Full wwPDB X-ray Structure Validation Report (i)

Feb 6, 2024 – 08:54 AM EST

PDB ID	:	2EXH
Title	:	Structure of the family43 beta-Xylosidase from geobacillus stearothermophilus
Authors	:	Brux, C.; Niefind, K.; Shallom-Shezifi, D.; Yuval, S.; Schomburg, D.
Deposited on	:	2005-11-08
Resolution	:	1.88 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

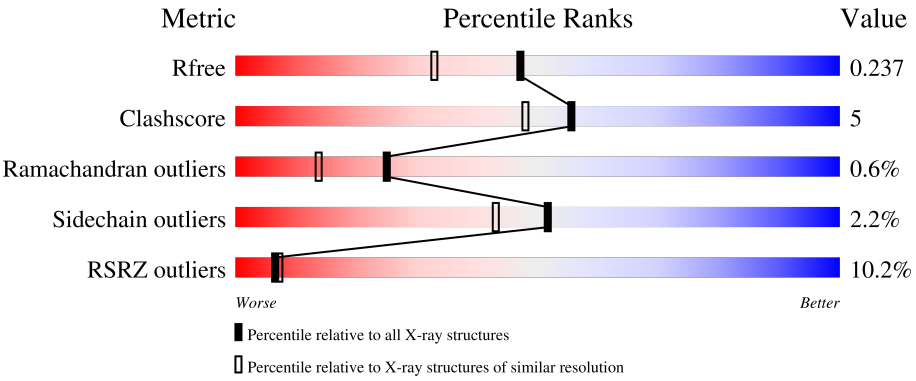
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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}	130704	9470 (1.90-1.86)
Clashscore	141614	10282 (1.90-1.86)
Ramachandran outliers	138981	10152 (1.90-1.86)
Sidechain outliers	138945	10152 (1.90-1.86)
RSRZ outliers	127900	9303 (1.90-1.86)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	535	3% 88% 11%
1	B	535	3% 89% 9%
1	C	535	31% 82% 17%
1	D	535	4% 88% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 19399 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.

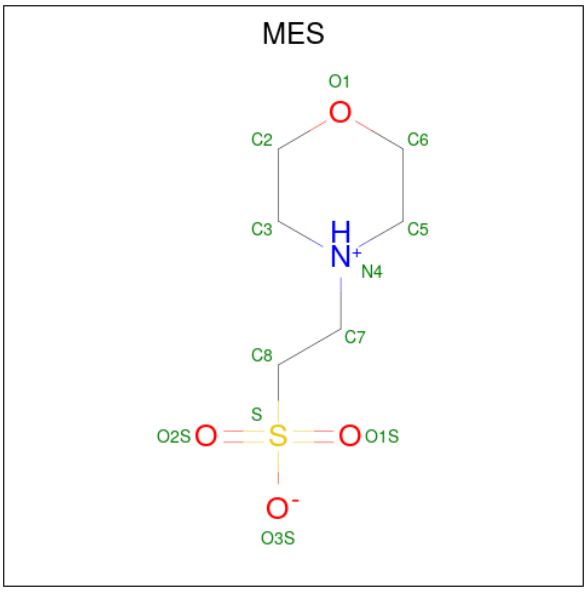
- Molecule 1 is a protein called beta-D-xylosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	533	Total	C	N	O	S	0	0	0
			4376	2814	748	804	10			
1	B	533	Total	C	N	O	S	0	0	0
			4376	2814	748	804	10			
1	C	533	Total	C	N	O	S	0	0	0
			4376	2814	748	804	10			
1	D	533	Total	C	N	O	S	0	0	0
			4376	2814	748	804	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

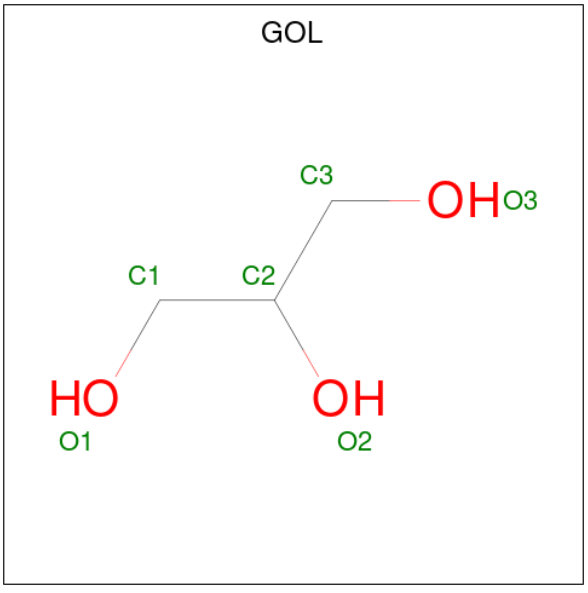
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 5 is water.

