1:1:452:SER:HA	2.54	0.43
1:1:581:ASN:HB2	1:1:583:ASN:ND2	2.34	0.42
1:3:824:GLN:HG2	1:3:825:CYS:N	2.33	0.42
1:4:533:LEU:HD23	1:4:533:LEU:C	2.38	0.42
1:1:755:ARG:HB2	1:1:769:TRP:HB2	2.01	0.42
1:1:730:LEU:H	1:1:730:LEU:HD12	1.84	0.42
1:2:749:ILE:HB	1:2:756:TRP:HB2	2.00	0.42
1:3:830:LEU:CD2	1:4:830:LEU:HD21	2.49	0.42
1:1:843:GLN:HA	1:1:847:LYS:O	2.19	0.42
1:3:815:HIS:HD2	1:3:849:LEU:HD13	1.85	0.42
1:2:777:LEU:HG	1:2:889:ALA:HA	2.02	0.42
1:1:524:LEU:HD11	1:1:562:LEU:HG	2.01	0.42
1:2:542:MET:CE	1:2:601:PHE:HA	2.49	0.42
1:2:337:ILE:HA	1:2:341:LEU:O	2.18	0.42
1:3:231:PHE:N	1:3:231:PHE:CD1	2.86	0.42
1:3:613:PRO:HB3	1:3:617:LEU:HD23	2.01	0.42
1:4:333:ARG:HA	1:4:345:ASN:OD1	2.19	0.42
1:2:240:LEU:C	1:2:240:LEU:HD23	2.40	0.42
1:1:128:ASN:HA	1:1:180:GLY:O	2.20	0.42
1:2:440:VAL:HG13	1:2:475:ILE:HD11	2.01	0.42
1:1:730:LEU:HD12	1:1:730:LEU:N	2.34	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:899:GLY:HA2	1:4:915:PHE:CD1	2.54	0.42
1:4:955:PHE:CD1	1:4:986:ILE:HG23	2.54	0.42
1:1:390:SER:HA	1:1:391:HIS:HA	1.80	0.42
1:1:163:GLN:O	1:1:164:ASP:HB3	2.20	0.42
1:1:19:PRO:HD3	1:1:112:PRO:CB	2.50	0.42
1:1:1020:TRP:HD1	1:1:1021:CYS:N	2.18	0.42
1:2:166:ARG:HG3	1:2:392:TYR:CB	2.50	0.42
1:3:652:LEU:O	1:3:667:GLU:HA	2.20	0.42
1:3:595:THR:HA	1:3:596:PRO:C	2.40	0.42
1:3:80:GLU:H	1:3:80:GLU:CD	2.21	0.42
1:2:200:GLN:HG2	1:2:391:HIS:HB2	2.02	0.42
1:3:59:ARG:HB2	1:3:124:SER:OG	2.20	0.42
1:1:580:GLU:HA	1:1:580:GLU:OE1	2.19	0.42
1:1:568:TRP:CD2	1:1:569:ASP:HB3	2.55	0.42
1:4:352:ARG:HG2	1:4:553:TRP:CH2	2.55	0.42
1:2:867:THR:HG23	1:2:1015:HIS:HE1	1.85	0.42
1:2:782:ASP:HB2	1:2:842:TRP:CZ2	2.55	0.42
1:2:842:TRP:HZ3	1:2:852:SER:HB3	1.84	0.42
1:1:200:GLN:HG2	1:1:391:HIS:HB2	2.02	0.42
1:4:737:ILE:HA	1:4:738:PRO:HD3	1.91	0.42
1:2:340:GLY:O	1:2:532:PRO:HB3	2.19	0.42
1:1:356:ARG:HH22	1:1:367:MET:HE2	1.85	0.41
1:1:619:GLU:HA	1:1:912:ALA:HB2	2.02	0.41
1:3:316:HIS:HB2	1:3:321:THR:O	2.20	0.41
1:2:995:GLY:C	1:2:997:ASP:N	2.72	0.41
1:3:127:PHE:CD1	1:3:127:PHE:N	2.88	0.41
1:1:502:MET:HA	1:1:537:GLU:O	2.20	0.41
1:3:793:ILE:HA	1:3:807:VAL:HG11	2.02	0.41
1:4:767:GLN:HA	1:4:776:LEU:HD12	2.01	0.41
1:4:59:ARG:HB2	1:4:124:SER:OG	2.20	0.41
1:1:955:PHE:HB2	1:1:987:ASP:O	2.21	0.41
1:1:587:ALA:HB1	1:1:591:ASP:CB	2.50	0.41
1:4:79:PRO:HD2	1:4:80:GLU:OE2	2.21	0.41
1:1:240:LEU:HD23	1:1:240:LEU:C	2.40	0.41
1:4:748:CYS:C	1:4:749:ILE:HD12	2.40	0.41
1:2:658:LEU:N	1:2:663:LEU:CD2	2.83	0.41
1:3:1006:GLU:HG2	1:3:1007:PHE:CD2	2.56	0.41
1:2:699:ARG:HB3	1:2:699:ARG:HE	1.67	0.41
1:2:500:CYS:HA	1:2:534:ILE:O	2.21	0.41
1:2:505:ARG:O	1:2:519:SER:HA	2.20	0.41
1:3:454:ILE:HG13	1:3:455:ILE:HG13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:696:LEU:HB2	1:4:722:LEU:HD11	2.02	0.41
1:2:146:VAL:HG11	1:2:150:PHE:CD1	2.55	0.41
1:3:782:ASP:OD1	1:3:842:TRP:HH2	2.04	0.41
1:2:319:ASP:C	1:2:319:ASP:OD2	2.58	0.41
1:3:995:GLY:C	1:3:997:ASP:N	2.73	0.41
1:1:768:MET:HE1	1:1:1020:TRP:CH2	2.56	0.41
1:3:793:ILE:HA	1:3:807:VAL:CG1	2.50	0.41
1:4:127:PHE:CE1	1:4:184:LEU:HG	2.56	0.41
1:3:429:ASP:OD1	1:3:431:ARG:HG3	2.21	0.41
1:3:163:GLN:O	1:3:164:ASP:HB3	2.21	0.41
1:1:800:ARG:C	1:1:801:ILE:HD12	2.41	0.41
1:2:703:PRO:O	1:2:711:ALA:HB1	2.20	0.41
1:2:501:PRO:HB3	1:2:523:TRP:CZ3	2.56	0.41
1:1:333:ARG:HA	1:1:345:ASN:OD1	2.21	0.41
1:4:650:GLU:HB3	1:4:670:LEU:HD12	2.03	0.41
1:4:441:THR:O	1:4:445:GLN:HG3	2.21	0.41
1:1:86:VAL:HG13	1:1:87:PRO:HA	2.02	0.41
1:4:73:TRP:CE2	1:4:122:CYS:HB3	2.55	0.41
1:1:746:ASP:OD1	1:1:759:ASN:HA	2.21	0.41
1:1:283:GLY:CA	5:1:5029:DMS:H12	2.44	0.41
1:1:755:ARG:O	1:1:768:MET:HA	2.21	0.41
1:2:542:MET:HE3	1:2:601:PHE:HA	2.03	0.41
1:2:454:ILE:O	1:2:483:PRO:HD2	2.21	0.41
1:1:754:LYS:HA	1:1:769:TRP:O	2.22	0.40
1:2:658:LEU:H	1:2:663:LEU:CD2	2.34	0.40
1:2:869:ASP:OD1	1:2:1015:HIS:ND1	2.50	0.40
1:4:652:LEU:O	1:4:667:GLU:HA	2.21	0.40
1:1:794:GLY:HA2	1:1:998:SER:O	2.22	0.40
