



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:49 PM 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 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

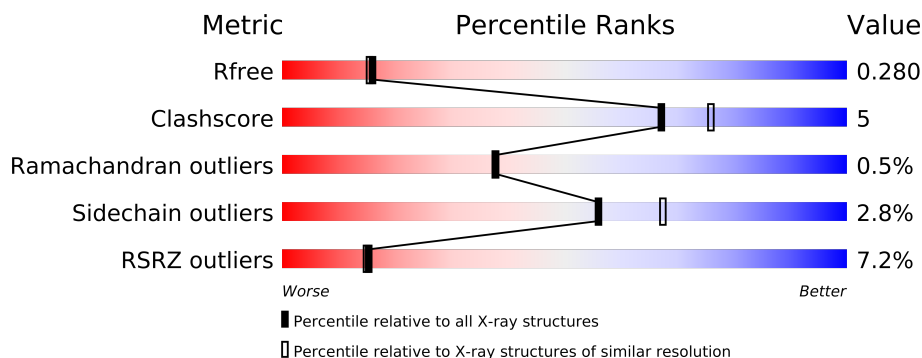
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MES	B	2014	-	X
4	MES	D	2015	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18715 atoms, of which 0 are hydrogen and 0 are deuterium.

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 a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	2	Total	C	O	0	0
			19	10	9		
2	B	2	Total	C	O	0	0
			19	10	9		
2	C	2	Total	C	O	0	0
			19	10	9		
2	D	2	Total	C	O	0	0
			19	10	9		

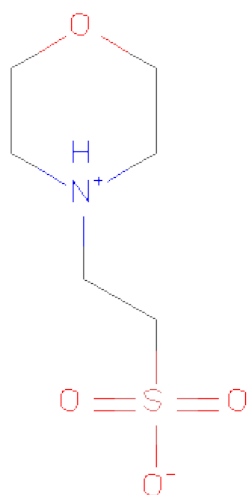
There are 8 discrepancies between the modelled and reference sequences:

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

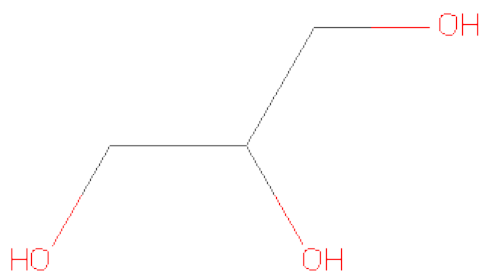
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

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

*Continued on next page...*

*Continued from previous page...*

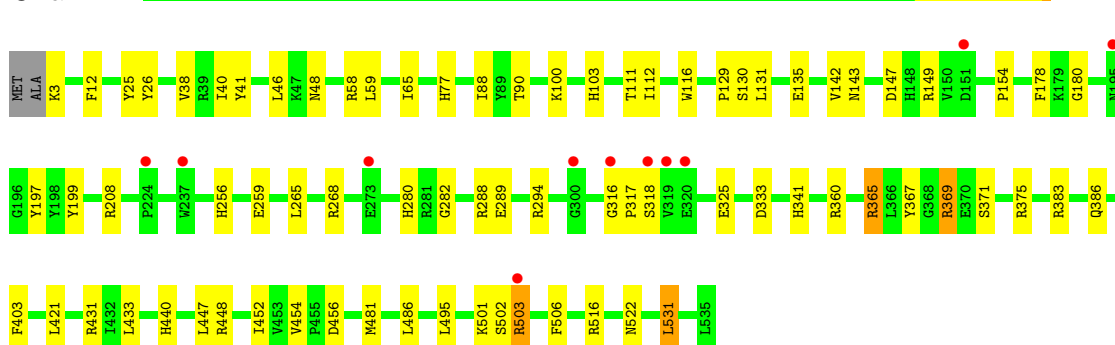
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	265	Total 265	O 265	0	0

### 3 Residue-property plots

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.