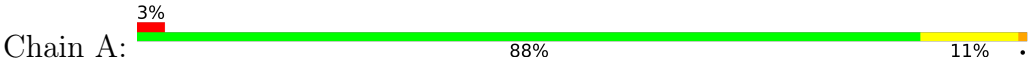
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	498	Total O 498 498	0	0
5	B	529	Total O 529 529	0	0
5	C	346	Total O 346 346	0	0
5	D	458	Total O 458 458	0	0

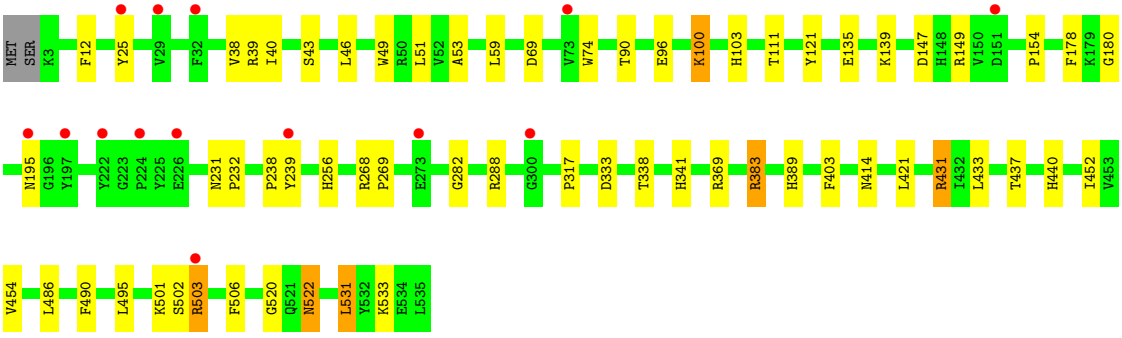
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 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

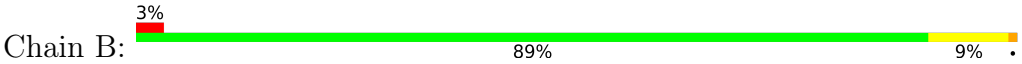
Chain A:

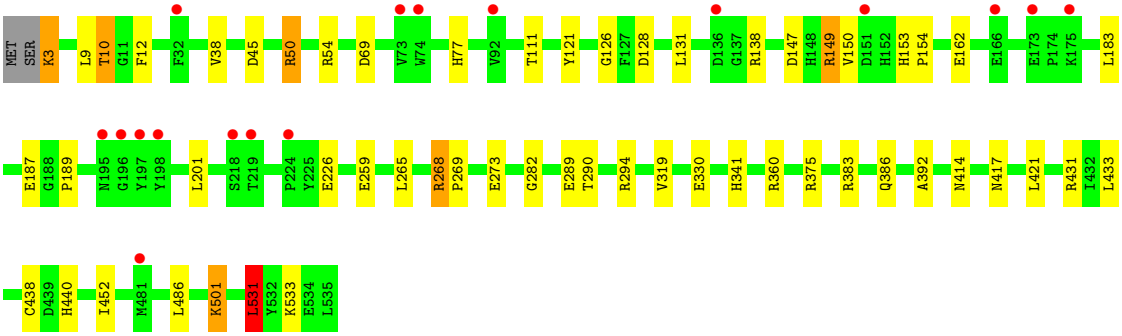




• Molecule 1: beta-D-xylosidase

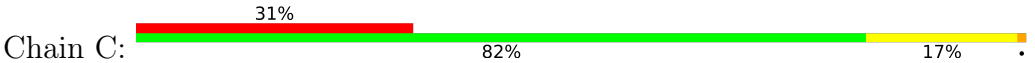
Chain B:

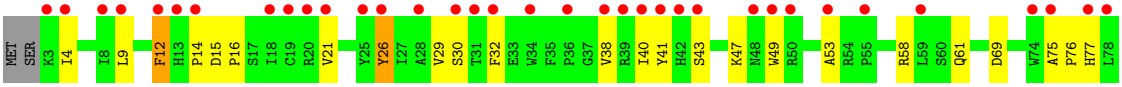


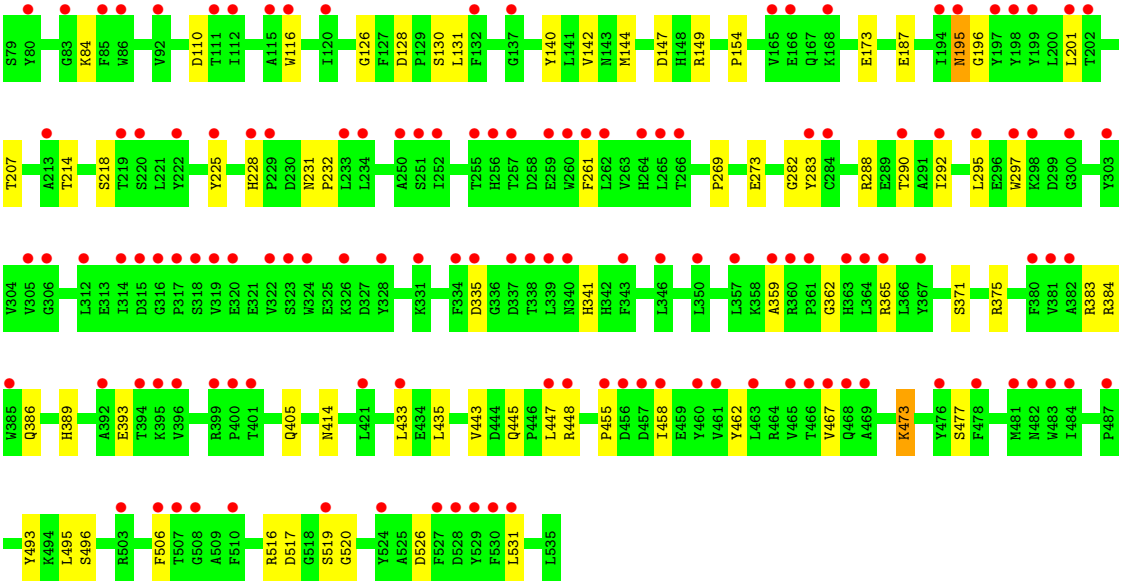


• Molecule 1: beta-D-xylosidase

Chain C:

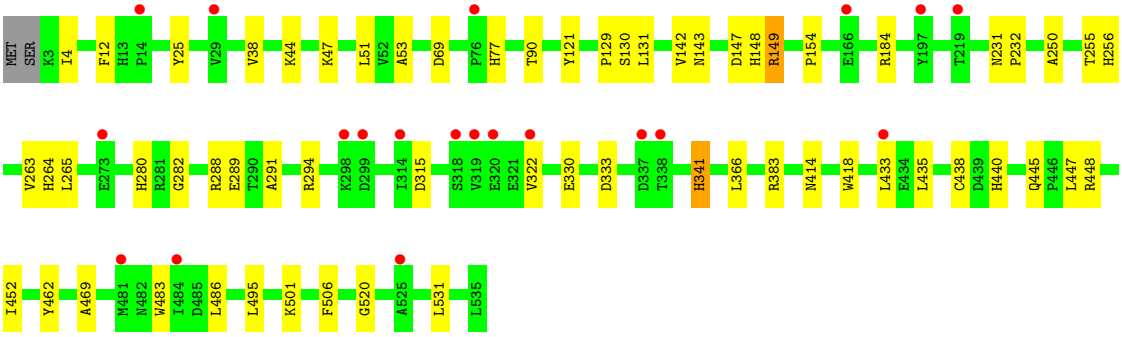






- Molecule 1: beta-D-xylosidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	140.03Å 140.03Å 231.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.88 38.63 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.88) 99.6 (38.63-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.90 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.286 0.237 , 0.237	Depositor DCC
R_{free} test set	9137 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19399	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, MES, GOL

