



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 06:00 am GMT

PDB ID : 2EXK  
Title : Structure of the family43 beta-Xylosidase E187G from geobacillus stearothermophilus in complex with xylobiose  
Authors : Brux, C.; Niefind, K.; Shallom-Shezifi, D.; Shoham, Y.; Schomburg, D.  
Deposited on : 2005-11-08  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

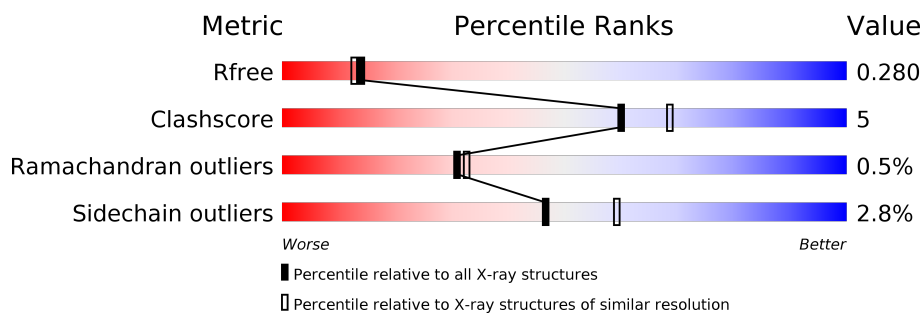
# 1 Overall quality at a glance

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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	535	
1	B	535	
1	C	535	
1	D	535	

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	XYS	A	2005	X	-	-	-
2	XYS	A	2006	X	-	-	-
2	XYS	B	2007	X	-	-	-
2	XYS	B	2008	X	-	-	-
2	XYS	C	2009	X	-	-	-
2	XYS	C	2010	X	-	-	-
2	XYS	D	2011	X	-	-	-
2	XYS	D	2012	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18715 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.

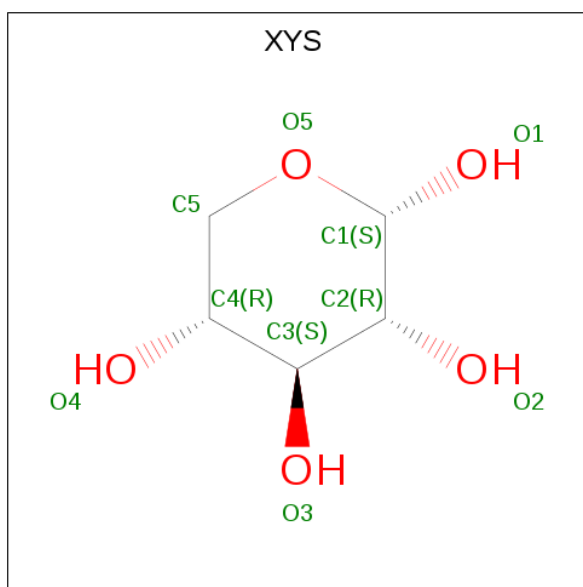
- Molecule 1 is a protein called beta-D-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	B	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	C	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			
1	D	533	Total	C	N	O	S	0	0	0
			4371	2811	748	802	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	ENGINEERED	UNP Q68HB3
A	187	GLY	GLU	ENGINEERED	UNP Q68HB3
B	2	ALA	SER	ENGINEERED	UNP Q68HB3
B	187	GLY	GLU	ENGINEERED	UNP Q68HB3
C	2	ALA	SER	ENGINEERED	UNP Q68HB3
C	187	GLY	GLU	ENGINEERED	UNP Q68HB3
D	2	ALA	SER	ENGINEERED	UNP Q68HB3
D	187	GLY	GLU	ENGINEERED	UNP Q68HB3

- Molecule 2 is XYLOPYRANOSE (three-letter code: YYS) (formula: C<sub>5</sub>H<sub>10</sub>O<sub>5</sub>).

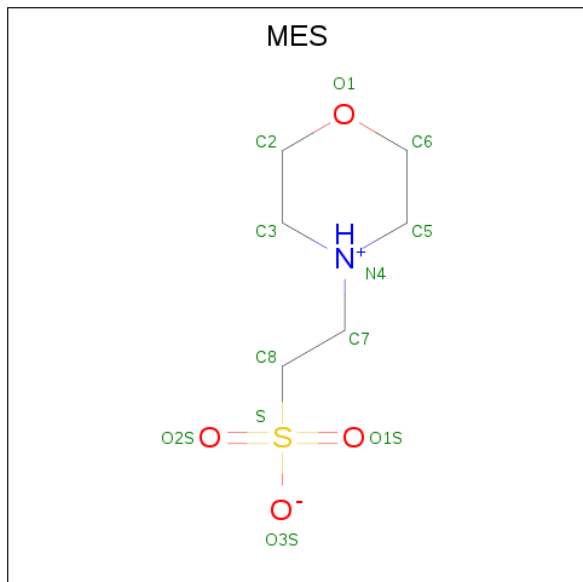


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 9 5 4	0	0
2	A	1	Total C O 10 5 5	0	0
2	B	1	Total C O 9 5 4	0	0
2	B	1	Total C O 10 5 5	0	0
2	C	1	Total C O 9 5 4	0	0
2	C	1	Total C O 10 5 5	0	0
2	D	1	Total C O 9 5 4	0	0
2	D	1	Total C O 10 5 5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