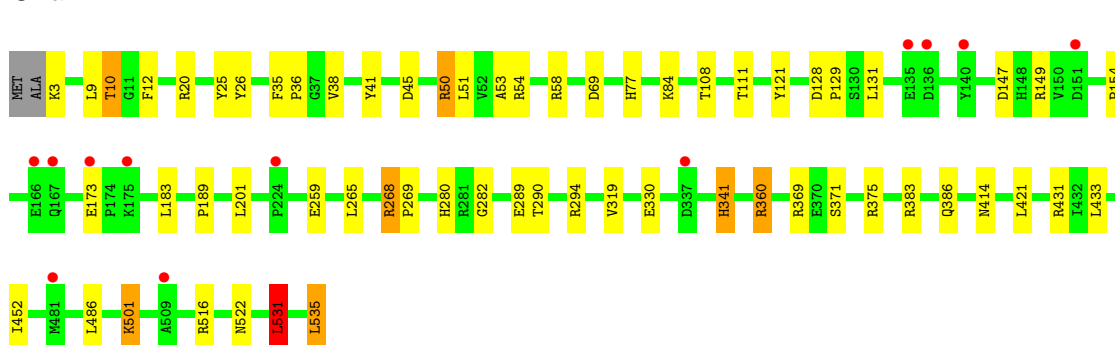
- Molecule 1: beta-D-xylosidase

Chain A:



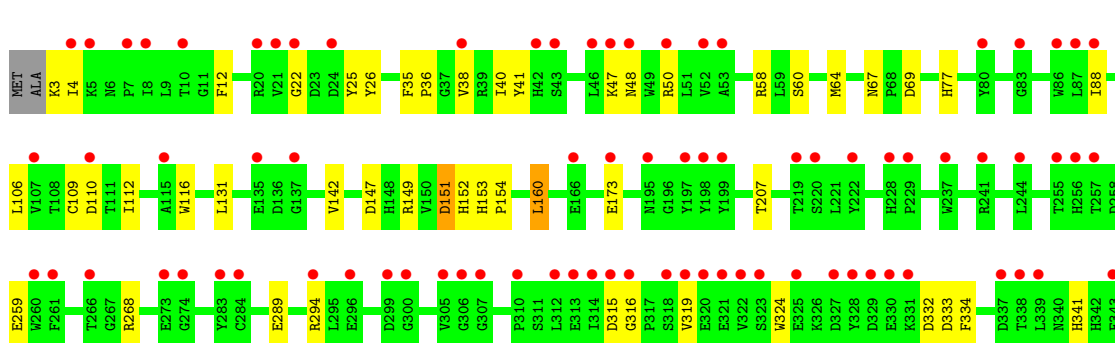
- Molecule 1: beta-D-xylosidase

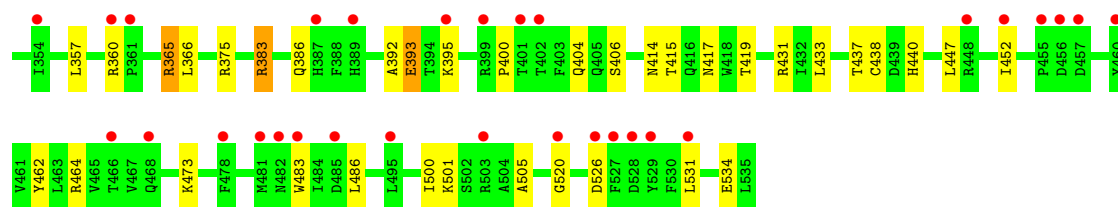
Chain B:



- Molecule 1: beta-D-xylosidase

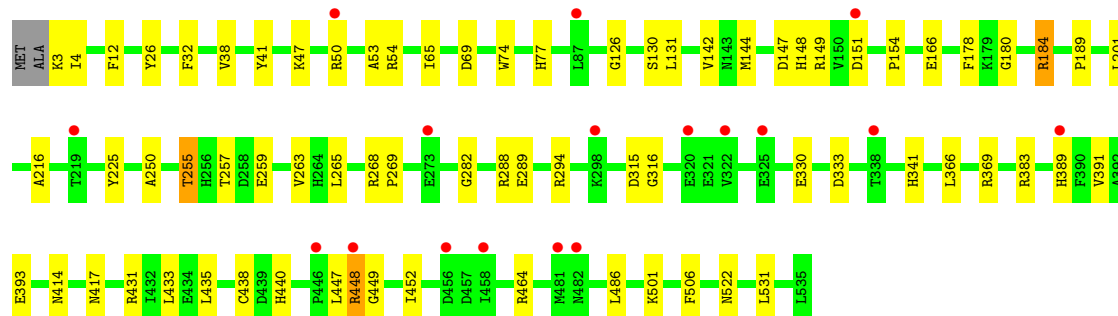
Chain C:





• Molecule 1: beta-D-xylosidase

Chain D:





## 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 5.2.0005	Depositor
R, $R_{free}$	0.185 , 0.238 0.240 , 0.280	Depositor DCC
$R_{free}$ test set	5800 reflections (5.01%)	DCC
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 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 115793 reflections	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.

