



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 10:50 PM GMT

PDB ID : 2EXJ  
Title : Structure of the family43 beta-Xylosidase D128G mutant 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>

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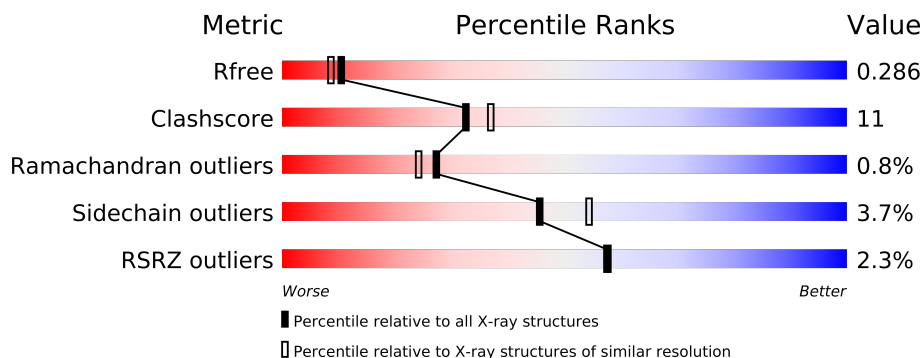
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 19279 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
			4372	2812	748	802	10			
1	B	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			
1	C	533	Total	C	N	O	S	0	0	0
			4372	2812	748	802	10			
1	D	533	Total	C	N	O	S	0	0	0
			4372	2812	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	128	GLY	ASP	ENGINEERED	UNP Q68HB3
B	2	ALA	SER	ENGINEERED	UNP Q68HB3
B	128	GLY	ASP	ENGINEERED	UNP Q68HB3
C	2	ALA	SER	ENGINEERED	UNP Q68HB3
C	128	GLY	ASP	ENGINEERED	UNP Q68HB3
D	2	ALA	SER	ENGINEERED	UNP Q68HB3
D	128	GLY	ASP	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		

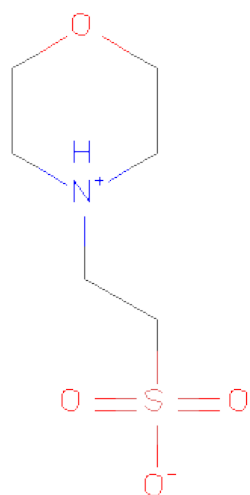
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	ENGINEERED	UNP Q68HB3
A	128	GLY	ASP	ENGINEERED	UNP Q68HB3
B	2	ALA	SER	ENGINEERED	UNP Q68HB3
B	128	GLY	ASP	ENGINEERED	UNP Q68HB3
C	2	ALA	SER	ENGINEERED	UNP Q68HB3
C	128	GLY	ASP	ENGINEERED	UNP Q68HB3
D	2	ALA	SER	ENGINEERED	UNP Q68HB3
D	128	GLY	ASP	ENGINEERED	UNP Q68HB3

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

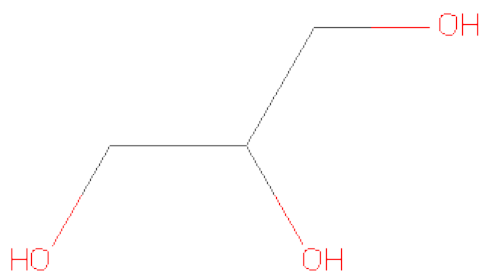
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0

- 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	451	Total	O	0	0
			451	451		
6	B	469	Total	O	0	0
			469	469		
6	C	316	Total	O	0	0
			316	316		

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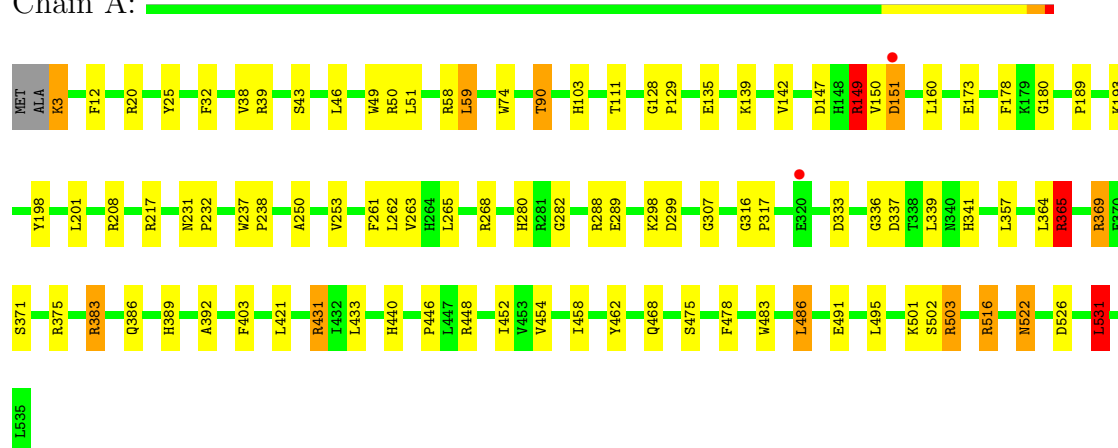
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	415	Total 415	O 415	0	0

### 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.

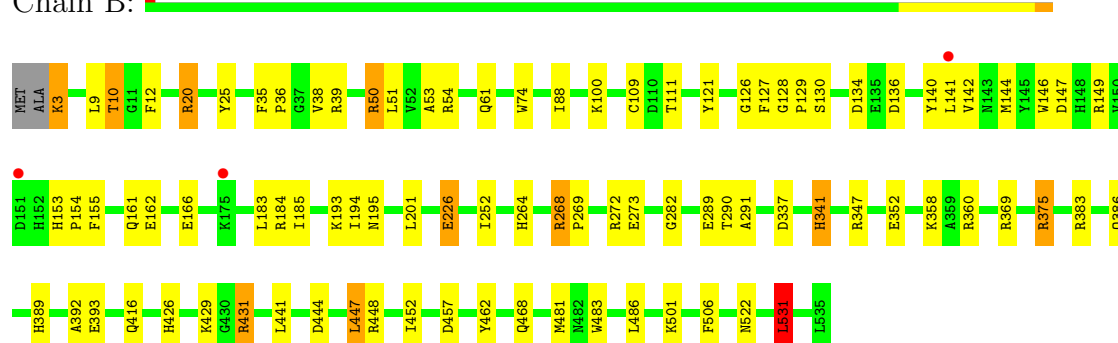
- Molecule 1: beta-D-xylosidase

Chain A:



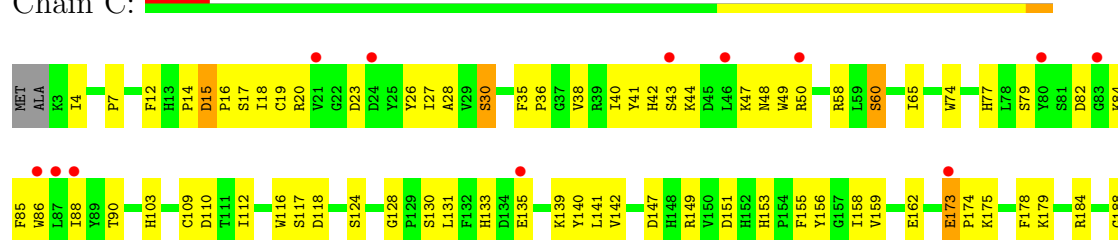
- Molecule 1: beta-D-xylosidase

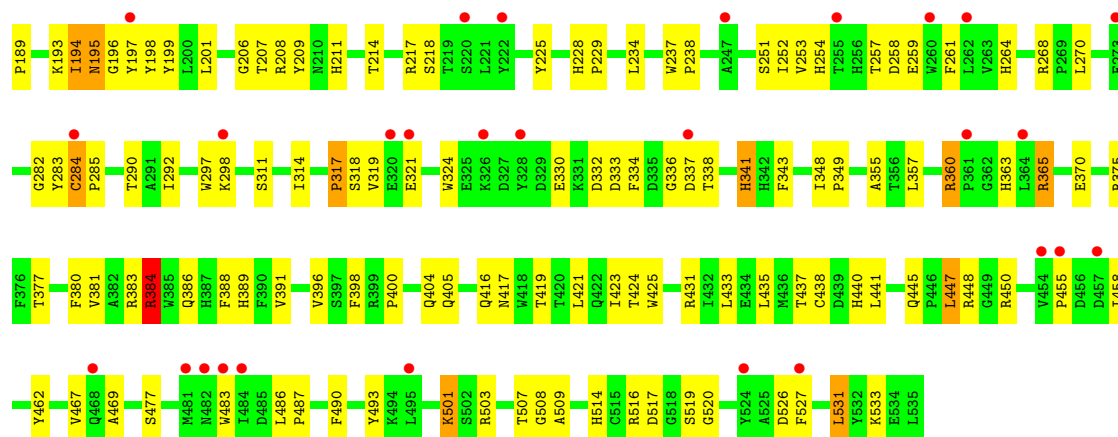
Chain B:



- 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, $\alpha$ , $\beta$ , $\gamma$	140.38Å 140.38Å 232.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.20) 99.8 (20.00-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.30 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.205 , 0.282 0.214 , 0.286	Depositor DCC
$R_{free}$ test set	5923 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 118188 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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	0.69	0/4516	0.80	10/6154 (0.2%)
1	B	0.72	0/4516	0.76	3/6154 (0.0%)
1	C	0.62	1/4516 (0.0%)	0.70	1/6154 (0.0%)
1	D	0.68	0/4516	0.73	3/6154 (0.0%)
All	All	0.68	1/18064 (0.0%)	0.75	17/24616 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	A	2	0
2	B	2	0
2	C	2	0
2	D	2	0
All	All	8	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	284	CYS	CB-SG	-7.56	1.69	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	ARG	NE-CZ-NH1	9.54	125.07	120.30
1	A	531	LEU	CA-CB-CG	9.18	136.41	115.30
1	A	365	ARG	NE-CZ-NH2	-8.14	116.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	268	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	369	ARG	NE-CZ-NH2	-7.29	116.65	120.30
1	B	531	LEU	CA-CB-CG	7.11	131.65	115.30
1	A	58	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	A	383	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	357	LEU	CA-CB-CG	5.88	128.82	115.30
1	D	39	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	149	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	B	268	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	383	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	149	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	449	GLY	N-CA-C	-5.21	100.07	113.10
1	A	486	LEU	CA-CB-CG	-5.08	103.63	115.30
1	C	531	LEU	CA-CB-CG	5.00	126.80	115.30

All (8) chirality outliers are listed below:

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

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	384	ARG	Peptide

## 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	4372	0	4162	75	0
1	B	4372	0	4162	75	0
1	C	4372	0	4162	160	0
1	D	4372	0	4162	78	0
2	A	19	0	17	2	0
2	B	19	0	17	2	0
2	C	19	0	17	0	0
2	D	19	0	17	4	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	5	0
4	D	12	0	12	6	0
5	A	6	0	8	0	0
5	B	6	0	8	1	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
6	A	451	0	0	20	0
6	B	469	0	0	29	0
6	C	316	0	0	34	0
6	D	415	0	0	17	0
All	All	19279	0	16784	387	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 11.