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	0.40	0/4520	0.58	1/6160 (0.0%)
1	B	0.42	0/4520	0.60	3/6160 (0.0%)
1	C	0.38	0/4520	0.54	0/6160
1	D	0.40	0/4520	0.58	1/6160 (0.0%)
All	All	0.40	0/18080	0.57	5/24640 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	531	LEU	CA-CB-CG	7.90	133.48	115.30
1	A	531	LEU	CA-CB-CG	7.28	132.05	115.30
1	B	268	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	D	149	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	268	ARG	NE-CZ-NH1	5.08	122.84	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	4376	0	4163	38	0
1	B	4376	0	4163	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4376	0	4163	64	0
1	D	4376	0	4163	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	12	0	0
3	B	12	0	12	2	0
3	D	12	0	12	1	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	498	0	0	8	0
5	B	529	0	0	4	0
5	C	346	0	0	16	0
5	D	458	0	0	2	0
All	All	19399	0	16720	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	1.47	1.11
1:B:50:ARG:HG2	1:B:50:ARG:HH11	1.23	1.02
1:C:30:SER:HB3	5:C:2160:HOH:O	1.58	1.02
1:C:16:PRO:HA	5:C:2115:HOH:O	1.70	0.91
1:C:195:ASN:HD22	1:C:196:GLY:H	0.93	0.90
1:A:90:THR:HB	5:A:2248:HOH:O	1.73	0.88
1:C:195:ASN:HD22	1:C:196:GLY:N	1.72	0.87
1:A:369:ARG:NH2	1:A:522:ASN:ND2	2.21	0.87
1:C:195:ASN:ND2	1:C:196:GLY:H	1.73	0.85
1:A:369:ARG:NH2	1:A:522:ASN:HD22	1.73	0.85
1:D:90:THR:HB	5:D:2419:HOH:O	1.75	0.85
1:C:58:ARG:NH2	1:C:116:TRP:O	2.13	0.82
1:C:362:GLY:HA2	5:C:2085:HOH:O	1.80	0.81
1:A:147:ASP:OD1	1:A:149:ARG:HD2	1.81	0.80
1:C:29:VAL:HG12	5:C:2115:HOH:O	1.82	0.79
1:C:384:ARG:HG3	1:C:384:ARG:HH11	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:ASP:OD1	1:D:149:ARG:HD3	1.83	0.78
1:A:369:ARG:HH22	1:A:522:ASN:HD21	1.30	0.76
1:B:3:LYS:N	5:B:2524:HOH:O	2.19	0.76
1:B:268:ARG:HD3	1:B:289:GLU:OE2	1.86	0.76
1:B:50:ARG:HG2	1:B:50:ARG:NH1	2.01	0.73
1:C:41:TYR:HD1	5:C:2344:HOH:O	1.71	0.72
1:C:75:ALA:HA	5:C:2160:HOH:O	1.93	0.69
1:D:25:TYR:OH	1:D:256:HIS:HD2	1.76	0.68
1:D:255:THR:HB	5:D:2211:HOH:O	1.96	0.65
1:B:10:THR:HG23	1:B:386:GLN:O	1.96	0.65
1:A:533:LYS:HE2	5:A:2444:HOH:O	1.98	0.63
1:C:473:LYS:HA	5:C:2270:HOH:O	1.99	0.63
1:D:294:ARG:NH1	1:D:315:ASP:O	2.26	0.62
1:C:147:ASP:OD1	1:C:149:ARG:HD3	2.00	0.61
1:A:178:PHE:CE2	1:A:180:GLY:HA2	2.36	0.61
1:C:53:ALA:HB2	5:C:2025:HOH:O	1.99	0.61
1:D:433:LEU:HB2	1:D:452:ILE:HB	1.82	0.61
1:A:502:SER:O	1:A:503:ARG:HB2	2.02	0.60
1:B:268:ARG:CD	1:B:289:GLU:OE2	2.49	0.60
1:C:30:SER:CB	5:C:2160:HOH:O	2.32	0.59
1:A:96:GLU:OE2	1:A:502:SER:HB2	2.04	0.58
1:B:421:LEU:HD13	1:B:486:LEU:CD1	2.34	0.58
1:A:46:LEU:HD12	1:A:317:PRO:HG3	1.85	0.57
1:B:77:HIS:CD2	1:B:131:LEU:H	2.23	0.57
1:D:280:HIS:HD2	1:D:282:GLY:H	1.52	0.57
1:D:53:ALA:HA	3:D:2007:MES:H71	1.88	0.56
1:C:393:GLU:HB3	1:C:531:LEU:HB3	1.86	0.56
1:C:495:LEU:HG	5:C:2263:HOH:O	2.06	0.56
1:A:39:ARG:NH2	1:A:51:LEU:HD22	2.22	0.55
1:D:440:HIS:NE2	1:D:501:LYS:HG2	2.22	0.55
1:A:431:ARG:HD3	1:A:454:VAL:HB	1.89	0.54
1:C:140:TYR:HD2	5:C:2208:HOH:O	1.90	0.54
1:C:295:LEU:HG	5:C:2210:HOH:O	2.07	0.54
1:B:259:GLU:OE1	1:B:294:ARG:NH2	2.37	0.54
1:B:128:ASP:OD2	1:B:187:GLU:HG2	2.08	0.54
1:A:389:HIS:HB3	5:A:2187:HOH:O	2.08	0.54
1:B:421:LEU:HD13	1:B:486:LEU:HD11	1.90	0.54
1:D:4:ILE:HG12	1:D:47:LYS:HB2	1.88	0.54
1:A:111:THR:HG22	5:A:2289:HOH:O	2.08	0.54
1:B:330:GLU:OE1	1:B:533:LYS:HE2	2.07	0.54
1:A:269:PRO:HB3	1:A:282:GLY:HA3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:PRO:HA	1:B:201:LEU:O	2.09	0.53
1:C:21:VAL:HG23	1:C:26:TYR:HE2	1.73	0.53
1:C:371:SER:HA	1:C:516:ARG:HD2	1.89	0.53
1:D:77:HIS:CD2	1:D:131:LEU:H	2.27	0.53
1:A:433:LEU:HB2	1:A:452:ILE:HB	1.91	0.52
1:B:126:GLY:C	5:B:2274:HOH:O	2.48	0.52
1:A:501:LYS:HE2	5:A:2205:HOH:O	2.08	0.52
1:C:261:PHE:HB3	1:C:292:ILE:HD11	1.92	0.52
1:D:147:ASP:OD1	1:D:149:ARG:CD	2.56	0.51
1:C:12:PHE:CD1	1:C:14:PRO:HD3	2.45	0.51
1:D:445:GLN:O	1:D:448:ARG:HB2	2.10	0.51
1:B:431:ARG:HD3	5:B:2533:HOH:O	2.10	0.51
1:C:43:SER:HB2	1:C:49:TRP:CD2	2.46	0.51
1:A:421:LEU:HD13	1:A:486:LEU:HD11	1.94	0.50
1:B:54:ARG:H	3:B:2006:MES:H51	1.76	0.50
1:C:26:TYR:HA	1:C:41:TYR:O	2.12	0.49
1:D:51:LEU:HD23	1:D:341:HIS:CD2	2.47	0.49
1:C:77:HIS:CD2	1:C:131:LEU:H	2.29	0.49
1:A:111:THR:HG21	5:A:2074:HOH:O	2.11	0.49
1:A:421:LEU:HD13	1:A:486:LEU:CD1	2.43	0.49
1:C:384:ARG:HG3	1:C:384:ARG:NH1	2.22	0.48
1:C:493:TYR:O	1:C:496:SER:OG	2.26	0.48