## 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%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A	4	0
2	B	4	0
2	C	4	0
2	D	4	0
All	All	16	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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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
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

All (16) chirality outliers are listed below:

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

There are no planarity outliers.

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (173) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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:369:ARG:HH22	1:A:522:ASN:HD21	1.32	0.75
1:A:25:TYR:OH	1:A:256:HIS:HD2	1.70	0.75
1:D:268:ARG:HD3	1:D:289:GLU:OE1	1.86	0.74
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.70	0.73
1:C:268:ARG:HD3	1:C:289:GLU:OE1	1.87	0.73
1:C:77:HIS:CD2	1:C:131:LEU:H	2.07	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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:D:255:THR:HG22	1:D:259:GLU:N	2.16	0.56
1:A:280:HIS:CD2	1:A:282:GLY:H	2.24	0.56
1:D:54:ARG:H	4:D:2015:MES:H32	1.71	0.55
1:C:375:ARG:HG3	1:C:415:THR:HG21	1.88	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:B:50:ARG:HH11	1:B:50:ARG:HB3	1.73	0.54
1:A:383:ARG:HD2	6:A:2164:HOH:O	2.06	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:147:ASP:O	1:D:154:PRO:HA	2.08	0.53
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: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:280:HIS:HE1	6:B:2194:HOH:O	1.91	0.53
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.08	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
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:C:147:ASP:O	1:C:154:PRO:HA	2.11	0.49
1:B:421:LEU:HD13	1:B:486:LEU:HD13	1.93	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:C:207:THR:N	2:C:2010:XYS:O3	2.47	0.47
1:A:3:LYS:HB3	1:A:316:GLY:H	1.80	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:421:LEU:HD13	1:B:486:LEU:CD1	2.45	0.46
1:A:40:ILE:HG21	1:A:112:ILE:HD11	1.97	0.46
1:D:126:GLY:HA3	1:D:144:MET:O	2.16	0.46
1:A:288:ARG:NH2	1:A:506:PHE:HB3	2.30	0.46
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.63	0.46
1:A:403:PHE:O	1:D:148:HIS:HE1	1.99	0.46
1:A:130:SER:HB3	1:A:142:VAL:HG23	1.97	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:51:LEU:HD23	1:B:341:HIS:CG	2.51	0.46
1:B:189:PRO:HA	1:B:201:LEU:O	2.16	0.46
1:D:250:ALA:HA	1:D:263:VAL:O	2.15	0.46
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.37	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
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:B:3:LYS:CE	6:B:2118:HOH:O	2.65	0.43
1:A:259:GLU:OE1	1:A:294:ARG:NH2	2.43	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:3:LYS:HE3	6:B:2118:HOH:O	2.18	0.43
1:B:265:LEU:HA	1:B:289:GLU:O	2.18	0.43
1:D:393:GLU:OE1	1:D:464:ARG:HD3	2.18	0.43
1:A:48:ASN:HB3	6:A:2236:HOH:O	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:389:HIS:HD2	6:D:2250:HOH:O	2.01	0.42
1:C:500:ILE:HB	1:C:505:ALA:HB2	2.00	0.42
1:B:69:ASP:CG	1:B:414:ASN:HB2	2.38	0.42
1:B:45:ASP:HA	1:B:319:VAL:HG21	2.01	0.42
1:C:3:LYS:HD3	1:C:316:GLY:N	2.31	0.42
1:C:35:PHE:CG	1:C:36:PRO:HA	2.54	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:B:330:GLU:O	1:B:531:LEU:HA	2.20	0.42
1:A:26:TYR:HA	1:A:41:TYR:O	2.20	0.42
1:C:64:MET:O	1:C:67:ASN:HB2	2.20	0.42
1:C:419:THR:HG22	1:C:437:THR:HG22	2.02	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:D:50:ARG:HA	6:D:2129:HOH:O	2.20	0.41
1:A:371:SER:HA	1:A:516:ARG:HD3	2.03	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
1:D:77:HIS:CD2	6:D:2055:HOH:O	2.74	0.41
1:B:128:ASP:N	1:B:129:PRO:CD	2.84	0.41
1:D:130:SER:HB3	1:D:142:VAL:HG23	2.02	0.41
1:B:35:PHE:CG	1:B:36:PRO:HA	2.55	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:32:PHE:CE2	1:D:74:TRP:CD1	3.10	0.40
1:D:26:TYR:HA	1:D:41:TYR:O	2.21	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