1:4:287:ASP:OD1	1:4:287:ASP:N	2.51	0.40
1:1:1011:ALA:HB3	1:1:1014:TYR:CZ	2.56	0.40
1:4:701:VAL:O	1:4:703:PRO:HD3	2.21	0.40
1:3:360:HIS:CE1	1:3:362:LEU:HB2	2.56	0.40
1:2:127:PHE:N	1:2:127:PHE:CD1	2.89	0.40
1:2:699:ARG:HD2	6:2:4846:HOH:O	2.19	0.40
1:2:598:ASP:OD1	1:2:797:GLU:HA	2.21	0.40
1:4:991:MET:CE	1:4:1003:VAL:HG21	2.50	0.40
1:1:292:ARG:HH11	1:1:292:ARG:HG3	1.86	0.40
1:4:499:ILE:HG22	1:4:501:PRO:HD3	2.03	0.40
1:4:664:ALA:CB	1:4:685:LEU:HD22	2.51	0.40
1:4:568:TRP:HA	1:4:569:ASP:HA	1.80	0.40
1:4:549:PHE:CE2	1:4:620:ALA:HA	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:807:VAL:HG13	1:2:808:GLU:N	2.36	0.40
1:4:482:ARG:HA	1:4:483:PRO:HD3	1.95	0.40
1:3:240:LEU:HD13	1:3:260:LEU:HD13	2.02	0.40
1:4:416:GLU:HA	1:4:460:ASN:O	2.22	0.40
1:1:883:GLY:HA3	1:1:987:ASP:HA	2.04	0.40
1:2:13:ARG:NH1	1:3:13:ARG:HD2	2.37	0.40
1:1:753:ASN:HB2	1:1:771:GLY:HA2	2.02	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%)	40 (4%)	1 (0%)	56	64
1	2	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
1	3	1009/1052 (96%)	966 (96%)	43 (4%)	0	100	100
1	4	1009/1052 (96%)	958 (95%)	51 (5%)	0	100	100
All	All	4036/4208 (96%)	3850 (95%)	185 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	798	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	863/897 (96%)	858 (99%)	5 (1%)	90	95
1	2	863/897 (96%)	859 (100%)	4 (0%)	92	96
1	3	863/897 (96%)	857 (99%)	6 (1%)	88	94
1	4	863/897 (96%)	857 (99%)	6 (1%)	88	94
All	All	3452/3588 (96%)	3431 (99%)	21 (1%)	90	95

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

Mol	Chain	Res	Type
1	1	333	ARG
1	1	519	SER
1	1	546	LEU
1	1	774	LYS
1	1	1017	GLN
1	2	333	ARG
1	2	519	SER
1	2	546	LEU
1	2	754	LYS
1	3	333	ARG
1	3	519	SER
1	3	546	LEU
1	3	761	GLN
1	3	772	ASP
1	3	773	LYS
1	4	333	ARG
1	4	519	SER
1	4	546	LEU
1	4	663	LEU
1	4	687	GLN
1	4	772	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	262	GLN
1	1	294	ASN
1	1	583	ASN
1	1	624	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	804	ASN
1	1	890	GLN
1	1	1017	GLN
1	1	1022	GLN
1	2	50	GLN
1	2	102	ASN
1	2	163	GLN
1	2	510	GLN
1	2	804	ASN
1	2	844	HIS
1	2	1017	GLN
1	2	1022	GLN
1	3	394	ASN
1	3	554	GLN
1	3	624	GLN
1	3	634	GLN
1	3	646	HIS
1	3	804	ASN
1	3	887	GLN
1	3	1022	GLN
1	4	163	GLN
1	4	294	ASN
1	4	653	HIS
1	4	687	GLN
1	4	757	GLN
1	4	804	ASN
1	4	863	GLN
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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 153 ligands modelled in this entry, 27 are monoatomic - leaving 126 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	149	1	2001	4	11,12,12	1.13	1 (9%)	13,17,17	0.84	0
5	DMS	1	5001	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	1	5002	-	3,3,3	0.18	0	3,3,3	0.58	0
5	DMS	1	5003	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	1	5004	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	1	5005	-	3,3,3	0.25	0	3,3,3	0.56	0
5	DMS	1	5006	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	1	5007	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	5008	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	1	5009	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	1	5010	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	1	5011	-	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	1	5012	-	3,3,3	0.20	0	3,3,3	0.56	0
5	DMS	1	5013	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	1	5014	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	1	5015	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	5016	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	1	5017	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	1	5018	4	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	1	5019	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	1	5020	-	3,3,3	0.20	0	3,3,3	0.59	0
5	DMS	1	5021	-	3,3,3	0.27	0	3,3,3	0.57	0