All (387) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:251:SER:HA	6:C:2142:HOH:O	1.20	1.31
4:D:2015:MES:S	4:D:2015:MES:O3S	1.92	1.26
1:B:3:LYS:HB3	6:B:2325:HOH:O	1.08	1.25
1:A:369:ARG:HH22	1:A:522:ASN:ND2	1.34	1.24
1:B:144:MET:SD	6:B:2468:HOH:O	1.92	1.23
1:C:419:THR:HG22	1:C:437:THR:HG22	1.34	1.04
1:A:3:LYS:HB3	6:A:2330:HOH:O	1.61	1.00
1:A:369:ARG:NH2	1:A:522:ASN:ND2	2.11	0.96
1:C:324:TRP:HA	6:C:2200:HOH:O	1.65	0.96
1:A:336:GLY:HA3	6:A:2242:HOH:O	1.65	0.95
1:D:53:ALA:HA	4:D:2015:MES:H82	1.50	0.94
1:B:134:ASP:OD1	6:B:2358:HOH:O	1.88	0.91
1:C:284:CYS:SG	6:C:2143:HOH:O	2.14	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:297:TRP:HB3	6:C:2092:HOH:O	1.71	0.90
1:A:369:ARG:NH2	1:A:522:ASN:HD22	1.70	0.90
1:A:369:ARG:HH22	1:A:522:ASN:HD21	1.17	0.87
1:B:431:ARG:NH1	6:B:2435:HOH:O	2.08	0.86
1:C:517:ASP:OD1	1:C:519:SER:OG	1.93	0.86
1:C:270:LEU:HD22	6:C:2121:HOH:O	1.73	0.85
1:A:369:ARG:HH22	1:A:522:ASN:HD22	1.21	0.85
1:C:455:PRO:HA	6:C:2285:HOH:O	1.77	0.84
1:D:431:ARG:NH1	6:D:2348:HOH:O	2.10	0.83
4:D:2015:MES:O2S	4:D:2015:MES:O3S	1.95	0.83
1:B:389:HIS:HB3	6:B:2278:HOH:O	1.77	0.82
1:C:7:PRO:HG3	1:C:268:ARG:HH11	1.44	0.82
1:A:389:HIS:HB3	6:A:2174:HOH:O	1.80	0.81
1:C:135:GLU:HG2	6:C:2173:HOH:O	1.79	0.81
1:C:58:ARG:NH2	1:C:116:TRP:O	2.14	0.81
1:C:147:ASP:OD1	1:C:149:ARG:HD3	1.85	0.77
1:D:288:ARG:HH12	2:D:2011:XYS:H52	1.50	0.76
1:B:166:GLU:HB2	6:B:2440:HOH:O	1.84	0.76
1:D:440:HIS:NE2	1:D:501:LYS:HG2	2.00	0.76
1:D:182:ASP:HB3	6:D:2308:HOH:O	1.86	0.75
1:C:7:PRO:CG	1:C:268:ARG:HH11	2.01	0.74
1:A:365:ARG:CG	1:A:526:ASP:OD1	2.36	0.74
1:C:77:HIS:CD2	1:C:131:LEU:H	2.05	0.73
1:A:250:ALA:HB1	1:A:262:LEU:HD11	1.71	0.73
1:C:400:PRO:HD2	1:C:431:ARG:HD2	1.69	0.73
1:D:53:ALA:CA	4:D:2015:MES:H82	2.18	0.72
1:C:365:ARG:HH11	1:C:365:ARG:CG	2.01	0.72
1:C:15:ASP:OD2	1:C:30:SER:OG	2.07	0.72
1:D:42:HIS:ND1	6:D:2380:HOH:O	2.22	0.72
1:C:261:PHE:CZ	1:C:317:PRO:HG3	2.25	0.72
1:C:334:PHE:HB3	1:C:357:LEU:CD1	2.20	0.71
1:C:77:HIS:HD2	1:C:131:LEU:H	1.36	0.71
1:B:54:ARG:HE	4:B:2014:MES:H82	1.55	0.70
1:D:53:ALA:HA	4:D:2015:MES:C8	2.20	0.70
1:C:17:SER:HB3	1:C:28:ALA:HB3	1.73	0.70
1:D:255:THR:HG23	1:D:257:THR:H	1.56	0.70
1:C:184:ARG:HD3	6:C:2112:HOH:O	1.90	0.70
1:C:254:HIS:HE1	1:C:258:ASP:HA	1.57	0.69
1:D:501:LYS:HE3	6:D:2273:HOH:O	1.90	0.69
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.27	0.69
1:B:53:ALA:HA	4:B:2014:MES:H51	1.73	0.69
1:B:50:ARG:HB3	1:B:50:ARG:HH11	1.56	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:255:THR:HG22	1:D:259:GLU:H	1.57	0.68
1:C:509:ALA:O	6:C:2106:HOH:O	2.11	0.68
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.75	0.68
1:A:365:ARG:HG3	1:A:526:ASP:OD1	1.92	0.68
1:C:334:PHE:CD2	1:C:527:PHE:O	2.47	0.68
1:A:440:HIS:NE2	1:A:501:LYS:HG2	2.09	0.67
1:C:30:SER:HB3	1:C:74:TRP:O	1.93	0.67
1:C:35:PHE:CE1	1:C:349:PRO:HG3	2.29	0.67
1:A:208:ARG:NH2	1:A:503:ARG:HG3	2.08	0.67
1:A:173:GLU:O	6:A:2459:HOH:O	2.13	0.66
1:B:146:TRP:HB2	6:B:2468:HOH:O	1.93	0.66
1:D:431:ARG:NH2	1:D:458:ILE:O	2.28	0.66
1:C:334:PHE:HB3	1:C:357:LEU:HD11	1.76	0.66
1:C:462:TYR:HB2	1:C:477:SER:HB3	1.77	0.66
1:B:369:ARG:NH2	1:B:522:ASN:OD1	2.28	0.66
1:C:384:ARG:HH11	1:C:384:ARG:CG	2.08	0.66
1:A:458:ILE:HD12	1:A:478:PHE:HB3	1.76	0.66
1:B:10:THR:CG2	1:B:386:GLN:HB3	2.25	0.66
1:C:109:CYS:HB3	6:C:2045:HOH:O	1.94	0.66
1:C:507:THR:O	6:C:2147:HOH:O	2.14	0.66
1:A:111:THR:HG22	6:A:2328:HOH:O	1.96	0.65
1:B:426:HIS:ND1	1:B:429:LYS:HG3	2.11	0.65
1:C:355:ALA:O	6:C:2189:HOH:O	2.14	0.65
1:D:272:ARG:HD2	6:D:2374:HOH:O	1.96	0.64
1:A:365:ARG:HG2	1:A:526:ASP:OD1	1.97	0.64
1:C:384:ARG:HH11	1:C:384:ARG:HG3	1.63	0.64
1:C:334:PHE:HD2	1:C:527:PHE:O	1.81	0.64
1:D:375:ARG:NH2	6:D:2130:HOH:O	2.31	0.64
1:C:12:PHE:CD1	1:C:14:PRO:HD3	2.32	0.63
1:C:23:ASP:O	1:C:44:LYS:HD3	1.97	0.63
1:C:270:LEU:HG	1:C:283:TYR:O	1.99	0.63
1:D:320:GLU:HG3	6:D:2298:HOH:O	1.97	0.63
1:C:341:HIS:HD2	6:C:2162:HOH:O	1.82	0.63
1:C:110:ASP:C	6:C:2211:HOH:O	2.36	0.63
1:A:3:LYS:N	6:A:2309:HOH:O	2.32	0.62
1:C:43:SER:HB2	1:C:49:TRP:CE3	2.34	0.62
1:D:288:ARG:HH12	2:D:2011:XYS:C5	2.12	0.62
1:C:319:VAL:HG22	6:C:2202:HOH:O	2.00	0.62
1:B:147:ASP:OD1	1:B:149:ARG:HD3	2.00	0.62
1:C:503:ARG:HB3	6:C:2253:HOH:O	1.99	0.62
1:B:448:ARG:HD3	6:B:2485:HOH:O	1.99	0.61
1:C:158:ILE:HD12	1:C:189:PRO:HB3	1.83	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:288:ARG:NH1	2:D:2011:XY5:H52	2.14	0.61
1:A:316:GLY:N	6:A:2330:HOH:O	2.29	0.61
1:C:7:PRO:CG	1:C:268:ARG:NH1	2.63	0.61
1:C:20:ARG:HD3	1:C:254:HIS:O	2.01	0.60
1:B:50:ARG:HD2	6:B:2359:HOH:O	2.00	0.60
1:A:20:ARG:HG3	1:A:25:TYR:CE1	2.36	0.60
1:C:462:TYR:HB3	1:C:483:TRP:CH2	2.36	0.60
1:C:16:PRO:HG3	1:C:290:THR:HG23	1.83	0.60
1:A:522:ASN:HA	6:A:2388:HOH:O	2.01	0.59
1:D:147:ASP:OD1	1:D:149:ARG:HD2	2.02	0.59
1:C:435:LEU:HD12	1:C:447:LEU:HD22	1.83	0.59
1:C:398:PHE:CD2	1:C:400:PRO:HD3	2.36	0.59
1:C:365:ARG:HG2	1:C:526:ASP:OD1	2.03	0.59
1:D:397:SER:HA	6:D:2402:HOH:O	2.01	0.59
1:A:250:ALA:HB1	1:A:262:LEU:CD1	2.32	0.59
1:C:26:TYR:HA	1:C:41:TYR:O	2.03	0.59
1:A:403:PHE:O	1:D:148:HIS:HE1	1.86	0.59
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.18	0.58
1:C:156:TYR:O	1:C:179:LYS:NZ	2.31	0.58
1:C:389:HIS:HA	1:C:467:VAL:O	2.03	0.58
1:C:85:PHE:HD2	6:C:2045:HOH:O	1.85	0.58
1:C:380:PHE:HB2	1:C:514:HIS:CD2	2.38	0.58
1:D:332:ASP:O	1:D:529:TYR:HB2	2.03	0.58
1:C:330:GLU:HG3	6:C:2100:HOH:O	2.03	0.58
1:C:197:TYR:HB2	1:C:199:TYR:HE1	1.69	0.58
1:D:50:ARG:NE	6:D:2380:HOH:O	2.35	0.58
1:D:447:LEU:HD21	1:D:486:LEU:HD22	1.86	0.57
1:A:502:SER:O	1:A:503:ARG:HB2	2.03	0.57
1:D:391:VAL:HG21	1:D:464:ARG:HD2	1.87	0.57
1:C:228:HIS:ND1	1:C:229:PRO:HD2	2.19	0.57
1:C:365:ARG:HG2	1:C:365:ARG:HH11	1.69	0.57
1:B:272:ARG:HD2	6:B:2102:HOH:O	2.05	0.56
1:A:151:ASP:N	1:A:151:ASP:OD1	2.36	0.56