### 5.3.1 Protein backbone ⓘ

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



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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	531/535 (99%)	505 (95%)	23 (4%)	3 (1%)	33	32
1	B	531/535 (99%)	508 (96%)	21 (4%)	2 (0%)	43	45
1	C	531/535 (99%)	503 (95%)	25 (5%)	3 (1%)	33	32
1	D	531/535 (99%)	501 (94%)	28 (5%)	2 (0%)	43	45
All	All	2124/2140 (99%)	2017 (95%)	97 (5%)	10 (0%)	38	38

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	38	VAL
1	B	12	PHE
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%)	53	64
1	B	468/469 (100%)	457 (98%)	11 (2%)	61	73
1	C	468/469 (100%)	452 (97%)	16 (3%)	49	59
1	D	468/469 (100%)	457 (98%)	11 (2%)	61	73
All	All	1872/1876 (100%)	1820 (97%)	52 (3%)	56	67

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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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 ⓘ

There are no RNA chains 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 ⓘ

8 carbohydrates are modelled in this entry.

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	8,9,10	1.03	1 (12%)	8,12,14	1.76	2 (25%)
2	XYS	A	2006	2	10,10,10	2.32	3 (30%)	14,14,14	2.77	5 (35%)
2	XYS	B	2007	2	8,9,10	1.16	1 (12%)	8,12,14	2.11	2 (25%)
2	XYS	B	2008	2	10,10,10	1.90	3 (30%)	14,14,14	1.93	2 (14%)
2	XYS	C	2009	2	8,9,10	1.07	0	8,12,14	0.63	0
2	XYS	C	2010	2	10,10,10	1.89	3 (30%)	14,14,14	1.67	2 (14%)
2	XYS	D	2011	2	8,9,10	0.86	0	8,12,14	1.36	1 (12%)
2	XYS	D	2012	2	10,10,10	2.11	3 (30%)	14,14,14	1.42	3 (21%)

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
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
2	XYS	C	2009	2	3/3/3/4	0/0/14/17	1/1/1/1
2	XYS	C	2010	2	1/1/4/4	0/0/17/17	0/1/1/1
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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2006	XYS	O5-C1	5.29	1.51	1.43
2	D	2012	XYS	O5-C1	4.43	1.49	1.43
2	B	2008	XYS	O5-C1	3.87	1.48	1.43
2	C	2010	XYS	O5-C1	3.47	1.48	1.43
2	A	2006	XYS	O4-C4	3.00	1.50	1.43
2	B	2008	XYS	O5-C5	2.79	1.48	1.43
2	D	2012	XYS	O4-C4	2.65	1.49	1.43
2	C	2010	XYS	O4-C4	2.50	1.49	1.43
2	D	2012	XYS	C4-C3	2.48	1.56	1.52
2	B	2008	XYS	O4-C4	2.32	1.48	1.43
2	B	2007	XYS	C4-C3	2.29	1.55	1.52
2	C	2010	XYS	O5-C5	2.28	1.47	1.43
2	A	2006	XYS	O5-C5	2.21	1.47	1.43
2	A	2005	XYS	C4-C3	2.11	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2006	XYS	O5-C1-C2	5.92	117.72	109.24
2	A	2006	XYS	O4-C4-C3	5.06	120.05	110.23
2	B	2008	XYS	O4-C4-C3	4.86	119.67	110.23
2	C	2010	XYS	O4-C4-C5	4.72	118.91	109.14
2	B	2007	XYS	C5-C4-C3	4.65	115.56	109.71
2	A	2005	XYS	C5-C4-C3	3.81	114.51	109.71
2	B	2008	XYS	O5-C5-C4	3.60	116.57	110.83
2	B	2007	XYS	C4-C3-C2	3.60	115.73	110.53
2	A	2006	XYS	C5-C4-C3	-3.59	105.18	109.71
2	A	2006	XYS	O5-C5-C4	-3.51	105.23	110.83
2	D	2012	XYS	O4-C4-C5	3.35	116.07	109.14
2	A	2006	XYS	O4-C4-C5	3.03	115.40	109.14
2	D	2011	XYS	C5-C4-C3	2.72	113.14	109.71
2	A	2005	XYS	O5-C5-C4	-2.63	107.60	111.74
2	C	2010	XYS	O5-C1-C2	2.53	112.86	109.24
2	D	2012	XYS	O4-C4-C3	2.48	115.04	110.23
2	D	2012	XYS	O5-C1-C2	2.14	112.31	109.24