5	DMS	1	5022	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	1	5023	-	3,3,3	0.20	0	3,3,3	0.55	0
5	DMS	1	5024	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	1	5025	-	3,3,3	0.16	0	3,3,3	0.49	0
5	DMS	1	5026	-	3,3,3	0.19	0	3,3,3	0.52	0
5	DMS	1	5028	-	3,3,3	0.28	0	3,3,3	0.58	0
5	DMS	1	5029	-	3,3,3	0.23	0	3,3,3	0.54	0
5	DMS	2	1024	-	3,3,3	0.27	0	3,3,3	0.61	0
2	149	2	2001	4	11,12,12	1.27	2 (18%)	13,17,17	0.82	0
5	DMS	2	5001	-	3,3,3	0.26	0	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	2	5002	-	3,3,3	0.22	0	3,3,3	0.55	0
5	DMS	2	5003	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	2	5004	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	2	5005	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	2	5006	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	2	5008	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	2	5009	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	2	5010	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	2	5011	-	3,3,3	0.24	0	3,3,3	0.55	0
5	DMS	2	5012	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	2	5014	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	5015	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	2	5016	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	5017	-	3,3,3	0.22	0	3,3,3	0.61	0
5	DMS	2	5019	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	2	5020	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	2	5021	4	3,3,3	0.25	0	3,3,3	0.59	0
5	DMS	2	5022	-	3,3,3	0.20	0	3,3,3	0.57	0
5	DMS	2	5023	-	3,3,3	0.23	0	3,3,3	0.61	0
5	DMS	2	5024	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	2	5025	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	2	5026	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	2	5027	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	2	5028	-	3,3,3	0.22	0	3,3,3	0.60	0
5	DMS	2	5029	-	3,3,3	0.28	0	3,3,3	0.56	0
5	DMS	2	5030	-	3,3,3	0.14	0	3,3,3	0.52	0
5	DMS	2	5031	-	3,3,3	0.29	0	3,3,3	0.60	0
5	DMS	2	5032	-	3,3,3	0.26	0	3,3,3	0.55	0
5	DMS	2	5033	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	1024	-	3,3,3	0.23	0	3,3,3	0.59	0
2	149	3	2001	4	11,12,12	1.15	2 (18%)	13,17,17	0.80	0
5	DMS	3	5001	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	3	5002	-	3,3,3	0.20	0	3,3,3	0.57	0
5	DMS	3	5003	-	3,3,3	0.25	0	3,3,3	0.58	0
5	DMS	3	5004	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	3	5005	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	3	5006	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5007	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	5008	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	5009	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5010	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	3	5011	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	3	5012	-	3,3,3	0.22	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	3	5013	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	3	5014	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	3	5015	-	3,3,3	0.20	0	3,3,3	0.58	0
5	DMS	3	5016	-	3,3,3	0.23	0	3,3,3	0.60	0
5	DMS	3	5017	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5018	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	3	5019	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5020	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	3	5021	4	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	5022	-	3,3,3	0.19	0	3,3,3	0.59	0
5	DMS	3	5023	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	3	5024	-	3,3,3	0.23	0	3,3,3	0.62	0
5	DMS	3	5025	-	3,3,3	0.22	0	3,3,3	0.58	0
5	DMS	3	5027	-	3,3,3	0.24	0	3,3,3	0.59	0
5	DMS	3	5028	-	3,3,3	0.24	0	3,3,3	0.56	0
5	DMS	3	5029	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	3	5030	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	3	5031	-	3,3,3	0.26	0	3,3,3	0.62	0