1:C:398:PHE:CE2	1:C:400:PRO:HB3	2.40	0.56
1:A:208:ARG:CZ	6:A:2447:HOH:O	2.53	0.56
1:C:197:TYR:HB2	1:C:199:TYR:CE1	2.40	0.56
1:C:424:THR:HG23	1:C:425:TRP:N	2.19	0.56
1:C:193:LYS:C	1:C:194:ILE:HG12	2.24	0.56
1:C:365:ARG:NH1	1:C:365:ARG:CG	2.63	0.56
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.53	0.56
1:B:201:LEU:HD22	1:B:252:ILE:HG13	1.88	0.56
1:C:174:PRO:O	1:C:175:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:77:HIS:CD2	1:D:131:LEU:H	2.23	0.56
1:D:391:VAL:CG2	1:D:464:ARG:HD2	2.36	0.56
1:B:128:GLY:N	1:B:129:PRO:CD	2.68	0.56
1:B:88:ILE:HG21	1:B:129:PRO:HB2	1.87	0.55
1:A:50:ARG:HG3	6:A:2177:HOH:O	2.05	0.55
1:C:336:GLY:HA3	6:C:2309:HOH:O	2.06	0.55
1:B:10:THR:HG23	1:B:386:GLN:O	2.07	0.55
1:C:421:LEU:HD13	1:C:486:LEU:HD13	1.88	0.55
1:A:316:GLY:HA3	6:A:2330:HOH:O	2.06	0.55
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.89	0.55
1:C:153:HIS:NE2	1:C:184:ARG:HB3	2.21	0.55
1:D:402:THR:HG23	1:D:405:GLN:HG3	1.89	0.55
1:A:365:ARG:HH11	1:A:365:ARG:HG3	1.72	0.54
1:C:261:PHE:HB3	1:C:292:ILE:HD11	1.89	0.54
1:C:404:GLN:NE2	1:C:519:SER:HA	2.22	0.54
1:C:252:ILE:HG22	6:C:2150:HOH:O	2.07	0.54
1:C:440:HIS:NE2	1:C:501:LYS:HD3	2.23	0.54
1:C:337:ASP:HA	6:C:2216:HOH:O	2.08	0.54
1:C:60:SER:HB2	1:C:118:ASP:OD1	2.08	0.54
1:B:268:ARG:HD3	1:B:289:GLU:OE2	2.08	0.54
1:A:250:ALA:CB	1:A:262:LEU:HD11	2.37	0.53
1:A:431:ARG:HD2	6:A:2075:HOH:O	2.08	0.53
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.89	0.53
1:D:126:GLY:HA3	1:D:144:MET:O	2.08	0.53
1:B:50:ARG:HG3	6:B:2142:HOH:O	2.07	0.53
1:C:330:GLU:O	1:C:531:LEU:HA	2.09	0.53
1:D:398:PHE:CD2	1:D:400:PRO:HD3	2.43	0.53
1:D:3:LYS:HG3	6:D:2214:HOH:O	2.09	0.53
1:D:440:HIS:CD2	1:D:501:LYS:HG2	2.43	0.53
1:C:261:PHE:CE2	1:C:317:PRO:HG3	2.44	0.53
1:B:20:ARG:HG3	1:B:25:TYR:CE1	2.43	0.53
1:C:58:ARG:NH1	1:C:118:ASP:OD1	2.42	0.53
1:C:365:ARG:HG3	1:C:365:ARG:NH1	2.23	0.53
1:B:126:GLY:HA2	6:B:2468:HOH:O	2.09	0.53
1:C:18:ILE:HG12	1:C:253:VAL:HB	1.90	0.52
1:C:380:PHE:HB2	1:C:514:HIS:HD2	1.74	0.52
1:D:431:ARG:HH12	1:D:456:ASP:HA	1.74	0.52
6:B:2242:HOH:O	1:C:375:ARG:CZ	2.57	0.52
1:B:39:ARG:NH2	6:B:2167:HOH:O	2.24	0.52
1:B:184:ARG:HD2	6:B:2143:HOH:O	2.09	0.52
1:B:126:GLY:HA3	1:B:144:MET:O	2.10	0.52
1:B:74:TRP:CE3	2:B:2007:XYS:H2	2.45	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:3:LYS:HD3	6:B:2325:HOH:O	2.10	0.51
1:C:58:ARG:HH12	1:C:118:ASP:CG	2.13	0.51
1:A:43:SER:HB2	1:A:49:TRP:CE3	2.45	0.51
1:A:231:ASN:CG	1:A:232:PRO:HA	2.31	0.51
1:B:54:ARG:HE	4:B:2014:MES:C8	2.24	0.51
1:C:360:ARG:HG2	1:C:363:HIS:CG	2.45	0.51
1:C:419:THR:CG2	1:C:437:THR:HG22	2.24	0.51
1:C:365:ARG:NH2	6:C:2167:HOH:O	2.43	0.51
1:C:254:HIS:CE1	1:C:258:ASP:HA	2.42	0.51
1:C:370:GLU:HB2	1:C:377:THR:O	2.11	0.51
1:D:294:ARG:NH1	1:D:315:ASP:O	2.36	0.51
1:C:206:GLY:C	1:C:208:ARG:H	2.14	0.51
1:A:316:GLY:CA	6:A:2330:HOH:O	2.59	0.50
1:C:338:THR:C	6:C:2064:HOH:O	2.49	0.50
1:C:17:SER:O	1:C:27:ILE:HA	2.11	0.50
1:B:273:GLU:O	6:B:2345:HOH:O	2.20	0.50
1:A:288:ARG:NH2	2:A:2005:XYS:O4	2.41	0.50
1:A:339:LEU:HD21	1:A:364:LEU:HD13	1.92	0.50
1:A:150:VAL:HG23	1:D:445:GLN:OE1	2.11	0.50
4:D:2015:MES:C8	4:D:2015:MES:O3S	2.59	0.50
1:A:383:ARG:HD2	6:A:2120:HOH:O	2.11	0.50
1:A:39:ARG:NH2	1:A:51:LEU:HD22	2.27	0.50
1:B:468:GLN:CD	6:B:2278:HOH:O	2.49	0.49
1:A:189:PRO:HA	1:A:201:LEU:O	2.12	0.49
1:A:371:SER:HA	1:A:516:ARG:HD3	1.94	0.49
1:B:416:GLN:HG2	1:B:441:LEU:HD13	1.94	0.49
1:B:10:THR:HG22	1:B:386:GLN:HB3	1.92	0.49
1:A:74:TRP:O	6:A:2028:HOH:O	2.18	0.49
1:C:435:LEU:HD12	1:C:447:LEU:CD2	2.43	0.49
1:B:39:ARG:NE	6:B:2167:HOH:O	2.34	0.49
1:B:51:LEU:HD23	1:B:341:HIS:ND1	2.27	0.49
1:C:334:PHE:N	6:C:2170:HOH:O	2.46	0.49
1:B:347:ARG:HD3	1:B:375:ARG:O	2.13	0.49
1:B:264:HIS:CE1	1:B:291:ALA:HB3	2.48	0.49
1:D:369:ARG:NH1	6:D:2223:HOH:O	2.46	0.49
1:C:285:PRO:HD2	6:C:2033:HOH:O	2.13	0.48
1:C:234:LEU:HD21	1:C:264:HIS:CD2	2.48	0.48
1:D:313:GLU:HB2	6:D:2141:HOH:O	2.12	0.48
1:B:121:TYR:OH	1:C:520:GLY:HA3	2.14	0.48
1:A:502:SER:O	1:A:503:ARG:NH1	2.47	0.48
1:B:9:LEU:HB2	1:B:290:THR:HB	1.95	0.48
1:D:26:TYR:HA	1:D:41:TYR:O	2.13	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:455:PRO:HB2	1:C:458:ILE:HG12	1.95	0.48
1:A:193:LYS:HD3	1:A:198:TYR:CE1	2.49	0.48
1:C:357:LEU:HD23	6:C:2064:HOH:O	2.13	0.48
1:A:90:THR:HA	1:A:103:HIS:O	2.14	0.47
1:D:433:LEU:HD21	1:D:461:VAL:HG11	1.96	0.47
1:A:421:LEU:HD13	1:A:486:LEU:HD13	1.96	0.47
1:C:405:GLN:HA	1:C:516:ARG:O	2.15	0.47
1:B:452:ILE:HD12	1:B:452:ILE:N	2.29	0.47
1:B:136:ASP:HB3	6:B:2227:HOH:O	2.13	0.47
1:A:365:ARG:NH1	1:A:365:ARG:HG3	2.29	0.47
1:C:209:TYR:OH	1:C:282:GLY:O	2.33	0.47
1:D:216:ALA:HB1	1:D:225:TYR:HB3	1.96	0.47
1:B:183:LEU:HD11	6:D:2364:HOH:O	2.14	0.47
1:C:386:GLN:NE2	6:C:2295:HOH:O	2.46	0.47
1:B:184:ARG:CD	6:B:2143:HOH:O	2.61	0.47
1:C:445:GLN:O	1:C:448:ARG:HG3	2.14	0.47
1:B:226:GLU:HB2	6:B:2403:HOH:O	2.15	0.47
1:C:283:TYR:CB	1:C:493:TYR:HB2	2.45	0.47
1:A:299:ASP:CG	6:A:2147:HOH:O	2.53	0.47
1:B:88:ILE:CG2	1:B:129:PRO:HB2	2.45	0.46
1:A:198:TYR:O	1:A:217:ARG:HA	2.15	0.46
1:A:446:PRO:HA	1:A:448:ARG:HH21	1.79	0.46
1:C:343:PHE:HB3	1:C:381:VAL:HG12	1.96	0.46
1:C:416:GLN:NE2	1:C:441:LEU:HD13	2.30	0.46
1:B:54:ARG:HH21	4:B:2014:MES:H82	1.81	0.46
1:D:228:HIS:ND1	1:D:229:PRO:HD2	2.31	0.46
1:B:109:CYS:SG	1:B:111:THR:O	2.73	0.46
1:B:444:ASP:OD1	6:B:2402:HOH:O	2.20	0.46
1:C:139:LYS:O	1:C:162:GLU:HG3	2.16	0.46
1:D:447:LEU:CD2	1:D:486:LEU:HD22	2.46	0.46
1:B:141:LEU:N	1:B:161:GLN:O	2.46	0.46
1:B:393:GLU:HB3	1:B:531:LEU:HG	1.97	0.46
1:B:375:ARG:NH2	6:B:2242:HOH:O	2.49	0.45
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.51	0.45
1:C:40:ILE:HG21	1:C:112:ILE:HD11	1.98	0.45
1:D:52:VAL:O	1:D:113:ASP:HB3	2.16	0.45
1:D:447:LEU:HD21	1:D:486:LEU:CD2	2.45	0.45
1:A:383:ARG:NH2	1:A:386:GLN:OE1	2.50	0.45