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2012	XYS	C1
2	D	2011	XYS	C2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
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.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	2009	XYS	C1-C2-C3-C4-C5-O5

## 5.6 Ligand geometry ⓘ

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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$
4	MES	A	2013	-	12,12,12	1.83	4 (33%)	16,16,16	5.32	11 (68%)
5	GOL	A	2016	-	5,5,5	0.41	0	5,5,5	0.62	0
4	MES	B	2014	-	12,12,12	2.00	4 (33%)	16,16,16	5.21	10 (62%)
5	GOL	B	2017	-	5,5,5	0.34	0	5,5,5	0.40	0
5	GOL	C	2018	-	5,5,5	0.28	0	5,5,5	0.32	0
4	MES	D	2015	-	12,12,12	4.69	4 (33%)	16,16,16	5.37	9 (56%)
5	GOL	D	2019	-	5,5,5	0.30	0	5,5,5	0.35	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
4	MES	A	2013	-	-	0/6/14/14	0/1/1/1
5	GOL	A	2016	-	-	0/4/4/4	0/0/0/0
4	MES	B	2014	-	-	0/6/14/14	0/1/1/1
5	GOL	B	2017	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2018	-	-	0/4/4/4	0/0/0/0
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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2015	MES	O1S-S	11.03	1.71	1.45
4	D	2015	MES	O3S-S	8.57	1.65	1.45
4	D	2015	MES	O2S-S	5.80	1.59	1.45
4	D	2015	MES	C8-S	5.20	1.87	1.78
4	B	2014	MES	C8-S	3.87	1.85	1.78
4	A	2013	MES	C8-S	3.53	1.84	1.78
4	B	2014	MES	O1S-S	3.26	1.53	1.45
4	A	2013	MES	O1S-S	3.14	1.52	1.45
4	B	2014	MES	O2S-S	2.65	1.51	1.45
4	A	2013	MES	O3S-S	2.60	1.51	1.45
4	A	2013	MES	O2S-S	2.36	1.51	1.45
4	B	2014	MES	O3S-S	2.16	1.50	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2013	MES	O3S-S-O2S	-12.05	81.50	112.48
4	D	2015	MES	O3S-S-O1S	-11.79	82.16	112.48
4	D	2015	MES	O3S-S-O2S	-11.35	83.28	112.48
4	B	2014	MES	O3S-S-O2S	-11.13	83.87	112.48
4	B	2014	MES	O3S-S-O1S	-10.79	84.74	112.48
4	A	2013	MES	O3S-S-O1S	-10.13	86.44	112.48
4	D	2015	MES	O3S-S-C8	-8.90	83.04	105.99
4	B	2014	MES	O3S-S-C8	-8.74	83.45	105.99
4	A	2013	MES	O3S-S-C8	-7.61	86.36	105.99
4	A	2013	MES	C5-N4-C3	7.09	123.82	109.75
4	D	2015	MES	O2S-S-O1S	6.57	125.10	112.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2013	MES	O2S-S-O1S	5.70	123.42	112.44
4	D	2015	MES	C5-N4-C3	5.54	120.73	109.75
4	B	2014	MES	C5-N4-C3	5.27	120.20	109.75
4	A	2013	MES	O1-C6-C5	-4.57	105.89	111.34
4	B	2014	MES	O2S-S-C8	4.33	119.70	106.36
4	B	2014	MES	O1-C6-C5	4.28	116.44	111.34
4	B	2014	MES	O1S-S-C8	4.09	118.97	106.36
4	A	2013	MES	O2S-S-C8	3.75	117.92	106.36
4	B	2014	MES	C7-N4-C5	3.61	121.09	111.66
4	D	2015	MES	C7-N4-C3	3.20	120.03	111.66
4	A	2013	MES	O1S-S-C8	3.17	116.13	106.36
4	B	2014	MES	O2S-S-O1S	2.95	118.12	112.44
4	D	2015	MES	C7-N4-C5	2.90	119.23	111.66
4	D	2015	MES	O2S-S-C8	2.88	115.25	106.36
4	D	2015	MES	O1S-S-C8	2.80	115.00	106.36
4	B	2014	MES	C7-N4-C3	2.68	118.67	111.66
4	A	2013	MES	C7-N4-C5	2.57	118.39	111.66
4	A	2013	MES	C7-N4-C3	2.35	117.79	111.66
4	A	2013	MES	O1-C2-C3	-2.03	108.92	111.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	533/535 (99%)	0.20	11 (2%) 60 61	32, 40, 49, 59	0