1:D:447:LEU:HD21	1:D:486:LEU:HD22	1.94	0.48
1:C:335:ASP:HB2	5:C:2195:HOH:O	2.14	0.47
1:A:440:HIS:NE2	1:A:501:LYS:HG2	2.29	0.47
1:B:50:ARG:HH11	1:B:50:ARG:CG	2.06	0.47
1:B:147:ASP:OD1	1:B:149:ARG:HD3	2.15	0.47
1:C:389:HIS:HA	1:C:467:VAL:O	2.14	0.47
1:A:147:ASP:O	1:A:154:PRO:HA	2.14	0.47
1:B:69:ASP:CG	1:B:414:ASN:HB2	2.35	0.46
1:D:435:LEU:HD12	1:D:447:LEU:HD13	1.97	0.46
1:D:330:GLU:O	1:D:531:LEU:HA	2.16	0.46
1:B:9:LEU:HB2	1:B:290:THR:HB	1.98	0.46
1:B:10:THR:CG2	1:B:386:GLN:O	2.62	0.46
1:C:359:ALA:HB3	1:C:365:ARG:HD2	1.98	0.46
1:A:288:ARG:NH2	1:A:506:PHE:HB3	2.31	0.46
1:A:520:GLY:HA3	1:D:121:TYR:OH	2.16	0.46
1:C:9:LEU:HB2	1:C:290:THR:HB	1.98	0.45
1:B:375:ARG:HH12	1:C:375:ARG:HH12	1.63	0.45
1:D:462:TYR:HB3	1:D:483:TRP:CH2	2.51	0.45
1:C:462:TYR:HB2	1:C:477:SER:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TYR:OH	1:A:256:HIS:HD2	2.00	0.45
1:D:231:ASN:CG	1:D:232:PRO:HA	2.37	0.45
1:B:111:THR:HG22	5:B:2209:HOH:O	2.17	0.45
1:B:269:PRO:HB3	1:B:282:GLY:HA3	1.98	0.45
1:C:126:GLY:HA3	1:C:144:MET:O	2.17	0.45
1:D:129:PRO:HA	1:D:143:ASN:HB3	1.99	0.45
1:D:250:ALA:HA	1:D:263:VAL:O	2.16	0.45
1:B:452:ILE:HD12	1:B:452:ILE:H	1.82	0.44
1:C:288:ARG:NH2	1:C:506:PHE:HB3	2.32	0.44
1:D:130:SER:HB3	1:D:142:VAL:HG23	1.99	0.44
1:D:147:ASP:O	1:D:154:PRO:HA	2.17	0.44
1:A:431:ARG:NH2	5:A:2242:HOH:O	2.49	0.44
1:C:455:PRO:HB2	1:C:458:ILE:HG12	1.99	0.44
1:A:40:ILE:HB	1:A:53:ALA:HB3	1.98	0.44
1:A:43:SER:HB2	1:A:49:TRP:CE3	2.51	0.44
1:A:231:ASN:CG	1:A:232:PRO:HA	2.38	0.44
1:C:147:ASP:O	1:C:154:PRO:HA	2.17	0.44
1:C:61:GLN:HE22	1:C:116:TRP:HB2	1.82	0.44
1:A:383:ARG:HD2	5:A:2082:HOH:O	2.17	0.44
1:D:44:LYS:HB2	1:D:322:VAL:HB	1.98	0.44
1:C:231:ASN:CG	1:C:232:PRO:HA	2.38	0.44
1:C:435:LEU:HD12	1:C:447:LEU:HD13	1.99	0.44
1:A:74:TRP:CH2	1:A:100:LYS:HD3	2.53	0.44
1:B:121:TYR:OH	1:C:520:GLY:HA3	2.18	0.44
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.38	0.44
1:C:128:ASP:OD2	1:C:187:GLU:HB2	2.18	0.44
1:B:54:ARG:HE	3:B:2006:MES:H82	1.83	0.43
1:B:330:GLU:O	1:B:531:LEU:HA	2.17	0.43
1:D:280:HIS:CD2	1:D:282:GLY:H	2.32	0.43
1:C:283:TYR:CB	1:C:493:TYR:HB2	2.47	0.43
1:D:288:ARG:NH2	1:D:506:PHE:HB3	2.33	0.43
1:B:10:THR:CG2	1:B:386:GLN:HB3	2.48	0.43
1:C:297:TRP:HB3	5:C:2175:HOH:O	2.19	0.43
1:A:238:PRO:HG2	1:A:239:TYR:CE2	2.53	0.43
1:C:201:LEU:HD12	1:C:214:THR:O	2.17	0.43
1:C:218:SER:HB2	1:C:225:TYR:HA	2.00	0.43
1:D:265:LEU:HA	1:D:289:GLU:O	2.19	0.43
1:D:418:TRP:CE2	1:D:438:CYS:HB2	2.53	0.43
1:C:4:ILE:HG12	1:C:47:LYS:HB2	2.01	0.43
1:C:269:PRO:HB3	1:C:282:GLY:HA3	2.01	0.43
1:D:25:TYR:OH	1:D:256:HIS:CD2	2.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASP:O	1:B:154:PRO:HA	2.18	0.43
1:C:30:SER:HG	1:C:32:PHE:HE1	1.66	0.43
1:C:40:ILE:HB	1:C:53:ALA:HB3	1.99	0.43
1:D:69:ASP:CG	1:D:414:ASN:HB2	2.39	0.42
1:B:421:LEU:CD1	1:B:486:LEU:HD11	2.48	0.42
1:D:264:HIS:CE1	1:D:291:ALA:HB3	2.55	0.42
1:B:150:VAL:CG2	1:C:443:VAL:HG12	2.50	0.42
1:B:45:ASP:HA	1:B:319:VAL:HG21	2.02	0.42
1:C:371:SER:HA	1:C:516:ARG:CD	2.50	0.42
1:C:517:ASP:OD1	1:C:519:SER:OG	2.22	0.42
1:A:403:PHE:O	1:D:148:HIS:HE1	2.03	0.42
1:B:153:HIS:HA	1:B:154:PRO:HD3	1.87	0.42
1:C:130:SER:HB3	1:C:142:VAL:HG23	2.01	0.41
1:B:50:ARG:NH1	1:B:50:ARG:CG	2.71	0.41
1:A:121:TYR:OH	1:D:520:GLY:HA3	2.21	0.41
1:A:437:THR:HG21	1:A:490:PHE:HE1	1.85	0.41
1:B:433:LEU:HB3	1:B:452:ILE:HB	2.01	0.41
1:B:138:ARG:HD2	1:B:162:GLU:OE2	2.20	0.41
1:B:392:ALA:HA	1:B:531:LEU:O	2.20	0.41
1:C:228:HIS:HB3	1:C:231:ASN:HB2	2.03	0.41
1:C:365:ARG:HG2	1:C:526:ASP:OD1	2.19	0.41
1:B:265:LEU:HA	1:B:289:GLU:O	2.20	0.41
1:B:417:ASN:HA	1:B:438:CYS:O	2.21	0.41
1:C:15:ASP:HB2	5:C:2160:HOH:O	2.20	0.41
1:C:43:SER:HB2	1:C:49:TRP:CE3	2.56	0.41
1:C:76:PRO:HD3	5:C:2160:HOH:O	2.21	0.41
1:B:3:LYS:HE3	1:B:3:LYS:HB3	1.85	0.41
1:B:440:HIS:NE2	1:B:501:LYS:HD3	2.36	0.41
1:D:418:TRP:CZ2	1:D:438:CYS:HB2	2.56	0.41
1:C:283:TYR:HB2	1:C:493:TYR:HB2	2.03	0.40
1:A:69:ASP:CG	1:A:414:ASN:HB2	2.41	0.40
1:C:445:GLN:O	1:C:448:ARG:HG3	2.21	0.40
1:A:90:THR:HA	1:A:103:HIS:O	2.22	0.40
1:C:405:GLN:HA	1:C:516:ARG:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	531/535 (99%)	502 (94%)	26 (5%)	3 (1%)	25 14
1	B	531/535 (99%)	506 (95%)	23 (4%)	2 (0%)	34 22
1	C	531/535 (99%)	495 (93%)	32 (6%)	4 (1%)	19 9
1	D	531/535 (99%)	503 (95%)	25 (5%)	3 (1%)	25 14
All	All	2124/2140 (99%)	2006 (94%)	106 (5%)	12 (1%)	25 14