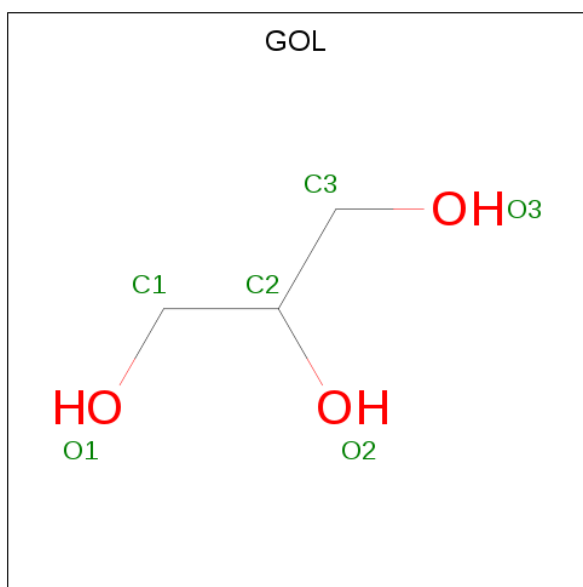
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
4	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

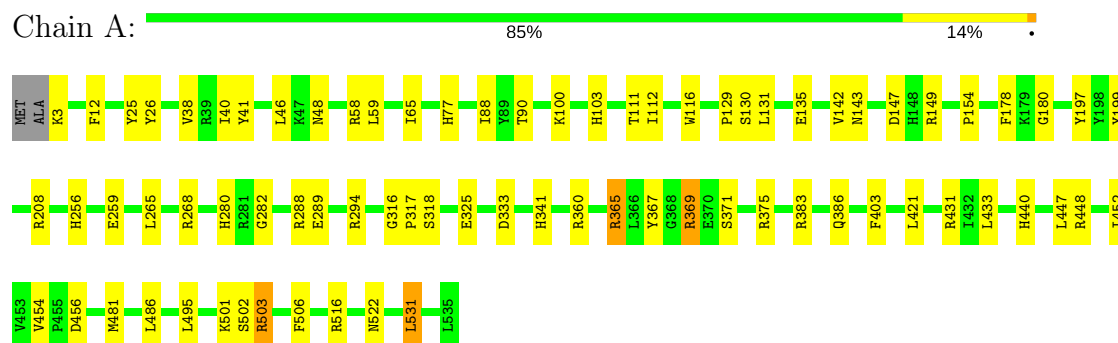
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	325	Total O 325 325	0	0
6	B	361	Total O 361 361	0	0
6	C	140	Total O 140 140	0	0
6	D	265	Total O 265 265	0	0

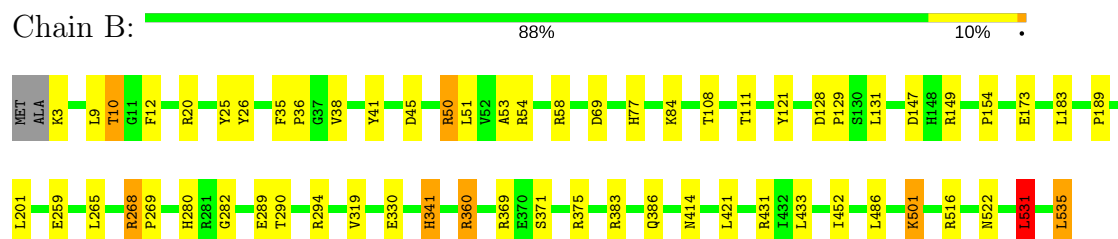
### 3 Residue-property plots [i](#)