5	DMS	3	5032	-	3,3,3	0.12	0	3,3,3	0.62	0
5	DMS	3	5033	-	3,3,3	0.30	0	3,3,3	0.59	0
5	DMS	3	5034	-	3,3,3	0.27	0	3,3,3	0.60	0
2	149	4	2001	4	11,12,12	0.96	1 (9%)	13,17,17	0.79	0
5	DMS	4	5001	-	3,3,3	0.22	0	3,3,3	0.59	0
5	DMS	4	5002	-	3,3,3	0.16	0	3,3,3	0.52	0
5	DMS	4	5003	-	3,3,3	0.20	0	3,3,3	0.59	0
5	DMS	4	5004	-	3,3,3	0.21	0	3,3,3	0.61	0
5	DMS	4	5005	-	3,3,3	0.23	0	3,3,3	0.56	0
5	DMS	4	5006	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	4	5007	-	3,3,3	0.23	0	3,3,3	0.57	0
5	DMS	4	5008	-	3,3,3	0.26	0	3,3,3	0.58	0
5	DMS	4	5009	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	4	5010	-	3,3,3	0.24	0	3,3,3	0.58	0
5	DMS	4	5011	-	3,3,3	0.23	0	3,3,3	0.58	0
5	DMS	4	5012	-	3,3,3	0.23	0	3,3,3	0.56	0
5	DMS	4	5013	-	3,3,3	0.22	0	3,3,3	0.57	0
5	DMS	4	5014	-	3,3,3	0.21	0	3,3,3	0.55	0
5	DMS	4	5016	-	3,3,3	0.21	0	3,3,3	0.58	0
5	DMS	4	5017	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	4	5018	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	5019	-	3,3,3	0.24	0	3,3,3	0.60	0
5	DMS	4	5020	-	3,3,3	0.24	0	3,3,3	0.57	0
5	DMS	4	5021	-	3,3,3	0.23	0	3,3,3	0.59	0
5	DMS	4	5022	-	3,3,3	0.19	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	5023	-	3,3,3	0.21	0	3,3,3	0.57	0
5	DMS	4	5024	-	3,3,3	0.21	0	3,3,3	0.60	0
5	DMS	4	5025	-	3,3,3	0.25	0	3,3,3	0.57	0
5	DMS	4	5026	-	3,3,3	0.22	0	3,3,3	0.56	0
5	DMS	4	5027	-	3,3,3	0.21	0	3,3,3	0.59	0
5	DMS	4	5028	-	3,3,3	0.31	0	3,3,3	0.55	0
5	DMS	4	5029	-	3,3,3	0.25	0	3,3,3	0.57	0
5	DMS	4	5030	-	3,3,3	0.29	0	3,3,3	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	149	1	2001	4	-	0/2/22/22	0/1/1/1
5	DMS	1	5001	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5002	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5003	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5004	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5005	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5006	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5007	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5008	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5009	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5010	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5011	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5012	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5013	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5014	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5015	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5016	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5017	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5018	4	-	0/0/0/0	0/0/0/0
5	DMS	1	5019	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5020	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5021	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5022	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5023	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5024	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5025	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5026	-	-	0/0/0/0	0/0/0/0
5	DMS	1	5028	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	1	5029	-	-	0/0/0/0	0/0/0/0
5	DMS	2	1024	-	-	0/0/0/0	0/0/0/0
2	149	2	2001	4	-	0/2/22/22	0/1/1/1
5	DMS	2	5001	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5002	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5003	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5004	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5005	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5006	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5008	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5009	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5010	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5011	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5012	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5014	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5015	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5016	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5017	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5019	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5020	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5021	4	-	0/0/0/0	0/0/0/0