1	B	533/535 (99%)	0.15	12 (2%) 57 58	32, 39, 47, 54	0
1	C	533/535 (99%)	1.20	111 (20%) 1 1	38, 50, 63, 68	0
1	D	533/535 (99%)	0.28	17 (3%) 45 46	32, 42, 51, 59	0
All	All	2132/2140 (99%)	0.46	151 (7%) 15 15	32, 42, 56, 68	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	PRO	6.3
1	B	151	ASP	5.3
1	C	337	ASP	4.9
1	C	306	GLY	4.9
1	C	22	GLY	4.7
1	C	4	ILE	4.5
1	C	338	THR	4.5
1	C	115	ALA	4.1
1	C	256	HIS	4.0
1	C	135	GLU	3.9
1	C	274	GLY	3.9
1	C	481	MET	3.9
1	C	199	TYR	3.8
1	A	151	ASP	3.8
1	C	320	GLU	3.7
1	C	21	VAL	3.7
1	C	137	GLY	3.7
1	C	318	SER	3.6
1	C	468	GLN	3.6
1	C	195	ASN	3.5
1	C	260	TRP	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	299	ASP	3.5
1	C	197	TYR	3.5
1	C	222	TYR	3.4
1	C	305	VAL	3.4
1	C	325	GLU	3.4
1	D	320	GLU	3.4
1	C	46	LEU	3.4
1	C	261	PHE	3.3
1	C	456	ASP	3.3
1	C	457	ASP	3.3
1	C	283	TYR	3.3
1	C	503	ARG	3.3
1	C	80	TYR	3.2
1	C	339	LEU	3.2
1	C	483	TRP	3.2
1	D	482	ASN	3.2
1	C	8	ILE	3.1
1	C	24	ASP	3.1
1	C	478	PHE	3.1
1	C	460	TYR	3.1
1	C	284	CYS	3.1
1	C	220	SER	3.0
1	C	313	GLU	3.0
1	C	482	ASN	3.0
1	D	481	MET	2.9
1	C	360	ARG	2.9
1	C	315	ASP	2.9
1	C	273	GLU	2.9
1	A	320	GLU	2.9
1	C	300	GLY	2.9
1	C	53	ALA	2.9
1	C	5	LYS	2.9
1	C	389	HIS	2.8
1	C	395	LYS	2.8
1	A	318	SER	2.8
1	C	50	ARG	2.8
1	D	273	GLU	2.8
1	C	219	THR	2.8
1	B	509	ALA	2.8
1	C	529	TYR	2.8
1	C	10	THR	2.8
1	D	338	THR	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	43	SER	2.7
1	C	52	VAL	2.6
1	D	458	ILE	2.6
1	C	455	PRO	2.6
1	C	322	VAL	2.6
1	A	273	GLU	2.6
1	C	86	TRP	2.6
1	A	224	PRO	2.6
1	B	173	GLU	2.6
1	C	323	SER	2.6
1	C	495	LEU	2.6
1	B	166	GLU	2.5
1	B	337	ASP	2.5
1	C	452	ILE	2.5
1	C	448	ARG	2.5
1	C	520	GLY	2.5
1	C	296	GLU	2.5
1	C	307	GLY	2.5
1	C	330	GLU	2.5
1	B	167	GLN	2.5
1	C	314	ILE	2.5
1	D	298	LYS	2.5
1	C	107	VAL	2.5
1	A	195	ASN	2.5
1	D	219	THR	2.4
1	B	140	TYR	2.4
1	A	300	GLY	2.4
1	C	294	ARG	2.4
1	A	316	GLY	2.4
1	C	266	THR	2.4
1	A	237	TRP	2.4
1	C	198	TYR	2.4
1	C	343	PHE	2.4
1	C	257	THR	2.3
1	C	173	GLU	2.3
1	D	322	VAL	2.3
1	C	526	ASP	2.3
1	C	401	THR	2.3
1	C	88	ILE	2.3
1	D	151	ASP	2.3
1	C	47	LYS	2.3
1	C	42	HIS	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	237	TRP	2.3
1	C	87	LEU	2.3
1	C	399	ARG	2.3
1	C	328	TYR	2.3
1	C	402	THR	2.3
1	C	485	ASP	2.3
1	C	316	GLY	2.2
1	C	531	LEU	2.2
1	B	481	MET	2.2
1	D	456	ASP	2.2
1	B	135	GLU	2.2
1	C	255	THR	2.2
1	C	329	ASP	2.2
1	C	331	LYS	2.2
1	B	224	PRO	2.2
1	B	175	LYS	2.2
1	D	448	ARG	2.2
1	C	387	HIS	2.2
1	C	38	VAL	2.2
1	D	50	ARG	2.1
1	D	389	HIS	2.1
1	C	244	LEU	2.1
1	C	354	ILE	2.1
1	C	527	PHE	2.1
1	C	110	ASP	2.1
1	C	528	ASP	2.1
1	C	229	PRO	2.1
1	C	48	ASN	2.1
1	A	319	VAL	2.1
1	B	136	ASP	2.1
1	C	466	THR	2.1
1	C	312	LEU	2.0
1	C	321	GLU	2.0
1	D	446	PRO	2.0
1	C	166	GLU	2.0
1	D	325	GLU	2.0
1	C	228	HIS	2.0
1	C	310	PRO	2.0
1	C	319	VAL	2.0
1	A	503	ARG	2.0
1	C	20	ARG	2.0
1	C	83	GLY	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	327	ASP	2.0
1	D	87	LEU	2.0
1	C	7	PRO	2.0
1	C	241	ARG	2.0