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

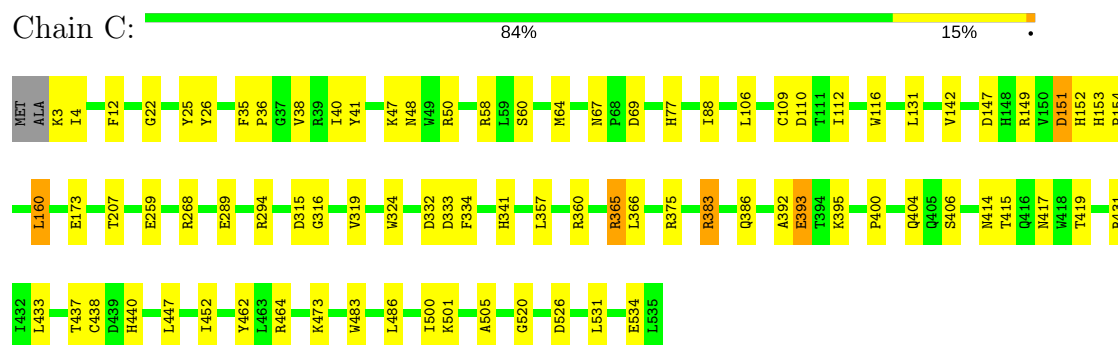
- Molecule 1: beta-D-xylosidase



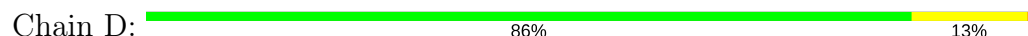
- Molecule 1: beta-D-xylosidase



- Molecule 1: beta-D-xylosidase



- Molecule 1: beta-D-xylosidase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.87Å 139.87Å 232.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	2.23 – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.4 (2.23-2.20) 99.5 (19.99-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.43 (at 2.21Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.185 , 0.238 0.240 , 0.280	Depositor DCC
$R_{free}$ test set	5803 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.0	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 39.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	18715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CA, XYS, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.45	0/4515	0.62	2/6153 (0.0%)
1	B	0.45	0/4515	0.62	2/6153 (0.0%)
1	C	0.72	13/4515 (0.3%)	0.62	3/6153 (0.0%)
1	D	0.44	0/4515	0.60	0/6153
All	All	0.53	13/18060 (0.1%)	0.61	7/24612 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	GLU	CD-OE2	12.34	1.39	1.25
1	C	50	ARG	CZ-NH1	9.67	1.45	1.33
1	C	393	GLU	CD-OE1	9.63	1.36	1.25
1	C	259	GLU	CD-OE1	9.59	1.36	1.25
1	C	383	ARG	CZ-NH1	9.37	1.45	1.33
1	C	319	VAL	C-O	8.28	1.39	1.23
1	C	393	GLU	CG-CD	7.52	1.63	1.51
1	C	393	GLU	CD-OE2	7.19	1.33	1.25
1	C	315	ASP	CG-OD2	6.92	1.41	1.25
1	C	294	ARG	NE-CZ	6.51	1.41	1.33
1	C	386	GLN	CD-OE1	5.73	1.36	1.24
1	C	534	GLU	CD-OE1	5.71	1.31	1.25
1	C	25	TYR	CG-CD2	5.20	1.46	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ARG	NE-CZ-NH2	-10.29	115.15	120.30
1	C	50	ARG	NE-CZ-NH2	-7.57	116.51	120.30
1	B	531	LEU	CA-CB-CG	7.38	132.27	115.30
1	A	531	LEU	CA-CB-CG	6.69	130.69	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	383	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	369	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	B	268	ARG	NE-CZ-NH2	-5.41	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4371	0	4160	48	0
1	B	4371	0	4160	47	0
1	C	4371	0	4160	38	0
1	D	4371	0	4160	41	0
2	A	19	0	16	1	0
2	B	19	0	16	0	0
2	C	19	0	16	2	0
2	D	19	0	16	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	4	0
4	D	12	0	12	2	0
5	A	6	0	8	0	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	325	0	0	11	0
6	B	361	0	0	14	0
6	C	140	0	0	0	0
6	D	265	0	0	5	0
All	All	18715	0	16772	173	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 (173) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:ARG:HH22	1:A:522:ASN:ND2	1.34	1.24