5	DMS	2	5022	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5023	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5024	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5025	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5026	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5027	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5028	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5029	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5030	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5031	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5032	-	-	0/0/0/0	0/0/0/0
5	DMS	2	5033	-	-	0/0/0/0	0/0/0/0
5	DMS	3	1024	-	-	0/0/0/0	0/0/0/0
2	149	3	2001	4	-	0/2/22/22	0/1/1/1
5	DMS	3	5001	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5002	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5003	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5004	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5005	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5006	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5007	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	3	5008	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5009	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5010	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5011	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5012	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5013	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5014	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5015	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5016	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5017	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5018	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5019	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5020	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5021	4	-	0/0/0/0	0/0/0/0
5	DMS	3	5022	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5023	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5024	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5025	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5027	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5028	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5029	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5030	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5031	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5032	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5033	-	-	0/0/0/0	0/0/0/0
5	DMS	3	5034	-	-	0/0/0/0	0/0/0/0
2	149	4	2001	4	-	0/2/22/22	0/1/1/1
5	DMS	4	5001	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5002	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5003	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5004	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5005	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5006	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5007	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5008	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5009	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5010	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5011	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5012	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5013	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5014	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5016	-	-	0/0/0/0	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMS	4	5017	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5018	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5019	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5020	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5021	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5022	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5023	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5024	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5025	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5026	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5027	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5028	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5029	-	-	0/0/0/0	0/0/0/0
5	DMS	4	5030	-	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	2001	149	O5-C5	2.05	1.49	1.46
2	4	2001	149	O5-C1	2.34	1.38	1.34
2	2	2001	149	O5-C5	2.38	1.49	1.46
2	3	2001	149	O5-C1	2.55	1.38	1.34
2	1	2001	149	O5-C1	2.68	1.38	1.34
2	2	2001	149	O5-C1	2.94	1.38	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	5012	DMS	2	0
5	1	5029	DMS	4	0
5	2	5033	DMS	1	0
5	3	5030	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%)	-0.16	37 (3%)	45	44	13, 25, 46, 74	0
1	2	1011/1052 (96%)	-0.24	31 (3%)	52	51	13, 24, 45, 75	0
1	3	1011/1052 (96%)	-0.22	34 (3%)	49	47	14, 24, 45, 75	0
1	4	1011/1052 (96%)	-0.18	40 (3%)	42	41	13, 25, 46, 74	0
All	All	4044/4208 (96%)	-0.20	142 (3%)	48	46	13, 25, 46, 75	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	3	732	ALA	9.5
1	1	772	ASP	8.3
1	2	733	ALA	8.2
1	4	735	HIS	7.6
1	1	735	HIS	7.5
1	2	731	PRO	7.1
1	1	732	ALA	6.6
1	3	733	ALA	6.6
1	2	734	SER	6.6
1	2	732	ALA	6.5
1	3	730	LEU	6.4
1	1	799	THR	6.2
1	3	799	THR	6.2
1	4	732	ALA	6.1
1	3	731	PRO	6.1
1	3	689	GLU	5.8
1	1	800	ARG	5.5
1	2	686	PRO	5.5
1	3	745	MET	5.3
1	4	731	PRO	5.3
1	4	686	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	4	689	GLU	5.0
1	1	689	GLU	5.0
1	1	730	LEU	5.0
1	4	772	ASP	4.9
1	1	686	PRO	4.9
1	4	730	LEU	4.7
1	1	731	PRO	4.6
1	4	800	ARG	4.6
1	2	689	GLU	4.4
1	1	71	GLU	4.4
1	2	800	ARG	4.4
1	1	684	GLU	4.3
1	4	799	THR	4.3
1	2	799	THR	4.3
1	3	800	ARG	4.2
1	1	1023	LYS	4.2
1	4	687	GLN	4.1
1	2	730	LEU	4.1
1	2	687	GLN	4.0
1	1	580	GLU	4.0
1	1	733	ALA	4.0
1	4	801	ILE	4.0
1	1	801	ILE	4.0
1	3	735	HIS	4.0
1	4	733	ALA	3.9
1	3	801	ILE	3.9
1	1	736	ALA	3.9
1	1	685	LEU	3.8
1	4	734	SER	3.8
1	1	687	GLN	3.8
1	3	772	ASP	3.7
1	1	729	THR	3.7
1	1	734	SER	3.6
1	3	734	SER	3.6
1	3	685	LEU	3.5
1	3	686	PRO	3.5
1	2	684	GLU	3.4
1	2	801	ILE	3.4
1	3	729	THR	3.3
1	2	846	GLY	3.3
1	2	688	PRO	3.3
1	4	79	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	2	831	ALA	3.3
1	3	798	ALA	3.2
1	3	684	GLU	3.2
1	2	845	GLN	3.2
1	2	735	HIS	3.1
1	2	729	THR	3.1
1	1	581	ASN	3.1
1	4	684	GLU	3.0
1	4	845	GLN	3.0
1	3	1023	LYS	2.9
1	3	687	GLN	2.9
1	1	771	GLY	2.9
1	4	831	ALA	2.9
1	2	772	ASP	2.8
1	1	630	ARG	2.8
1	2	761	GLN	2.8
1	3	744	GLU	2.8
1	3	761	GLN	2.7
1	1	798	ALA	2.7
1	4	580	GLU	2.7
1	4	634	GLN	2.7
1	1	846	GLY	2.7
1	4	729	THR	2.7
1	4	71	GLU	2.7
1	2	264	GLU	2.7
1	1	773	LYS	2.7
1	2	745	MET	2.6
1	3	817	GLN	2.6
1	4	653	HIS	2.6
1	4	739	HIS	2.6
1	2	1022	GLN	2.6
1	1	130	ASP	2.6
1	4	319	ASP	2.6
1	1	634	GLN	2.6
1	1	745	MET	2.6
1	2	819	GLU	2.5
1	2	580	GLU	2.5
1	3	832	ASP	2.5
1	4	685	LEU	2.5
1	1	959	ILE	2.5
1	1	977	HIS	2.5
1	2	80	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	4	135	GLN	2.5
1	2	798	ALA	2.4
1	1	845	GLN	2.4
1	4	832	ASP	2.4
1	3	580	GLU	2.4
1	3	76	CYS	2.4
1	4	583	ASN	2.4
1	3	75	GLU	2.4
1	3	845	GLN	2.4
1	3	186	VAL	2.4
1	3	802	ASP	2.4
1	4	846	GLY	2.4
1	3	736	ALA	2.4
1	4	1023	LYS	2.4
1	3	581	ASN	2.3
1	2	737	ILE	2.3
1	4	630	ARG	2.3
1	4	753	ASN	2.3