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	12	PHE
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	C	273	GLU
1	D	38	VAL
1	A	195	ASN
1	C	207	THR
1	D	469	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	469/471 (100%)	455 (97%)	14 (3%)	41 30
1	B	469/471 (100%)	457 (97%)	12 (3%)	46 36
1	C	469/471 (100%)	459 (98%)	10 (2%)	53 45
1	D	469/471 (100%)	463 (99%)	6 (1%)	69 64
All	All	1876/1884 (100%)	1834 (98%)	42 (2%)	52 43

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	100	LYS
1	A	135	GLU
1	A	139	LYS
1	A	268	ARG
1	A	333	ASP
1	A	338	THR
1	A	341	HIS
1	A	383	ARG
1	A	431	ARG
1	A	495	LEU
1	A	503	ARG
1	A	522	ASN
1	A	531	LEU
1	B	3	LYS
1	B	10	THR
1	B	50	ARG
1	B	149	ARG
1	B	183	LEU
1	B	226	GLU
1	B	273	GLU
1	B	341	HIS
1	B	360	ARG
1	B	383	ARG
1	B	501	LYS
1	B	531	LEU
1	C	26	TYR
1	C	84	LYS
1	C	110	ASP
1	C	173	GLU
1	C	195	ASN
1	C	341	HIS
1	C	383	ARG

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Mol	Chain	Res	Type
1	C	386	GLN
1	C	433	LEU
1	C	473	LYS
1	D	184	ARG
1	D	333	ASP
1	D	341	HIS
1	D	366	LEU
1	D	383	ARG
1	D	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	210	ASN
1	A	256	HIS
1	A	422	GLN
1	A	522	ASN
1	B	77	HIS
1	C	61	GLN
1	C	77	HIS
1	C	195	ASN
1	C	249	HIS
1	C	280	HIS
1	C	468	GLN
1	D	77	HIS
1	D	256	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	MES	D	2007	-	12,12,12	1.72	2 (16%)	14,16,16	10.27	9 (64%)
4	GOL	C	2010	-	5,5,5	0.39	0	5,5,5	0.31	0
4	GOL	D	2011	-	5,5,5	0.42	0	5,5,5	0.31	0
3	MES	B	2006	-	12,12,12	2.51	4 (33%)	14,16,16	7.03	8 (57%)
3	MES	A	2005	-	12,12,12	1.65	3 (25%)	14,16,16	6.58	8 (57%)
4	GOL	B	2009	-	5,5,5	0.36	0	5,5,5	0.48	0
4	GOL	A	2008	-	5,5,5	0.33	0	5,5,5	0.68	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
3	MES	D	2007	-	-	3/6/14/14	0/1/1/1
4	GOL	C	2010	-	-	2/4/4/4	-
4	GOL	D	2011	-	-	0/4/4/4	-
3	MES	B	2006	-	-	2/6/14/14	0/1/1/1
3	MES	A	2005	-	-	3/6/14/14	0/1/1/1
4	GOL	B	2009	-	-	3/4/4/4	-
4	GOL	A	2008	-	-	3/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2006	MES	C8-S	5.87	1.85	1.77
3	D	2007	MES	C8-S	4.87	1.84	1.77
3	B	2006	MES	O1S-S	4.61	1.58	1.45
3	A	2005	MES	C8-S	4.45	1.83	1.77
3	B	2006	MES	O2S-S	2.99	1.53	1.45
3	B	2006	MES	O3S-S	2.62	1.56	1.47
3	A	2005	MES	O2S-S	2.30	1.51	1.45
3	A	2005	MES	O1S-S	2.11	1.51	1.45
3	D	2007	MES	O1S-S	2.03	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2007	MES	O1S-S-C8	-19.77	83.11	106.92
3	D	2007	MES	O2S-S-C8	-19.22	83.77	106.92
3	D	2007	MES	O3S-S-C8	15.89	131.47	105.77
3	D	2007	MES	O3S-S-O2S	-14.30	76.32	111.27
3	B	2006	MES	O3S-S-C8	-14.25	82.72	105.77
3	D	2007	MES	O3S-S-O1S	-13.51	78.26	111.27
3	A	2005	MES	O3S-S-O2S	-11.65	82.81	111.27
3	B	2006	MES	O3S-S-O1S	-11.58	82.98	111.27
3	A	2005	MES	O3S-S-C8	-11.52	87.14	105.77
3	B	2006	MES	O3S-S-O2S	-11.28	83.71	111.27
3	A	2005	MES	O3S-S-O1S	-11.22	83.86	111.27
3	B	2006	MES	O1S-S-C8	10.03	118.99	106.92
3	A	2005	MES	O1S-S-C8	8.63	117.31	106.92
3	B	2006	MES	O2S-S-C8	8.52	117.17	106.92
3	A	2005	MES	O2S-S-C8	7.77	116.27	106.92
3	A	2005	MES	C5-N4-C3	7.10	124.81	108.83
3	D	2007	MES	C5-N4-C3	5.56	121.34	108.83
3	B	2006	MES	C5-N4-C3	5.32	120.81	108.83
3	D	2007	MES	O2S-S-O1S	5.07	131.50	113.95
3	B	2006	MES	C7-N4-C3	3.43	119.99	111.23
3	D	2007	MES	C7-N4-C3	3.36	119.83	111.23
3	B	2006	MES	C7-N4-C5	3.11	119.18	111.23
3	A	2005	MES	C7-N4-C5	3.07	119.08	111.23
3	D	2007	MES	C7-N4-C5	2.97	118.83	111.23
3	A	2005	MES	O2S-S-O1S	2.82	123.73	113.95