1:A:369:ARG:HH22	1:A:522:ASN:HD22	1.08	1.02
1:B:54:ARG:HE	4:B:2014:MES:H82	1.27	0.98
1:A:369:ARG:NH2	1:A:522:ASN:HD22	1.63	0.97
1:A:369:ARG:NH2	1:A:522:ASN:ND2	2.14	0.95
1:D:255:THR:HG22	1:D:259:GLU:H	1.37	0.88
1:A:503:ARG:HG3	6:A:2241:HOH:O	1.81	0.79
1:A:360:ARG:HB2	1:A:365:ARG:HH12	1.50	0.76
1:A:25:TYR:OH	1:A:256:HIS:HD2	1.70	0.75
1:A:369:ARG:HH22	1:A:522:ASN:HD21	1.32	0.75
1:D:268:ARG:HD3	1:D:289:GLU:OE1	1.86	0.74
1:C:268:ARG:HD3	1:C:289:GLU:OE1	1.87	0.73
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.70	0.73
1:C:77:HIS:CD2	1:C:131:LEU:H	2.07	0.72
1:B:3:LYS:HG3	6:B:2093:HOH:O	1.89	0.71
1:B:53:ALA:HA	4:B:2014:MES:H51	1.71	0.71
1:B:10:THR:CG2	1:B:386:GLN:O	2.40	0.69
1:D:53:ALA:HA	4:D:2015:MES:H81	1.76	0.68
1:B:147:ASP:OD1	1:B:149:ARG:HD3	1.93	0.68
1:A:111:THR:HG21	6:A:2193:HOH:O	1.93	0.68
1:B:10:THR:HG23	1:B:386:GLN:O	1.94	0.68
1:C:58:ARG:NH2	1:C:116:TRP:O	2.26	0.68
1:D:147:ASP:OD1	1:D:149:ARG:HD3	1.94	0.67
1:B:111:THR:HG22	6:B:2101:HOH:O	1.94	0.67
1:D:294:ARG:NH1	1:D:315:ASP:O	2.29	0.66
1:C:3:LYS:HD3	1:C:316:GLY:H	1.62	0.65
1:B:121:TYR:OH	1:C:520:GLY:HA3	1.98	0.64
1:C:40:ILE:HG21	1:C:112:ILE:HD11	1.81	0.63
1:C:433:LEU:HB2	1:C:452:ILE:HB	1.83	0.61
1:B:77:HIS:CD2	1:B:131:LEU:H	2.19	0.61
1:D:433:LEU:HB2	1:D:452:ILE:HB	1.82	0.60
1:A:365:ARG:HD3	1:A:367:TYR:CZ	2.37	0.59
1:A:502:SER:O	1:A:503:ARG:HB2	2.03	0.58
1:C:147:ASP:OD1	1:C:149:ARG:HD3	2.03	0.58
1:B:54:ARG:NE	4:B:2014:MES:H82	2.08	0.57
1:B:58:ARG:NH1	6:B:2032:HOH:O	2.19	0.57
1:D:77:HIS:CD2	1:D:131:LEU:H	2.21	0.57
1:C:365:ARG:HD3	1:C:526:ASP:OD1	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:417:ASN:HA	1:C:438:CYS:O	2.04	0.57
1:B:10:THR:HG22	1:B:386:GLN:HB3	1.87	0.57
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.53	0.57
1:D:435:LEU:HD12	1:D:447:LEU:HD13	1.85	0.56
1:D:255:THR:HG23	1:D:257:THR:H	1.69	0.56
1:A:433:LEU:HB2	1:A:452:ILE:HB	1.88	0.56
1:A:280:HIS:CD2	1:A:282:GLY:H	2.24	0.56
1:D:255:THR:HG22	1:D:259:GLU:N	2.16	0.56
1:C:375:ARG:HG3	1:C:415:THR:HG21	1.88	0.55
1:D:54:ARG:H	4:D:2015:MES:H32	1.71	0.55
1:B:84:LYS:HD3	1:B:108:THR:HB	1.87	0.55
1:D:330:GLU:O	1:D:531:LEU:HA	2.07	0.55
1:A:147:ASP:O	1:A:154:PRO:HA	2.07	0.55
1:C:392:ALA:HA	1:C:531:LEU:O	2.08	0.54
1:D:178:PHE:CE2	1:D:180:GLY:HA2	2.43	0.54
1:A:147:ASP:OD1	1:A:149:ARG:HD3	2.08	0.54
1:A:383:ARG:HD2	6:A:2164:HOH:O	2.06	0.54
1:B:50:ARG:HH11	1:B:50:ARG:HB3	1.73	0.54
1:A:58:ARG:NH2	1:A:116:TRP:O	2.31	0.53
1:C:334:PHE:HB3	1:C:357:LEU:HD22	1.89	0.53
1:D:147:ASP:O	1:D:154:PRO:HA	2.08	0.53
1:C:393:GLU:HG3	1:C:464:ARG:HB2	1.90	0.53
1:A:208:ARG:CZ	6:A:2241:HOH:O	2.55	0.53