1:D:462:TYR:HB3	1:D:483:TRP:CH2	2.51	0.45
1:C:208:ARG:O	1:C:211:HIS:HB2	2.17	0.45
1:B:35:PHE:CG	1:B:36:PRO:HA	2.51	0.45
1:C:4:ILE:HB	1:C:314:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:43:SER:OG	1:C:48:ASN:O	2.08	0.45
1:D:506:PHE:CD1	2:D:2011:XY5:H51	2.52	0.45
1:C:42:HIS:O	1:C:49:TRP:HA	2.17	0.45
1:D:418:TRP:CZ2	1:D:438:CYS:HB2	2.52	0.45
1:B:54:ARG:NE	4:B:2014:MES:H82	2.29	0.45
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.64	0.45
1:B:447:LEU:HD21	1:B:486:LEU:HD22	1.99	0.45
1:A:280:HIS:CD2	1:A:282:GLY:H	2.35	0.45
1:C:86:TRP:CD1	1:C:86:TRP:N	2.85	0.45
1:C:234:LEU:CD2	1:C:264:HIS:CD2	3.00	0.45
1:D:265:LEU:HA	1:D:289:GLU:O	2.16	0.45
1:D:109:CYS:SG	1:D:114:GLY:HA3	2.57	0.45
1:C:109:CYS:HB2	1:C:116:TRP:CD2	2.52	0.44
1:C:142:VAL:HA	1:C:159:VAL:O	2.17	0.44
1:C:128:GLY:O	1:C:189:PRO:HD2	2.17	0.44
1:B:462:TYR:HB3	1:B:483:TRP:CH2	2.52	0.44
1:A:491:GLU:HG2	6:A:2301:HOH:O	2.16	0.44
1:C:388:PHE:O	1:C:467:VAL:HG12	2.17	0.44
1:C:201:LEU:HD12	1:C:214:THR:O	2.18	0.44
1:A:142:VAL:CG1	1:A:160:LEU:HD12	2.48	0.44
1:C:195:ASN:HB3	1:C:196:GLY:H	1.68	0.44
1:A:375:ARG:HE	1:A:375:ARG:HB2	1.59	0.44
1:B:3:LYS:CD	6:B:2325:HOH:O	2.65	0.44
1:B:352:GLU:OE1	1:B:358:LYS:HD2	2.17	0.44
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.98	0.44
1:A:392:ALA:HA	1:A:531:LEU:O	2.18	0.44
1:C:103:HIS:ND1	1:C:124:SER:OG	2.39	0.44
1:D:431:ARG:HG2	1:D:454:VAL:HB	1.99	0.44
1:A:59:LEU:HD22	6:A:2406:HOH:O	2.18	0.44
1:D:250:ALA:HA	1:D:263:VAL:O	2.18	0.44
1:B:3:LYS:CB	6:B:2325:HOH:O	1.96	0.44
1:B:153:HIS:HA	1:B:154:PRO:HD3	1.84	0.44
1:D:269:PRO:HB3	1:D:282:GLY:HA3	2.00	0.44
1:C:153:HIS:O	6:C:2037:HOH:O	2.21	0.43
1:A:462:TYR:HB3	1:A:483:TRP:CH2	2.52	0.43
6:B:2401:HOH:O	1:C:173:GLU:HG2	2.17	0.43
1:C:450:ARG:NH1	1:C:487:PRO:HG2	2.32	0.43
1:D:184:ARG:NH1	6:D:2119:HOH:O	2.51	0.43
1:D:86:TRP:HE3	1:D:106:LEU:HD11	1.83	0.43
1:B:140:TYR:HA	1:B:162:GLU:HA	2.00	0.43
1:D:79:SER:CB	1:D:133:HIS:HE2	2.32	0.43
1:C:234:LEU:HD21	1:C:264:HIS:CG	2.54	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:392:ALA:HA	1:D:531:LEU:O	2.19	0.43
1:A:522:ASN:HD22	1:A:522:ASN:HA	1.72	0.43
1:C:435:LEU:HD22	1:C:490:PHE:HZ	1.84	0.43
1:C:360:ARG:HG2	1:C:363:HIS:HB2	2.00	0.43
1:A:265:LEU:HA	1:A:289:GLU:O	2.18	0.43
1:A:43:SER:HB2	1:A:49:TRP:CD2	2.54	0.43
1:C:88:ILE:HG21	1:C:141:LEU:HD11	2.01	0.43
1:A:501:LYS:HE2	6:A:2453:HOH:O	2.18	0.43
1:D:197:TYR:HB2	1:D:199:TYR:CE1	2.54	0.43
1:B:166:GLU:CB	6:B:2440:HOH:O	2.56	0.43
1:C:341:HIS:CD2	6:C:2162:HOH:O	2.65	0.43
1:D:369:ARG:NH2	1:D:522:ASN:OD1	2.51	0.43
1:C:155:PHE:N	1:C:155:PHE:CD2	2.85	0.43
1:C:7:PRO:HG2	1:C:268:ARG:NH1	2.34	0.43
1:C:42:HIS:HB3	1:C:50:ARG:HG3	2.01	0.42
1:A:32:PHE:HZ	2:A:2005:XYS:H4	1.83	0.42
1:C:19:CYS:SG	6:C:2073:HOH:O	2.54	0.42
1:C:268:ARG:HH21	1:C:388:PHE:HE2	1.67	0.42
1:C:435:LEU:HD22	1:C:490:PHE:CZ	2.54	0.42
1:C:4:ILE:HG12	1:C:47:LYS:HB2	2.01	0.42
1:A:147:ASP:OD1	1:A:149:ARG:HD2	2.19	0.42
1:B:468:GLN:NE2	6:B:2278:HOH:O	2.52	0.42
1:C:259:GLU:OE2	1:C:317:PRO:HB3	2.19	0.42
1:C:17:SER:O	1:C:28:ALA:N	2.44	0.42
1:C:375:ARG:NH2	6:C:2028:HOH:O	2.51	0.42
1:B:506:PHE:CD1	2:B:2007:XYS:H52	2.55	0.42
1:A:433:LEU:HB2	1:A:452:ILE:HB	2.00	0.42
1:D:435:LEU:HB2	1:D:446:PRO:HG2	2.02	0.42
1:D:35:PHE:CG	1:D:36:PRO:HA	2.55	0.42
1:C:79:SER:OG	1:C:133:HIS:NE2	2.43	0.42
1:D:399:ARG:CD	6:D:2258:HOH:O	2.67	0.42
1:D:12:PHE:CE1	1:D:507:THR:HA	2.54	0.42
1:C:391:VAL:HG13	1:C:533:LYS:HB3	2.02	0.42
1:D:40:ILE:HB	1:D:53:ALA:HB3	2.01	0.42
1:D:3:LYS:HB2	1:D:316:GLY:H	1.85	0.42
1:C:469:ALA:C	6:C:2121:HOH:O	2.58	0.42
1:B:121:TYR:OH	1:C:520:GLY:CA	2.68	0.42
1:A:421:LEU:HD13	1:A:486:LEU:CD1	2.50	0.42
1:D:447:LEU:HD11	1:D:487:PRO:HD2	2.01	0.41
1:D:234:LEU:O	1:D:235:THR:HB	2.19	0.41
1:D:264:HIS:CE1	1:D:291:ALA:HB3	2.55	0.41
1:C:324:TRP:HE3	6:C:2200:HOH:O	2.04	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:392:ALA:HA	1:B:531:LEU:O	2.20	0.41
1:C:417:ASN:HA	1:C:438:CYS:O	2.21	0.41
1:D:448:ARG:HA	1:D:449:GLY:HA2	1.84	0.41
1:A:253:VAL:CG1	1:A:261:PHE:HB2	2.50	0.41
1:B:100:LYS:HG2	1:B:127:PHE:CE2	2.56	0.41
1:C:35:PHE:HE1	1:C:349:PRO:HG3	1.81	0.41
1:C:65:ILE:HD12	1:C:348:ILE:HG21	2.02	0.41
1:A:298:LYS:O	1:A:299:ASP:HB2	2.20	0.41
1:C:90:THR:HA	1:C:103:HIS:O	2.21	0.41
1:D:251:SER:HB2	6:D:2294:HOH:O	2.20	0.41
1:C:218:SER:HB2	1:C:225:TYR:HA	2.03	0.41
1:C:131:LEU:HA	1:C:140:TYR:O	2.21	0.41
1:C:365:ARG:HG3	1:C:365:ARG:HH11	1.77	0.41
1:D:402:THR:CG2	1:D:405:GLN:HG3	2.50	0.41
1:A:337:ASP:HB2	6:A:2178:HOH:O	2.20	0.41
1:B:130:SER:HB3	1:B:142:VAL:HG23	2.03	0.41
1:C:16:PRO:HB3	1:C:290:THR:CG2	2.51	0.41
1:C:421:LEU:HD13	1:C:486:LEU:CD1	2.49	0.41
1:B:153:HIS:NE2	1:B:184:ARG:HB3	2.36	0.41
1:D:84:LYS:HE2	6:D:2337:HOH:O	2.21	0.41
1:D:189:PRO:HA	1:D:201:LEU:O	2.21	0.41
1:B:155:PHE:CG	1:B:185:ILE:HA	2.56	0.41
1:C:237:TRP:HB3	1:C:238:PRO:HD3	2.01	0.41
1:A:250:ALA:HA	1:A:263:VAL:O	2.21	0.41
1:C:321:GLU:HB2	6:C:2227:HOH:O	2.20	0.41
1:B:193:LYS:C	1:B:194:ILE:HG13	2.41	0.41
1:D:350:LEU:HD22	1:D:354:ILE:HG21	2.02	0.41
1:C:396:VAL:HG13	1:C:423:ILE:HD11	2.03	0.40
1:D:32:PHE:CE2	1:D:74:TRP:CD1	3.09	0.40
1:D:395:LYS:HD2	1:D:462:TYR:CE1	2.56	0.40
1:D:395:LYS:HG3	1:D:460:TYR:HB3	2.03	0.40
1:B:61:GLN:O	5:B:2017:GOL:H12	2.21	0.40
1:A:128:GLY:N	1:A:129:PRO:CD	2.84	0.40
1:C:198:TYR:O	1:C:217:ARG:HA	2.22	0.40
1:C:58:ARG:HH22	1:C:117:SER:C	2.25	0.40
1:C:35:PHE:CG	1:C:36:PRO:HA	2.56	0.40
1:A:237:TRP:HB3	1:A:238:PRO:HD3	2.04	0.40
1:C:12:PHE:HB2	1:C:508:GLY:HA3	2.02	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%)	493 (93%)	35 (7%)	3 (1%)	33	32
1	B	531/535 (99%)	492 (93%)	36 (7%)	3 (1%)	33	32
1	C	531/535 (99%)	479 (90%)	44 (8%)	8 (2%)	15	10
1	D	531/535 (99%)	495 (93%)	32 (6%)	4 (1%)	27	24
All	All	2124/2140 (99%)	1959 (92%)	147 (7%)	18 (1%)	27	24