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2005	MES	C7-C8-S-O2S
3	B	2006	MES	C7-C8-S-O3S
3	D	2007	MES	N4-C7-C8-S
3	D	2007	MES	C7-C8-S-O3S
4	A	2008	GOL	O1-C1-C2-C3
4	B	2009	GOL	O1-C1-C2-C3
3	A	2005	MES	C7-C8-S-O3S
4	C	2010	GOL	O1-C1-C2-C3
4	A	2008	GOL	O1-C1-C2-O2
4	B	2009	GOL	O1-C1-C2-O2
3	A	2005	MES	C8-C7-N4-C3
3	B	2006	MES	C8-C7-N4-C5
4	B	2009	GOL	O2-C2-C3-O3
4	A	2008	GOL	O2-C2-C3-O3
4	C	2010	GOL	O1-C1-C2-O2
3	D	2007	MES	C8-C7-N4-C5

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2007	MES	1	0
3	B	2006	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

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	533/535 (99%)	0.32	14 (2%) 56 57	16, 29, 43, 49	0
1	B	533/535 (99%)	0.32	17 (3%) 47 49	16, 29, 43, 48	0
1	C	533/535 (99%)	1.60	167 (31%) 0 0	26, 46, 59, 66	0
1	D	533/535 (99%)	0.47	20 (3%) 40 42	17, 32, 46, 51	0
All	All	2132/2140 (99%)	0.68	218 (10%) 6 7	16, 34, 54, 66	0