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.08	0.53
1:B:280:HIS:HE1	6:B:2194:HOH:O	1.91	0.53
1:D:3:LYS:HD3	1:D:316:GLY:H	1.73	0.53
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.44	0.52
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.92	0.52
1:B:58:ARG:NH2	6:B:2032:HOH:O	2.36	0.52
1:A:448:ARG:NH2	6:A:2269:HOH:O	2.42	0.52
1:B:433:LEU:HB3	1:B:452:ILE:HB	1.91	0.52
1:B:369:ARG:NH2	1:B:522:ASN:OD1	2.43	0.51
1:D:151:ASP:HB3	6:D:2159:HOH:O	2.09	0.51
1:B:375:ARG:NH2	6:B:2171:HOH:O	2.43	0.51
1:A:421:LEU:HD13	1:A:486:LEU:HD13	1.92	0.51
1:B:9:LEU:HB2	1:B:290:THR:HB	1.91	0.51
1:A:365:ARG:HH11	1:A:365:ARG:HB2	1.75	0.51
1:A:431:ARG:HD2	6:A:2092:HOH:O	2.10	0.51
1:C:4:ILE:HG12	1:C:47:LYS:HB2	1.93	0.50
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.93	0.50
1:C:395:LYS:HD2	1:C:462:TYR:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:184:ARG:HD3	6:D:2161:HOH:O	2.10	0.49
1:C:142:VAL:HG13	1:C:160:LEU:HD12	1.93	0.49
1:C:334:PHE:HB3	1:C:357:LEU:CD2	2.43	0.49
1:B:421:LEU:HD13	1:B:486:LEU:HD13	1.93	0.49
1:C:147:ASP:O	1:C:154:PRO:HA	2.11	0.49
6:B:2063:HOH:O	1:C:404:GLN:HG2	2.13	0.48
1:A:375:ARG:NH2	6:A:2142:HOH:O	2.46	0.48
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.96	0.48
2:A:2005:XYS:O4	6:A:2136:HOH:O	2.19	0.48
1:D:216:ALA:HB1	1:D:225:TYR:HB3	1.96	0.48
1:A:3:LYS:HB3	1:A:316:GLY:H	1.80	0.47
1:C:207:THR:N	2:C:2010:XYS:O3	2.47	0.47
1:D:259:GLU:OE1	1:D:294:ARG:NH2	2.47	0.47
1:A:383:ARG:NH2	1:A:386:GLN:OE1	2.47	0.47
1:A:501:LYS:HE2	6:A:2076:HOH:O	2.14	0.47
1:D:189:PRO:HA	1:D:201:LEU:O	2.14	0.47
1:B:20:ARG:HG3	1:B:25:TYR:CE1	2.49	0.47
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.97	0.47
1:A:440:HIS:NE2	1:A:501:LYS:HG2	2.30	0.47
1:A:40:ILE:HG21	1:A:112:ILE:HD11	1.97	0.46
1:A:288:ARG:NH2	1:A:506:PHE:HB3	2.30	0.46
1:B:421:LEU:HD13	1:B:486:LEU:CD1	2.45	0.46
1:D:126:GLY:HA3	1:D:144:MET:O	2.16	0.46
1:A:130:SER:HB3	1:A:142:VAL:HG23	1.97	0.46
1:A:403:PHE:O	1:D:148:HIS:HE1	1.99	0.46
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.63	0.46
1:A:90:THR:HA	1:A:103:HIS:O	2.15	0.46
1:B:54:ARG:H	4:B:2014:MES:H51	1.80	0.46
1:C:26:TYR:HA	1:C:41:TYR:O	2.15	0.46
1:C:151:ASP:OD2	1:C:152:HIS:CE1	2.69	0.46
1:B:189:PRO:HA	1:B:201:LEU:O	2.16	0.46
1:B:51:LEU:HD23	1:B:341:HIS:CG	2.51	0.46
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.37	0.46
1:D:250:ALA:HA	1:D:263:VAL:O	2.15	0.46
1:B:371:SER:HA	1:B:516:ARG:HD3	1.98	0.45
1:B:501:LYS:HD2	6:B:2075:HOH:O	2.15	0.45
1:D:69:ASP:CG	1:D:414:ASN:HB2	2.36	0.45
1:A:197:TYR:HB2	1:A:199:TYR:CE1	2.52	0.45
1:A:265:LEU:HA	1:A:289:GLU:O	2.16	0.45
1:B:360:ARG:HD3	6:B:2257:HOH:O	2.16	0.45