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

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

## 6.3 Carbohydrates ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	XYS	D	2011	9/10	0.46	15.37	55,58,62,63	1
2	XYS	C	2010	10/10	0.59	13.35	74,77,78,79	0
2	XYS	B	2007	9/10	0.34	11.98	58,62,66,66	1
2	XYS	A	2005	9/10	0.37	10.40	56,60,65,65	1
2	XYS	D	2012	10/10	0.46	9.52	62,65,67,69	0
2	XYS	A	2006	10/10	0.35	4.94	66,69,70,71	0
2	XYS	B	2008	10/10	0.31	4.30	68,70,71,72	0
2	XYS	C	2009	9/10	0.30	3.98	68,69,71,71	1

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	MES	D	2015	12/12	0.45	15.60	125,125,126,126	0
4	MES	B	2014	12/12	0.30	8.55	78,78,79,79	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	GOL	B	2017	6/6	0.15	0.64	49,51,52,52	0
4	MES	A	2013	12/12	0.15	0.59	47,50,51,52	0
5	GOL	C	2018	6/6	0.14	-0.45	52,54,54,55	0
3	CA	D	2004	1/1	0.14	-0.56	56,56,56,56	0
5	GOL	A	2016	6/6	0.10	-1.18	37,39,41,41	0
3	CA	C	2003	1/1	0.18	-1.44	75,75,75,75	0
3	CA	A	2001	1/1	0.08	-1.61	36,36,36,36	0
5	GOL	D	2019	6/6	0.09	-1.66	36,41,42,44	0
3	CA	B	2002	1/1	0.04	-4.01	38,38,38,38	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.