All (218) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	261	PHE	6.4
1	C	255	THR	5.5
1	C	4	ILE	5.3
1	C	85	PHE	5.1
1	C	306	GLY	5.1
1	C	21	VAL	4.9
1	C	343	PHE	4.6
1	C	363	HIS	4.6
1	C	199	TYR	4.6
1	C	305	VAL	4.5
1	C	361	PRO	4.5
1	C	484	ILE	4.5
1	B	224	PRO	4.4
1	C	364	LEU	4.4
1	C	300	GLY	4.4
1	C	137	GLY	4.3
1	C	314	ILE	4.3
1	C	222	TYR	4.2
1	C	483	TRP	4.2
1	C	256	HIS	4.1
1	C	460	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	529	TYR	4.0
1	C	32	PHE	3.9
1	C	312	LEU	3.9
1	D	314	ILE	3.9
1	C	219	THR	3.9
1	C	40	ILE	3.8
1	C	197	TYR	3.8
1	C	508	GLY	3.8
1	D	320	GLU	3.7
1	C	233	LEU	3.6
1	A	195	ASN	3.6
1	A	151	ASP	3.6
1	C	262	LEU	3.6
1	C	385	TRP	3.5
1	C	531	LEU	3.5
1	C	468	GLN	3.5
1	C	25	TYR	3.5
1	C	26	TYR	3.5
1	C	339	LEU	3.5
1	C	38	VAL	3.4
1	B	173	GLU	3.3
1	C	257	THR	3.3
1	C	481	MET	3.3
1	C	18	ILE	3.3
1	C	319	VAL	3.3
1	B	197	TYR	3.3
1	C	86	TRP	3.3
1	C	50	ARG	3.3
1	C	334	PHE	3.2
1	C	8	ILE	3.2
1	C	360	ARG	3.2
1	C	455	PRO	3.2
1	C	12	PHE	3.2
1	C	41	TYR	3.2
1	C	324	TRP	3.1
1	B	219	THR	3.1
1	D	219	THR	3.1
1	C	74	TRP	3.1
1	C	9	LEU	3.1
1	C	527	PHE	3.1
1	C	318	SER	3.1
1	C	447	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	478	PHE	3.0
1	C	198	TYR	3.0
1	A	503	ARG	3.0
1	C	461	VAL	3.0
1	C	213	ALA	3.0
1	C	421	LEU	3.0
1	B	151	ASP	3.0
1	C	220	SER	3.0
1	D	299	ASP	3.0
1	C	338	THR	2.9
1	C	328	TYR	2.9
1	C	524	TYR	2.9
1	C	132	PHE	2.9
1	C	283	TYR	2.9
1	C	3	LYS	2.9
1	C	290	THR	2.9
1	C	322	VAL	2.9
1	C	381	VAL	2.8
1	C	448	ARG	2.8
1	D	197	TYR	2.8
1	C	487	PRO	2.8
1	A	224	PRO	2.8
1	C	359	ALA	2.8
1	C	292	ILE	2.8
1	B	175	LYS	2.8
1	D	318	SER	2.8
1	A	73	VAL	2.8
1	C	78	LEU	2.8
1	C	194	ILE	2.8
1	C	317	PRO	2.7
1	A	32	PHE	2.7
1	C	510	PHE	2.7
1	C	250	ALA	2.7
1	C	396	VAL	2.7
1	C	400	PRO	2.7
1	C	476	TYR	2.7
1	C	20	ARG	2.7
1	C	458	ILE	2.7
1	C	469	ALA	2.7
1	D	525	ALA	2.7
1	A	222	TYR	2.7
1	C	506	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	234	LEU	2.7
1	C	112	ILE	2.6
1	C	457	ASP	2.6
1	D	298	LYS	2.6
1	C	463	LEU	2.6
1	C	202	THR	2.6
1	C	456	ASP	2.6
1	C	30	SER	2.6
1	C	260	TRP	2.6
1	C	350	LEU	2.6
1	C	394	THR	2.6
1	D	433	LEU	2.6
1	C	335	ASP	2.6
1	C	14	PRO	2.6
1	C	55	PRO	2.6
1	C	92	VAL	2.6
1	B	198	TYR	2.6
1	C	195	ASN	2.6
1	C	28	ALA	2.6
1	C	382	ALA	2.6
1	C	39	ARG	2.6
1	A	197	TYR	2.6
1	C	116	TRP	2.6
1	D	76	PRO	2.6
1	C	507	THR	2.6
1	C	259	GLU	2.6
1	C	482	ASN	2.5
1	D	337	ASP	2.5
1	C	48	ASN	2.5
1	C	357	LEU	2.5
1	C	49	TRP	2.5
1	A	29	VAL	2.5
1	B	166	GLU	2.5
1	B	74	TRP	2.5
1	C	295	LEU	2.4
1	C	251	SER	2.4
1	C	466	THR	2.4
1	C	519	SER	2.4
1	C	346	LEU	2.4
1	C	229	PRO	2.4
1	C	201	LEU	2.4
1	A	239	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	218	SER	2.4
1	C	392	ALA	2.4
1	C	166	GLU	2.4
1	C	165	VAL	2.4
1	C	59	LEU	2.3
1	C	53	ALA	2.3
1	C	316	GLY	2.3
1	C	331	LYS	2.3
1	C	77	HIS	2.3
1	A	300	GLY	2.3
1	C	528	ASP	2.3
1	B	73	VAL	2.3
1	D	319	VAL	2.3
1	C	75	ALA	2.3
1	A	273	GLU	2.3
1	C	298	LYS	2.3
1	D	484	ILE	2.3
1	C	115	ALA	2.3
1	B	195	ASN	2.3
1	C	13	HIS	2.3
1	C	399	ARG	2.3
1	C	467	VAL	2.3
1	D	322	VAL	2.3
1	D	338	THR	2.3
1	C	225	TYR	2.2
1	C	228	HIS	2.3
1	C	303	TYR	2.2
1	B	481	MET	2.2
1	C	31	THR	2.2
1	C	252	ILE	2.2
1	C	365	ARG	2.2
1	C	264	HIS	2.2
1	B	196	GLY	2.2
1	C	80	TYR	2.2
1	D	481	MET	2.2
1	B	92	VAL	2.2
1	D	29	VAL	2.2
1	C	34	TRP	2.2
1	C	297	TRP	2.2
1	C	433	LEU	2.2
1	D	14	PRO	2.2
1	C	395	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	226	GLU	2.2
1	C	320	GLU	2.2
1	B	136	ASP	2.2
1	C	380	PHE	2.2
1	C	43	SER	2.1
1	C	503	ARG	2.1
1	B	32	PHE	2.1
1	C	266	THR	2.1
1	C	337	ASP	2.1
1	C	265	LEU	2.1
1	C	42	HIS	2.1
1	C	36	PRO	2.1
1	C	401	THR	2.1
1	C	465	VAL	2.1
1	C	326	LYS	2.1
1	C	120	ILE	2.1
1	C	83	GLY	2.1
1	A	25	TYR	2.1
1	C	367	TYR	2.1
1	C	530	PHE	2.1
1	C	315	ASP	2.1
1	C	284	CYS	2.1
1	C	323	SER	2.0
1	D	166	GLU	2.0
1	D	273	GLU	2.0
1	C	340	ASN	2.0
1	C	168	LYS	2.0
1	C	111	THR	2.0
1	C	19	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MES	B	2006	12/12	0.62	0.30	76,77,78,78	0
3	MES	D	2007	12/12	0.71	0.39	96,97,97,98	0
2	CA	C	2003	1/1	0.80	0.10	61,61,61,61	0
4	GOL	B	2009	6/6	0.83	0.22	38,38,39,39	0
4	GOL	C	2010	6/6	0.89	0.11	33,36,36,37	0
4	GOL	A	2008	6/6	0.90	0.13	24,26,27,27	0
2	CA	D	2004	1/1	0.94	0.09	35,35,35,35	0
3	MES	A	2005	12/12	0.96	0.11	29,33,34,34	0
4	GOL	D	2011	6/6	0.96	0.09	24,26,28,29	0
2	CA	A	2001	1/1	0.97	0.03	27,27,27,27	0
2	CA	B	2002	1/1	0.99	0.05	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.