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PRO:HA	1:A:143:ASN:HB3	1.98	0.44
1:A:88:ILE:HG21	1:A:129:PRO:HB2	1.98	0.44
1:B:26:TYR:HA	1:B:41:TYR:O	2.18	0.44
1:A:280:HIS:HD2	1:A:282:GLY:H	1.63	0.44
1:A:447:LEU:HD11	1:A:486:LEU:HD22	2.00	0.44
1:D:391:VAL:CG2	1:D:464:ARG:HD2	2.48	0.44
1:B:259:GLU:OE1	1:B:294:ARG:NH2	2.47	0.44
1:B:535:LEU:HD11	6:B:2097:HOH:O	2.17	0.44
1:A:259:GLU:OE1	1:A:294:ARG:NH2	2.43	0.43
1:B:3:LYS:CE	6:B:2118:HOH:O	2.65	0.43
1:D:448:ARG:HA	1:D:449:GLY:HA2	1.83	0.43
1:B:501:LYS:NZ	6:B:2192:HOH:O	2.51	0.43
1:C:48:ASN:HB3	1:C:324:TRP:CD1	2.53	0.43
1:B:265:LEU:HA	1:B:289:GLU:O	2.18	0.43
1:B:3:LYS:HE3	6:B:2118:HOH:O	2.18	0.43
1:A:48:ASN:HB3	6:A:2236:HOH:O	2.18	0.43
1:D:393:GLU:OE1	1:D:464:ARG:HD3	2.18	0.43
1:C:88:ILE:HD13	1:C:106:LEU:HD13	2.01	0.43
1:C:440:HIS:NE2	1:C:501:LYS:HD3	2.34	0.43
1:A:77:HIS:CD2	1:A:131:LEU:H	2.37	0.42
1:B:69:ASP:CG	1:B:414:ASN:HB2	2.38	0.42
1:C:500:ILE:HB	1:C:505:ALA:HB2	2.00	0.42
1:D:389:HIS:HD2	6:D:2250:HOH:O	2.01	0.42
1:B:45:ASP:HA	1:B:319:VAL:HG21	2.01	0.42
1:C:35:PHE:CG	1:C:36:PRO:HA	2.54	0.42
1:C:3:LYS:HD3	1:C:316:GLY:N	2.31	0.42
1:C:77:HIS:HD2	1:C:131:LEU:H	1.64	0.42
1:D:440:HIS:NE2	1:D:501:LYS:HG2	2.35	0.42
1:D:417:ASN:HA	1:D:438:CYS:O	2.20	0.42
1:A:365:ARG:HD3	1:A:367:TYR:CE2	2.55	0.42
1:A:26:TYR:HA	1:A:41:TYR:O	2.20	0.42
1:B:330:GLU:O	1:B:531:LEU:HA	2.20	0.42
1:C:419:THR:HG22	1:C:437:THR:HG22	2.02	0.42
1:C:64:MET:O	1:C:67:ASN:HB2	2.20	0.42
1:C:109:CYS:HB2	1:C:116:TRP:CD2	2.55	0.41
1:B:147:ASP:O	1:B:154:PRO:HA	2.20	0.41
1:C:207:THR:HG22	2:C:2010:XYS:H3	2.02	0.41
1:A:371:SER:HA	1:A:516:ARG:HD3	2.03	0.41
1:D:50:ARG:HA	6:D:2129:HOH:O	2.20	0.41
1:C:153:HIS:HA	1:C:154:PRO:HD3	1.95	0.41
1:D:265:LEU:HD12	1:D:265:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ASP:N	1:B:129:PRO:CD	2.84	0.41
1:D:77:HIS:CD2	6:D:2055:HOH:O	2.74	0.41
1:B:35:PHE:CG	1:B:36:PRO:HA	2.55	0.41
1:D:130:SER:HB3	1:D:142:VAL:HG23	2.02	0.41
1:B:280:HIS:CD2	1:B:282:GLY:H	2.39	0.40
1:C:462:TYR:HB3	1:C:483:TRP:CH2	2.56	0.40
1:D:26:TYR:HA	1:D:41:TYR:O	2.21	0.40
1:D:32:PHE:CE2	1:D:74:TRP:CD1	3.10	0.40
1:A:111:THR:HG22	6:A:2183:HOH:O	2.22	0.40
1:D:369:ARG:NH2	1:D:522:ASN:OD1	2.41	0.40
1:B:50:ARG:HD2	6:B:2083:HOH:O	2.20	0.40
1:D:269:PRO:HB3	1:D:282:GLY:HA3	2.03	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	A	531/535 (99%)	505 (95%)	23 (4%)	3 (1%)	27	28
1	B	531/535 (99%)	508 (96%)	21 (4%)	2 (0%)	36	39
1	C	531/535 (99%)	503 (95%)	25 (5%)	3 (1%)	27	28
1	D	531/535 (99%)	501 (94%)	28 (5%)	2 (0%)	36	39
All	All	2124/2140 (99%)	2017 (95%)	97 (5%)	10 (0%)	31	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	38	VAL
1	B	12	PHE