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	38	VAL
1	A	38	VAL
1	B	12	PHE
1	B	38	VAL
1	C	188	GLY
1	C	318	SER
1	D	38	VAL
1	D	456	ASP
1	A	12	PHE
1	A	307	GLY
1	C	178	PHE
1	D	12	PHE
1	D	450	ARG
1	C	207	THR
1	C	298	LYS
1	B	195	ASN
1	C	195	ASN
1	C	317	PRO

### 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%)	449 (96%)	19 (4%)	41	49
1	B	468/469 (100%)	452 (97%)	16 (3%)	49	59
1	C	468/469 (100%)	447 (96%)	21 (4%)	38	44
1	D	468/469 (100%)	454 (97%)	14 (3%)	53	64
All	All	1872/1876 (100%)	1802 (96%)	70 (4%)	45	54

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	59	LEU
1	A	90	THR
1	A	135	GLU
1	A	139	LYS
1	A	149	ARG
1	A	151	ASP
1	A	268	ARG
1	A	333	ASP
1	A	341	HIS
1	A	365	ARG
1	A	431	ARG
1	A	468	GLN
1	A	475	SER
1	A	495	LEU
1	A	503	ARG
1	A	516	ARG
1	A	522	ASN
1	A	531	LEU
1	B	3	LYS
1	B	10	THR
1	B	20	ARG
1	B	50	ARG
1	B	226	GLU
1	B	337	ASP
1	B	341	HIS
1	B	360	ARG
1	B	375	ARG
1	B	383	ARG
1	B	431	ARG
1	B	447	LEU

