



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:23 AM UTC

PDB ID : 2EXH / pdb_00002exh
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

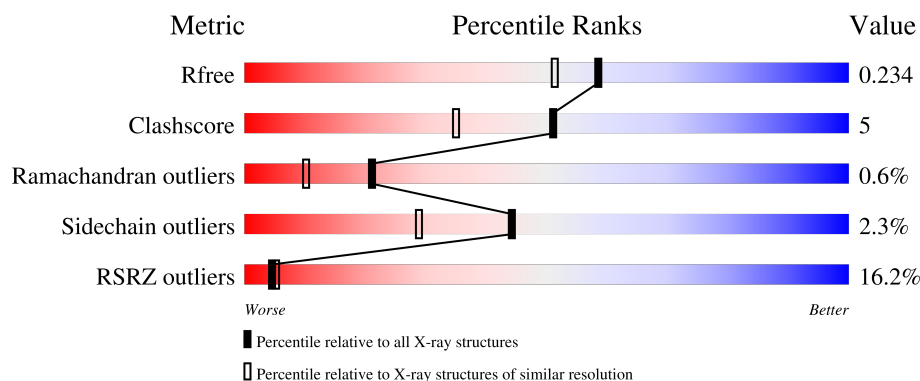
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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 $\leq 5\%$. 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% 10%
1	B	535	6% 90% 9%
1	C	535	51% 81% 17%
1	D	535	4% 88% 12%

2 Entry composition

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 (CCD ID: 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 (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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 (CCD ID: GOL) (formula: C₃H₈O₃).



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	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

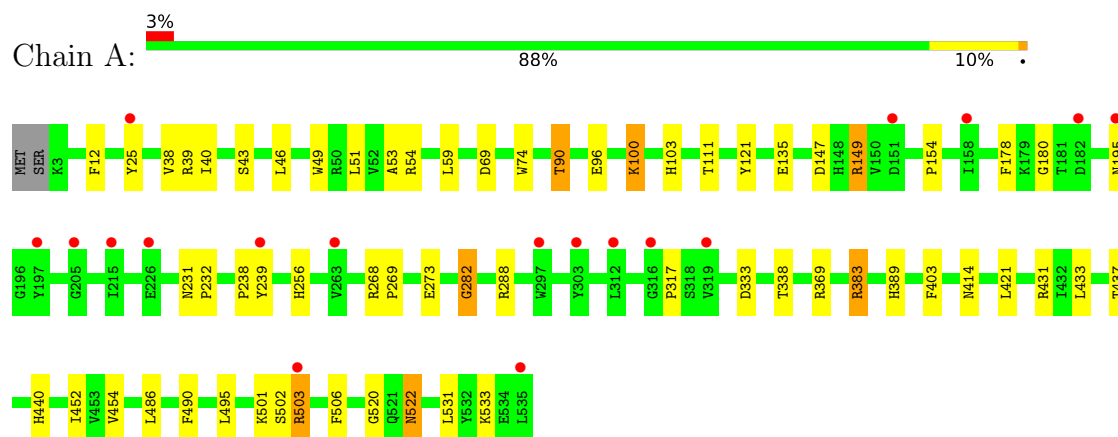
- Molecule 5 is water.

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

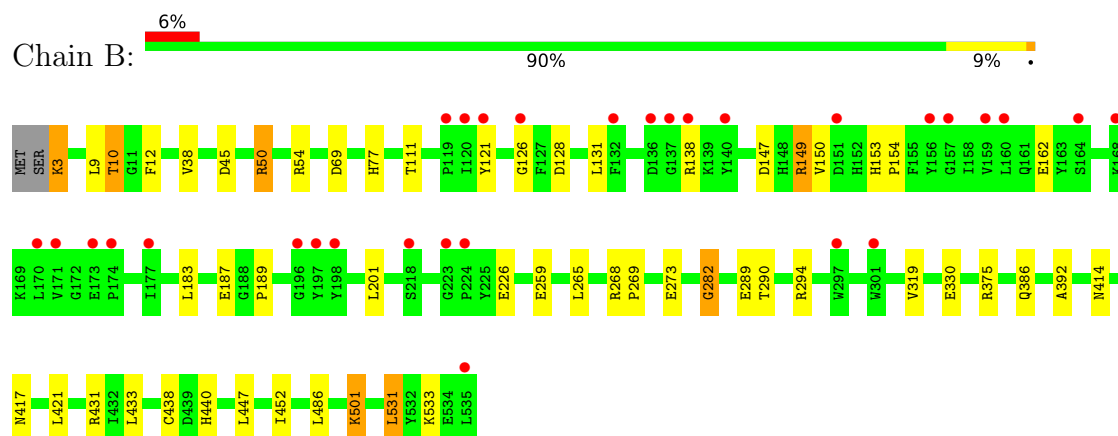
3 Residue-property plots

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.