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Mol	Chain	Res	Type
1	B	38	VAL
1	C	12	PHE
1	C	38	VAL
1	D	38	VAL
1	C	22	GLY
1	D	12	PHE
1	A	318	SER

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	468/469 (100%)	454 (97%)	14 (3%)	44	56
1	B	468/469 (100%)	457 (98%)	11 (2%)	52	65
1	C	468/469 (100%)	452 (97%)	16 (3%)	40	50
1	D	468/469 (100%)	457 (98%)	11 (2%)	52	65
All	All	1872/1876 (100%)	1820 (97%)	52 (3%)	47	59

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	65	ILE
1	A	100	LYS
1	A	135	GLU
1	A	268	ARG
1	A	325	GLU
1	A	333	ASP
1	A	341	HIS
1	A	365	ARG
1	A	456	ASP
1	A	481	MET
1	A	495	LEU
1	A	503	ARG
1	A	531	LEU

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Mol	Chain	Res	Type
1	B	10	THR
1	B	50	ARG
1	B	173	GLU
1	B	183	LEU
1	B	341	HIS
1	B	360	ARG
1	B	383	ARG
1	B	431	ARG
1	B	501	LYS
1	B	531	LEU
1	B	535	LEU
1	C	60	SER
1	C	110	ASP
1	C	151	ASP
1	C	160	LEU
1	C	173	GLU
1	C	332	ASP
1	C	333	ASP
1	C	341	HIS
1	C	360	ARG
1	C	365	ARG
1	C	366	LEU
1	C	383	ARG
1	C	406	SER
1	C	447	LEU
1	C	473	LYS
1	C	486	LEU
1	D	65	ILE
1	D	166	GLU
1	D	184	ARG
1	D	255	THR
1	D	333	ASP
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	431	ARG
1	D	448	ARG
1	D	486	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	210	ASN
1	A	254	HIS
1	A	256	HIS
1	A	280	HIS
1	A	422	GLN
1	A	522	ASN
1	B	77	HIS
1	B	254	HIS
1	B	280	HIS
1	C	77	HIS
1	C	152	HIS
1	C	195	ASN
1	C	254	HIS
1	C	280	HIS
1	C	411	ASN
1	C	422	GLN
1	D	77	HIS
1	D	280	HIS
1	D	422	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	XYS	A	2005	2	9,9,10	1.03	1 (11%)	10,12,14	1.41	1 (10%)
2	XYS	A	2006	2	10,10,10	2.44	4 (40%)	14,14,14	2.82	6 (42%)
4	MES	A	2013	-	12,12,12	1.81	3 (25%)	14,16,16	6.63	10 (71%)
5	GOL	A	2016	-	5,5,5	0.45	0	5,5,5	0.53	0
2	XYS	B	2007	2	9,9,10	1.22	1 (11%)	10,12,14	2.14	3 (30%)
2	XYS	B	2008	2	10,10,10	1.99	3 (30%)	14,14,14	1.94	3 (21%)
4	MES	B	2014	-	12,12,12	1.99	3 (25%)	14,16,16	7.11	9 (64%)
5	GOL	B	2017	-	5,5,5	0.38	0	5,5,5	0.32	0
2	XYS	C	2009	2	9,9,10	1.27	1 (11%)	10,12,14	1.02	1 (10%)
2	XYS	C	2010	2	10,10,10	1.95	3 (30%)	14,14,14	1.71	2 (14%)
5	GOL	C	2018	-	5,5,5	0.30	0	5,5,5	0.29	0
2	XYS	D	2011	2	9,9,10	0.97	0	10,12,14	1.29	2 (20%)
2	XYS	D	2012	2	10,10,10	2.19	3 (30%)	14,14,14	1.45	3 (21%)
4	MES	D	2015	-	12,12,12	3.88	4 (33%)	14,16,16	6.68	9 (64%)
5	GOL	D	2019	-	5,5,5	0.34	0	5,5,5	0.36	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	XYS	A	2005	2	3/3/3/4	0/0/14/17	0/1/1/1
2	XYS	A	2006	2	1/1/4/4	0/0/17/17	0/1/1/1
4	MES	A	2013	-	-	0/6/14/14	0/1/1/1
5	GOL	A	2016	-	-	0/4/4/4	0/0/0/0
2	XYS	B	2007	2	3/3/3/4	0/0/14/17	0/1/1/1
2	XYS	B	2008	2	1/1/4/4	0/0/17/17	0/1/1/1
4	MES	B	2014	-	-	0/6/14/14	0/1/1/1
5	GOL	B	2017	-	-	0/4/4/4	0/0/0/0
2	XYS	C	2009	2	3/3/3/4	0/0/14/17	0/1/1/1
2	XYS	C	2010	2	1/1/4/4	0/0/17/17	0/1/1/1
5	GOL	C	2018	-	-	0/4/4/4	0/0/0/0
2	XYS	D	2011	2	3/3/3/4	0/0/14/17	0/1/1/1
2	XYS	D	2012	2	1/1/4/4	0/0/17/17	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	D	2015	-	-	0/6/14/14	0/1/1/1
5	GOL	D	2019	-	-	0/4/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2005	XYS	C4-C3	2.00	1.55	1.52
4	A	2013	MES	O2S-S	2.03	1.51	1.45
2	A	2006	XYS	O1-C1	2.12	1.46	1.39
2	B	2007	XYS	C4-C3	2.18	1.55	1.52
2	A	2006	XYS	O5-C5	2.25	1.47	1.43
4	B	2014	MES	O2S-S	2.27	1.51	1.45
2	C	2010	XYS	O5-C5	2.32	1.47	1.43
2	C	2009	XYS	O5-C5	2.32	1.47	1.42
2	D	2012	XYS	C4-C3	2.35	1.56	1.52
2	B	2008	XYS	O4-C4	2.48	1.48	1.43
4	A	2013	MES	O1S-S	2.65	1.52	1.45
2	C	2010	XYS	O4-C4	2.67	1.49	1.43
4	B	2014	MES	O1S-S	2.75	1.53	1.45
2	D	2012	XYS	O4-C4	2.83	1.49	1.43
2	B	2008	XYS	O5-C5	2.83	1.48	1.43
2	A	2006	XYS	O4-C4	3.20	1.50	1.43
2	C	2010	XYS	O5-C1	3.64	1.48	1.43
2	B	2008	XYS	O5-C1	4.07	1.48	1.43
2	D	2012	XYS	O5-C1	4.67	1.49	1.43
4	D	2015	MES	O2S-S	4.75	1.59	1.45
4	A	2013	MES	C8-S	4.92	1.84	1.77
4	D	2015	MES	O3S-S	4.94	1.65	1.47
4	B	2014	MES	C8-S	5.35	1.85	1.77
2	A	2006	XYS	O5-C1	5.60	1.51	1.43
4	D	2015	MES	C8-S	7.01	1.87	1.77
4	D	2015	MES	O1S-S	8.87	1.71	1.45