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Mol	Chain	Res	Type
1	B	457	ASP
1	B	481	MET
1	B	501	LYS
1	B	531	LEU
1	C	15	ASP
1	C	30	SER
1	C	60	SER
1	C	82	ASP
1	C	84	LYS
1	C	130	SER
1	C	151	ASP
1	C	173	GLU
1	C	194	ILE
1	C	257	THR
1	C	311	SER
1	C	332	ASP
1	C	333	ASP
1	C	341	HIS
1	C	360	ARG
1	C	365	ARG
1	C	383	ARG
1	C	384	ARG
1	C	433	LEU
1	C	447	LEU
1	C	501	LYS
1	D	59	LEU
1	D	65	ILE
1	D	142	VAL
1	D	151	ASP
1	D	173	GLU
1	D	255	THR
1	D	320	GLU
1	D	333	ASP
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	447	LEU
1	D	448	ARG
1	D	495	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	77	HIS
1	A	254	HIS
1	A	256	HIS
1	A	280	HIS
1	A	422	GLN
1	A	522	ASN
1	B	195	ASN
1	B	254	HIS
1	B	275	GLN
1	C	77	HIS
1	C	190	HIS
1	C	341	HIS
1	C	387	HIS
1	C	404	GLN
1	C	416	GLN
1	C	422	GLN
1	C	514	HIS
1	D	77	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	0.72	0	8,12,14	2.12	3 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	XYS	A	2006	2	10,10,10	1.85	3 (30%)	14,14,14	2.62	4 (28%)
2	XYS	B	2007	2	8,9,10	1.23	0	8,12,14	1.60	3 (37%)
2	XYS	B	2008	2	10,10,10	1.79	3 (30%)	14,14,14	2.69	4 (28%)
2	XYS	C	2009	2	8,9,10	0.77	0	8,12,14	1.29	1 (12%)
2	XYS	C	2010	2	10,10,10	2.42	6 (60%)	14,14,14	2.17	3 (21%)
2	XYS	D	2011	2	8,9,10	0.50	0	8,12,14	1.52	1 (12%)
2	XYS	D	2012	2	10,10,10	2.21	4 (40%)	14,14,14	2.23	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	1/1/3/4	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	1/1/3/4	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	1/1/3/4	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	1/1/3/4	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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2010	XYS	O5-C1	4.31	1.49	1.43
2	D	2012	XYS	C4-C3	3.83	1.57	1.52
2	A	2006	XYS	O4-C4	3.52	1.51	1.43
2	C	2010	XYS	O4-C4	3.48	1.51	1.43
2	B	2008	XYS	O5-C1	3.22	1.47	1.43
2	D	2012	XYS	O5-C1	3.11	1.47	1.43
2	C	2010	XYS	C4-C3	3.05	1.56	1.52
2	D	2012	XYS	O4-C4	2.95	1.50	1.43
2	B	2008	XYS	O4-C4	2.73	1.49	1.43
2	D	2012	XYS	C1-C2	2.60	1.57	1.52
2	B	2008	XYS	C4-C3	2.55	1.56	1.52
2	A	2006	XYS	O5-C1	2.37	1.46	1.43
2	A	2006	XYS	C4-C3	2.24	1.55	1.52
2	C	2010	XYS	C1-C2	2.20	1.57	1.52
2	C	2010	XYS	C5-C4	2.18	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2010	XYS	O5-C5	2.12	1.47	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2006	XYS	O5-C1-C2	7.32	119.72	109.24
2	B	2008	XYS	O4-C4-C3	6.58	123.00	110.23
2	D	2012	XYS	O4-C4-C3	5.96	121.80	110.23
2	B	2008	XYS	O4-C4-C5	-5.56	97.63	109.14
2	C	2010	XYS	O5-C1-C2	5.13	116.59	109.24
2	C	2010	XYS	O4-C4-C3	4.99	119.92	110.23
2	A	2006	XYS	O4-C4-C3	4.74	119.43	110.23
2	A	2005	XYS	C4-C3-C2	4.07	116.41	110.53
2	D	2012	XYS	O5-C1-C2	3.94	114.87	109.24
2	A	2005	XYS	C5-C4-C3	3.44	114.04	109.71
2	C	2009	XYS	O5-C5-C4	3.15	116.70	111.74
2	B	2008	XYS	O5-C5-C4	3.05	115.68	110.83
2	D	2011	XYS	O5-C5-C4	2.67	115.94	111.74
2	B	2007	XYS	O3-C3-C2	2.63	114.74	109.94
2	A	2006	XYS	O1-C1-O5	-2.49	103.07	109.88
2	B	2008	XYS	O5-C1-C2	2.43	112.72	109.24
2	A	2006	XYS	C1-C2-C3	2.42	114.37	110.53
2	B	2007	XYS	O4-C4-C3	-2.32	105.72	110.23
2	B	2007	XYS	O3-C3-C4	-2.28	105.92	110.03
2	C	2010	XYS	O5-C5-C4	2.18	114.30	110.83
2	A	2005	XYS	O2-C2-C3	-2.07	105.70	110.18
2	D	2012	XYS	C1-C2-C3	2.01	113.71	110.53

All (8) chirality outliers are listed below:

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

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	1.84	4 (33%)	16,16,16	5.35	9 (56%)
5	GOL	A	2016	-	5,5,5	0.37	0	5,5,5	0.91	0
4	MES	B	2014	-	12,12,12	2.07	4 (33%)	16,16,16	5.21	11 (68%)
5	GOL	B	2017	-	5,5,5	0.43	0	5,5,5	0.27	0
5	GOL	C	2018	-	5,5,5	0.29	0	5,5,5	0.35	0
4	MES	D	2015	-	12,12,12	8.47	4 (33%)	16,16,16	6.14	9 (56%)
5	GOL	D	2019	-	5,5,5	0.53	0	5,5,5	0.42	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	1/1/1/1
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	O3S-S	20.57	1.92	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2015	MES	O1S-S	15.24	1.81	1.45
4	D	2015	MES	O2S-S	13.11	1.76	1.45
4	D	2015	MES	C8-S	4.81	1.86	1.78
4	B	2014	MES	C8-S	4.11	1.85	1.78
4	A	2013	MES	O1S-S	3.81	1.54	1.45
4	B	2014	MES	O1S-S	3.36	1.53	1.45
4	A	2013	MES	C8-S	3.23	1.84	1.78
4	B	2014	MES	O3S-S	2.42	1.51	1.45
4	B	2014	MES	O2S-S	2.38	1.51	1.45
4	A	2013	MES	O3S-S	2.37	1.50	1.45
4	A	2013	MES	O2S-S	2.23	1.50	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2015	MES	O3S-S-O2S	-18.91	63.84	112.48
4	A	2013	MES	O3S-S-O2S	-13.00	79.05	112.48
4	B	2014	MES	O3S-S-O1S	-10.79	84.74	112.48
4	B	2014	MES	O3S-S-O2S	-10.68	85.01	112.48
4	A	2013	MES	O3S-S-O1S	-9.04	89.24	112.48
4	D	2015	MES	O3S-S-O1S	-8.87	89.66	112.48
4	B	2014	MES	O3S-S-C8	-8.71	83.52	105.99
4	A	2013	MES	O3S-S-C8	-7.90	85.61	105.99
4	D	2015	MES	O3S-S-C8	-7.64	86.30	105.99
4	A	2013	MES	C5-N4-C3	7.37	124.37	109.75
4	A	2013	MES	O2S-S-O1S	6.48	124.92	112.44
4	D	2015	MES	C5-N4-C3	6.20	122.06	109.75
4	D	2015	MES	O2S-S-C8	5.43	123.10	106.36
4	B	2014	MES	C5-N4-C3	5.23	120.11	109.75
4	B	2014	MES	O1S-S-C8	4.54	120.34	106.36
4	B	2014	MES	O1-C6-C5	4.38	116.56	111.34
4	B	2014	MES	O2S-S-C8	4.35	119.78	106.36
4	A	2013	MES	O2S-S-C8	3.67	117.66	106.36
4	D	2015	MES	O2S-S-O1S	3.43	119.06	112.44
4	B	2014	MES	C7-N4-C5	3.39	120.53	111.66
4	D	2015	MES	C7-N4-C3	3.28	120.23	111.66
4	B	2014	MES	O1-C2-C3	3.22	115.17	111.34
4	D	2015	MES	O1-C6-C5	2.97	114.89	111.34
4	B	2014	MES	C7-N4-C3	2.94	119.34	111.66
4	A	2013	MES	C7-N4-C5	2.87	119.15	111.66
4	A	2013	MES	O1S-S-C8	2.71	114.72	106.36
4	A	2013	MES	O1-C2-C3	-2.62	108.22	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2014	MES	O2S-S-O1S	2.40	117.07	112.44
4	D	2015	MES	C7-N4-C5	2.31	117.71	111.66

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2014	MES	C2-C3-C5-C6-N4-O1

## 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%)	-0.31	2 (0%) 90 92	13, 31, 47, 59	0
1	B	533/535 (99%)	-0.34	3 (0%) 86 88	15, 30, 46, 52	0
1	C	533/535 (99%)	0.59	40 (7%) 14 13	23, 49, 65, 73	0
1	D	533/535 (99%)	-0.21	3 (0%) 86 88	16, 33, 49, 56	0
All	All	2132/2140 (99%)	-0.07	48 (2%) 57 58	13, 35, 58, 73	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	151	ASP	4.0
1	C	21	VAL	3.5
1	C	364	LEU	3.4
1	C	482	ASN	3.4
1	C	326	LYS	3.2
1	C	46	LEU	3.1
1	A	151	ASP	3.0
1	C	481	MET	2.8
1	C	455	PRO	2.7
1	C	361	PRO	2.7
1	C	87	LEU	2.6
1	C	284	CYS	2.6
1	C	247	ALA	2.6
1	C	135	GLU	2.5
1	C	43	SER	2.5
1	C	483	TRP	2.5
1	C	173	GLU	2.5
1	C	484	ILE	2.5
1	C	524	TYR	2.4
1	D	273	GLU	2.4
1	C	50	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	337	ASP	2.4
1	C	220	SER	2.4
1	C	527	PHE	2.3
1	C	255	THR	2.3
1	C	454	VAL	2.3
1	C	262	LEU	2.3
1	C	468	GLN	2.3
1	C	260	TRP	2.2
1	A	320	GLU	2.2
1	D	151	ASP	2.2
1	C	83	GLY	2.2
1	C	273	GLU	2.2
1	C	298	LYS	2.2
1	C	328	TYR	2.2
1	C	457	ASP	2.1
1	B	141	LEU	2.1
1	C	86	TRP	2.1
1	C	222	TYR	2.1
1	D	481	MET	2.1
1	C	320	GLU	2.1
1	C	80	TYR	2.1
1	C	321	GLU	2.1
1	C	495	LEU	2.1
1	C	24	ASP	2.1
1	C	88	ILE	2.1
1	C	197	TYR	2.0
1	B	175	LYS	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( $\text{\AA}^2$ )	Q<0.9
2	XYS	B	2007	9/10	0.33	18.97	51,54,55,56	1
2	XYS	D	2011	9/10	0.35	14.89	55,56,57,59	1
2	XYS	C	2009	9/10	0.38	12.17	66,68,69,69	1
2	XYS	A	2005	9/10	0.29	8.64	55,57,58,58	1
2	XYS	A	2006	10/10	0.23	7.13	54,56,58,61	0
2	XYS	C	2010	10/10	0.48	5.84	67,70,71,72	0
2	XYS	D	2012	10/10	0.23	3.31	46,52,53,54	0
2	XYS	B	2008	10/10	0.23	2.31	47,54,57,58	0

## 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( $\text{\AA}^2$ )	Q<0.9
4	MES	D	2015	12/12	0.43	14.48	116,116,118,118	0
4	MES	B	2014	12/12	0.32	9.29	81,83,84,85	0
4	MES	A	2013	12/12	0.13	1.84	34,36,37,38	0
5	GOL	B	2017	6/6	0.14	1.38	40,41,43,46	0
5	GOL	A	2016	6/6	0.10	0.39	26,28,29,31	0
5	GOL	D	2019	6/6	0.09	0.03	25,25,27,32	0
5	GOL	C	2018	6/6	0.13	-0.07	33,37,40,41	0
3	CA	A	2001	1/1	0.06	-1.47	28,28,28,28	0
3	CA	D	2004	1/1	0.06	-1.98	37,37,37,37	0
3	CA	C	2003	1/1	0.08	-2.59	50,50,50,50	0
3	CA	B	2002	1/1	0.04	-3.88	29,29,29,29	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.