1	4	829	THR	2.3
1	3	819	GLU	2.3
1	4	581	ASN	2.3
1	1	753	ASN	2.2
1	4	663	LEU	2.2
1	3	582	GLY	2.2
1	2	1023	LYS	2.2
1	1	80	GLU	2.2
1	4	860	GLY	2.2
1	2	319	ASP	2.1
1	4	131	GLU	2.1
1	4	582	GLY	2.1
1	1	817	GLN	2.1
1	4	179	ALA	2.0
1	3	237	ARG	2.0
1	1	582	GLY	2.0
1	4	186	VAL	2.0
1	2	744	GLU	2.0
1	1	76	CYS	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	4	5007	4/4	0.32	0.51	29.90	113,113,113,114	0
5	DMS	2	5025	4/4	0.81	0.29	12.96	93,93,93,94	0
5	DMS	1	5007	4/4	0.65	0.26	9.76	90,90,90,91	0
5	DMS	1	5029	4/4	0.97	0.22	9.16	51,52,53,54	0
5	DMS	3	1024	4/4	0.91	0.19	7.73	74,74,75,75	0
5	DMS	2	5021	4/4	0.92	0.36	7.39	89,89,89,90	0
5	DMS	3	5018	4/4	0.84	0.23	7.05	73,74,75,75	0
5	DMS	2	5020	4/4	0.86	0.18	6.37	69,70,70,70	0
5	DMS	3	5006	4/4	0.82	0.21	5.60	85,85,85,86	0
5	DMS	2	5033	4/4	0.92	0.26	4.82	72,72,73,73	0
5	DMS	2	5006	4/4	0.89	0.22	3.96	92,92,92,93	0
5	DMS	1	5016	4/4	0.95	0.12	3.92	65,65,65,65	0
5	DMS	1	5001	4/4	0.99	0.18	3.90	26,27,28,29	0
5	DMS	3	5024	4/4	0.83	0.32	3.61	76,77,77,77	0
5	DMS	4	5020	4/4	0.93	0.15	3.58	72,72,72,72	0
5	DMS	2	1024	4/4	0.95	0.15	3.55	59,60,61,61	0
5	DMS	2	5026	4/4	0.91	0.13	3.51	63,63,63,65	0
5	DMS	4	5028	4/4	0.96	0.15	3.43	41,42,42,43	0
5	DMS	3	5030	4/4	0.90	0.24	3.28	79,79,80,80	0
5	DMS	2	5023	4/4	0.94	0.21	3.21	57,58,58,59	0
5	DMS	3	5020	4/4	0.93	0.16	3.20	64,64,64,65	0
5	DMS	3	5017	4/4	0.91	0.18	3.19	83,83,84,84	0
5	DMS	3	5028	4/4	0.87	0.17	3.11	83,83,84,84	0
5	DMS	4	5024	4/4	0.89	0.20	3.00	80,81,81,81	0
5	DMS	4	5003	4/4	0.98	0.14	2.98	42,42,43,44	0
5	DMS	3	5004	4/4	0.94	0.13	2.95	49,50,52,52	0
5	DMS	3	5021	4/4	0.92	0.23	2.71	64,64,65,66	0
5	DMS	1	5006	4/4	0.91	0.20	2.71	74,75,75,75	0
5	DMS	3	5016	4/4	0.80	0.22	2.64	71,72,72,73	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	3	5010	4/4	0.98	0.15	2.51	40,41,42,42	0
5	DMS	3	5003	4/4	0.99	0.18	2.31	35,36,36,37	0
5	DMS	3	5033	4/4	0.93	0.20	2.30	59,60,61,61	0
5	DMS	3	5034	4/4	0.86	0.21	2.18	66,66,66,67	0
5	DMS	1	5015	4/4	0.89	0.17	2.08	65,65,66,66	0
5	DMS	2	5004	4/4	0.94	0.13	2.05	49,50,51,52	0
5	DMS	4	5026	4/4	0.74	0.29	2.03	102,102,102,102	0
5	DMS	2	5017	4/4	0.61	0.28	1.95	92,92,93,94	0
5	DMS	4	5008	4/4	0.96	0.23	1.84	49,50,50,51	0
5	DMS	2	5005	4/4	0.96	0.15	1.74	38,38,39,40	0
5	DMS	4	5027	4/4	0.92	0.30	1.71	81,82,82,82	0
5	DMS	1	5021	4/4	0.85	0.30	1.60	70,71,72,72	0
5	DMS	2	5010	4/4	0.94	0.14	1.60	87,87,87,87	0
5	DMS	1	5025	4/4	0.94	0.16	1.49	45,46,47,49	0
5	DMS	4	5004	4/4	0.93	0.13	1.45	53,53,55,55	0
5	DMS	3	5032	4/4	0.96	0.15	1.37	42,43,44,46	0
4	NA	4	3103	1/1	0.94	0.16	1.35	34,34,34,34	0
5	DMS	2	5028	4/4	0.92	0.16	1.31	59,61,61,61	0
5	DMS	1	5003	4/4	0.98	0.12	1.27	38,39,39,39	0
2	149	1	2001	12/12	0.95	0.11	1.20	17,19,21,25	0
5	DMS	2	5003	4/4	0.98	0.15	1.17	38,38,39,40	0
4	NA	3	3103	1/1	0.96	0.20	1.02	42,42,42,42	0
5	DMS	2	5008	4/4	0.95	0.14	0.92	53,54,55,55	0
5	DMS	2	5001	4/4	0.97	0.14	0.89	29,29,30,33	0
5	DMS	3	5005	4/4	0.98	0.12	0.89	43,43,44,45	0
5	DMS	4	5017	4/4	0.91	0.20	0.86	72,73,73,74	0
5	DMS	2	5024	4/4	0.91	0.16	0.78	78,78,78,79	0
2	149	2	2001	12/12	0.96	0.10	0.73	13,15,18,24	0
5	DMS	2	5011	4/4	0.98	0.11	0.70	38,39,39,40	0
5	DMS	4	5005	4/4	0.99	0.15	0.63	36,36,37,38	0
5	DMS	1	5026	4/4	0.98	0.16	0.59	60,61,61,61	0
5	DMS	3	5001	4/4	0.98	0.13	0.54	31,31,31,35	0
2	149	3	2001	12/12	0.96	0.09	0.50	16,19,22,25	0
5	DMS	4	5006	4/4	0.91	0.14	0.45	46,47,48,49	0
5	DMS	1	5012	4/4	0.94	0.17	0.42	61,61,62,62	0
4	NA	2	3103	1/1	0.91	0.13	0.27	29,29,29,29	0
5	DMS	1	5004	4/4	0.93	0.12	0.18	49,50,51,51	0
5	DMS	3	5002	4/4	0.96	0.12	0.18	26,29,30,33	0
5	DMS	4	5001	4/4	0.98	0.11	0.17	28,30,30,33	0
5	DMS	4	5018	4/4	0.94	0.11	0.17	72,72,73,73	0
5	DMS	4	5012	4/4	0.97	0.14	0.10	54,54,54,54	0
4	NA	1	3102	1/1	0.96	0.10	0.08	29,29,29,29	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	149	4	2001	12/12	0.97	0.09	0.05	13,17,19,24	0