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2015	MES	O3S-S-C8	-14.05	83.04	105.77
4	B	2014	MES	O3S-S-C8	-13.80	83.45	105.77
4	A	2013	MES	O3S-S-O2S	-12.18	81.50	111.27
4	A	2013	MES	O3S-S-C8	-12.00	86.36	105.77
4	D	2015	MES	O3S-S-O1S	-11.91	82.16	111.27
4	D	2015	MES	O3S-S-O2S	-11.46	83.28	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2014	MES	O3S-S-O2S	-11.22	83.87	111.27
4	B	2014	MES	O3S-S-O1S	-10.86	84.74	111.27
4	A	2013	MES	O3S-S-O1S	-10.17	86.44	111.27
2	A	2006	XYS	O5-C5-C4	-3.56	105.23	110.78
2	A	2006	XYS	C5-C4-C3	-3.54	105.18	109.66
4	A	2013	MES	O1-C6-C5	-2.69	105.89	111.81
2	D	2011	XYS	O2-C2-C1	-2.03	105.08	109.17
2	B	2008	XYS	O1-C1-O5	2.08	115.32	109.74
4	B	2014	MES	O1-C6-C5	2.11	116.44	111.81
2	A	2006	XYS	C5-O5-C1	2.11	116.46	112.80
2	B	2007	XYS	C1-C2-C3	2.22	112.47	109.66
2	D	2012	XYS	O5-C1-C2	2.24	112.31	109.31
2	C	2009	XYS	C5-O5-C1	2.37	115.18	111.55
2	D	2012	XYS	O4-C4-C3	2.49	115.04	110.19
4	A	2013	MES	C7-N4-C3	2.51	117.79	111.24
2	C	2010	XYS	O5-C1-C2	2.65	112.86	109.31
4	A	2013	MES	O2S-S-O1S	2.74	123.42	113.95
4	A	2013	MES	C7-N4-C5	2.74	118.39	111.24
2	D	2011	XYS	C5-C4-C3	2.75	113.14	109.66
4	B	2014	MES	C7-N4-C3	2.85	118.67	111.24
4	D	2015	MES	C7-N4-C5	3.06	119.23	111.24
2	A	2006	XYS	O4-C4-C5	3.09	115.40	109.17
4	D	2015	MES	O2S-S-O1S	3.22	125.10	113.95
4	D	2015	MES	C7-N4-C3	3.37	120.03	111.24
2	D	2012	XYS	O4-C4-C5	3.42	116.07	109.17
2	B	2008	XYS	O5-C5-C4	3.71	116.57	110.78
4	B	2014	MES	C7-N4-C5	3.78	121.09	111.24
2	A	2005	XYS	C5-C4-C3	3.83	114.51	109.66
2	B	2007	XYS	C4-C3-C2	4.19	115.73	110.86
2	B	2007	XYS	C5-C4-C3	4.66	115.56	109.66
2	C	2010	XYS	O4-C4-C5	4.83	118.91	109.17
2	B	2008	XYS	O4-C4-C3	4.86	119.67	110.19
2	A	2006	XYS	O4-C4-C3	5.06	120.05	110.19
4	B	2014	MES	C5-N4-C3	5.13	120.20	108.87
4	D	2015	MES	C5-N4-C3	5.36	120.73	108.87
2	A	2006	XYS	O5-C1-C2	6.27	117.72	109.31
4	D	2015	MES	O1S-S-C8	6.71	115.00	106.92
4	A	2013	MES	C5-N4-C3	6.76	123.82	108.87
4	D	2015	MES	O2S-S-C8	6.92	115.25	106.92
4	A	2013	MES	O1S-S-C8	7.65	116.13	106.92
4	A	2013	MES	O2S-S-C8	9.14	117.92	106.92
4	B	2014	MES	O1S-S-C8	10.01	118.97	106.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2014	MES	O2S-S-C8	10.62	119.70	106.92

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2012	XYS	C1
2	D	2011	XYS	C2
2	D	2011	XYS	C3
2	D	2011	XYS	C4
2	C	2010	XYS	C1
2	A	2006	XYS	C1
2	A	2005	XYS	C2
2	A	2005	XYS	C3
2	A	2005	XYS	C4
2	B	2008	XYS	C1
2	B	2007	XYS	C2
2	B	2007	XYS	C3
2	B	2007	XYS	C4
2	C	2009	XYS	C2
2	C	2009	XYS	C3
2	C	2009	XYS	C4

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2005	XYS	1	0
4	B	2014	MES	4	0
2	C	2010	XYS	2	0
4	D	2015	MES	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.