5	DMS	1	5018	4/4	0.94	0.17	0.04	68,68,69,69	0
5	DMS	2	5030	4/4	0.97	0.12	0.02	38,39,39,39	0
5	DMS	2	5029	4/4	0.96	0.11	-0.03	56,56,57,57	0
5	DMS	1	5002	4/4	0.95	0.12	-0.07	45,46,46,47	0
5	DMS	1	5005	4/4	0.98	0.10	-0.07	39,39,40,40	0
5	DMS	1	5008	4/4	0.96	0.13	-0.08	46,47,47,48	0
5	DMS	4	5011	4/4	0.98	0.11	-0.18	41,41,42,43	0
4	NA	1	3103	1/1	0.97	0.13	-0.18	47,47,47,47	0
5	DMS	3	5007	4/4	0.92	0.12	-0.21	61,62,62,63	0
4	NA	3	3102	1/1	0.99	0.10	-0.22	24,24,24,24	0
3	MG	1	3001	1/1	0.98	0.09	-0.33	20,20,20,20	0
5	DMS	3	5025	4/4	0.95	0.12	-0.34	76,76,76,76	0
5	DMS	4	5002	4/4	0.97	0.10	-0.38	39,39,39,39	0
4	NA	3	3101	1/1	0.98	0.09	-0.44	20,20,20,20	0
5	DMS	2	5012	4/4	0.97	0.10	-0.44	42,44,44,46	0
5	DMS	3	5011	4/4	0.97	0.10	-0.45	47,49,49,50	0
5	DMS	4	5022	4/4	0.94	0.11	-0.53	61,62,62,62	0
5	DMS	1	5020	4/4	0.95	0.12	-0.62	54,55,55,56	0
4	NA	4	3104	1/1	0.94	0.11	-0.94	41,41,41,41	0
5	DMS	1	5023	4/4	0.97	0.10	-0.95	63,63,64,64	0
4	NA	4	3102	1/1	0.97	0.07	-1.06	20,20,20,20	0
4	NA	2	3104	1/1	0.94	0.08	-1.11	34,34,34,34	0
5	DMS	4	5025	4/4	0.97	0.10	-1.11	57,57,58,58	0
5	DMS	2	5002	4/4	0.98	0.08	-1.16	32,33,34,37	0
4	NA	1	3104	1/1	0.88	0.08	-1.22	55,55,55,55	0
4	NA	3	3104	1/1	0.97	0.07	-1.92	42,42,42,42	0
3	MG	4	3001	1/1	0.98	0.06	-2.48	23,23,23,23	0
4	NA	2	3102	1/1	0.98	0.04	-2.51	18,18,18,18	0
5	DMS	3	5023	4/4	0.99	0.07	-2.69	46,46,47,47	0
3	MG	1	3002	1/1	0.97	0.05	-3.05	24,24,24,24	0
4	NA	4	3101	1/1	0.99	0.05	-3.23	16,16,16,16	0
3	MG	3	3002	1/1	0.99	0.06	-3.41	20,20,20,20	0
3	MG	4	3002	1/1	0.97	0.05	-3.76	25,25,25,25	0
3	MG	2	3002	1/1	0.97	0.04	-3.82	30,30,30,30	0
3	MG	3	3001	1/1	0.96	0.04	-4.21	19,19,19,19	0
4	NA	2	3101	1/1	0.97	0.07	-4.29	18,18,18,18	0
4	NA	1	3101	1/1	0.98	0.05	-4.60	21,21,21,21	0
3	MG	2	3001	1/1	0.98	0.03	-12.71	22,22,22,22	0
5	DMS	3	5019	4/4	0.95	0.19	-	63,63,64,64	0
5	DMS	2	5014	4/4	0.97	0.18	-	48,49,49,49	0
3	MG	2	3003	1/1	0.87	0.13	-	45,45,45,45	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	DMS	2	5016	4/4	0.96	0.30	-	54,54,54,55	0
5	DMS	1	5028	4/4	0.93	0.31	-	65,66,66,66	0
5	DMS	4	5013	4/4	0.90	0.40	-	86,86,86,86	0
5	DMS	4	5014	4/4	0.93	0.25	-	66,67,67,67	0
5	DMS	2	5009	4/4	0.97	0.14	-	56,56,56,56	0
5	DMS	4	5021	4/4	0.97	0.21	-	68,68,68,68	0
5	DMS	1	5024	4/4	0.92	0.16	-	86,86,86,86	0
5	DMS	4	5023	4/4	0.92	0.23	-	90,90,90,91	0
5	DMS	4	5029	4/4	0.97	0.16	-	60,61,61,61	0
3	MG	3	3003	1/1	0.52	0.13	-	78,78,78,78	0
5	DMS	3	5027	4/4	0.89	0.28	-	79,80,80,80	0
5	DMS	3	5015	4/4	0.83	0.38	-	67,67,67,68	0
5	DMS	1	5011	4/4	0.95	0.12	-	47,48,49,50	0
5	DMS	1	5010	4/4	0.91	0.18	-	71,72,72,72	0
5	DMS	3	5013	4/4	0.94	0.17	-	55,56,56,56	0
5	DMS	1	5017	4/4	0.94	0.25	-	61,61,61,62	0
5	DMS	2	5022	4/4	0.96	0.15	-	61,61,61,62	0
5	DMS	4	5019	4/4	0.94	0.18	-	64,64,64,64	0
5	DMS	1	5013	4/4	0.73	0.35	-	96,96,97,97	0
5	DMS	1	5022	4/4	0.93	0.42	-	82,82,82,83	0
5	DMS	1	5019	4/4	0.93	0.25	-	82,83,83,83	0
5	DMS	1	5009	4/4	0.92	0.14	-	55,55,55,56	0
5	DMS	3	5008	4/4	0.96	0.14	-	62,62,63,63	0
5	DMS	2	5019	4/4	0.96	0.21	-	69,70,70,70	0
5	DMS	3	5031	4/4	0.93	0.21	-	58,59,60,60	0
5	DMS	3	5029	4/4	0.83	0.24	-	81,82,82,82	0
5	DMS	1	5014	4/4	0.94	0.13	-	65,65,66,66	0
5	DMS	2	5015	4/4	0.94	0.14	-	56,56,56,57	0
5	DMS	4	5010	4/4	0.91	0.23	-	78,78,78,79	0
5	DMS	3	5012	4/4	0.67	0.33	-	108,108,109,109	0
5	DMS	2	5031	4/4	0.88	0.24	-	61,62,62,63	0
5	DMS	3	5014	4/4	0.86	0.27	-	68,69,70,70	0
5	DMS	4	5016	4/4	0.83	0.23	-	59,59,61,62	0
5	DMS	2	5032	4/4	0.95	0.17	-	54,54,54,54	0
3	MG	4	3003	1/1	0.75	0.22	-	68,68,68,68	0
5	DMS	3	5022	4/4	0.96	0.14	-	66,66,66,66	0
5	DMS	3	5009	4/4	0.89	0.24	-	88,88,89,89	0
5	DMS	4	5009	4/4	0.94	0.12	-	60,60,60,61	0
5	DMS	4	5030	4/4	0.95	0.23	-	58,59,59,60	0
5	DMS	2	5027	4/4	0.96	0.12	-	71,71,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.