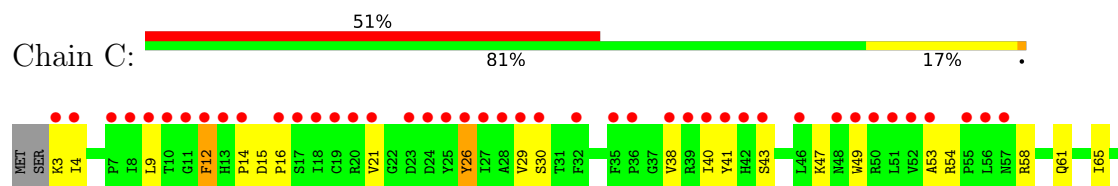
- Molecule 1: beta-D-xylosidase

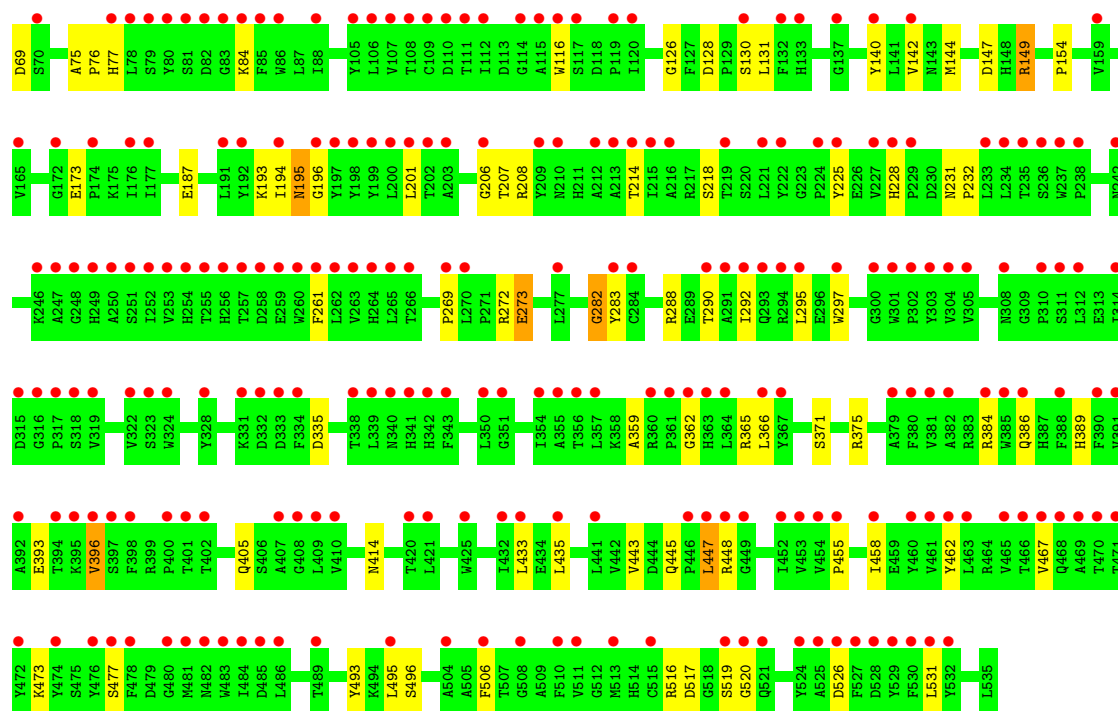


- Molecule 1: beta-D-xylosidase

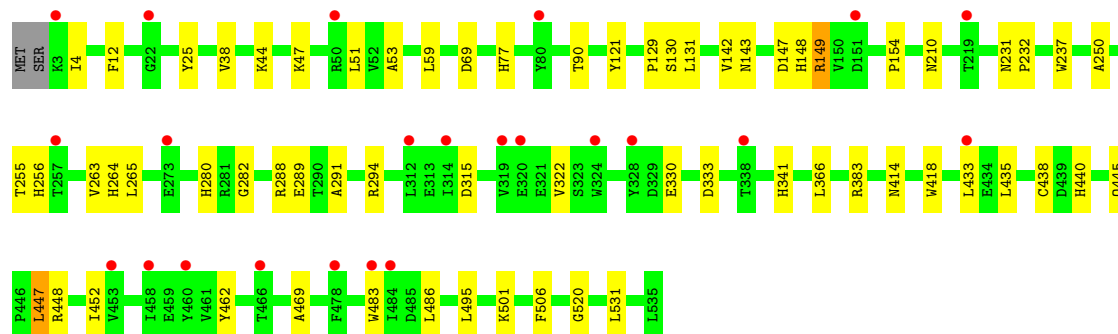
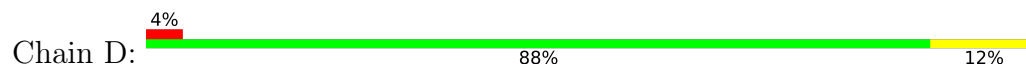


- Molecule 1: beta-D-xylosidase





● Molecule 1: beta-D-xylosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.03Å 140.03Å 231.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.88 40.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-1.88) 99.7 (40.00-1.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 1.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.233 , 0.286 0.235 , 0.234	Depositor DCC
R_{free} test set	9137 reflections (4.90%)	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 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	0/4520	0.73	3/6160 (0.0%)
1	B	0.51	0/4520	0.76	1/6160 (0.0%)
1	C	0.48	0/4520	0.73	4/6160 (0.1%)
1	D	0.51	0/4520	0.74	0/6160
All	All	0.50	0/18080	0.74	8/24640 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	282	GLY	N-CA-C	6.86	119.12	111.85
1	B	282	GLY	N-CA-C	6.04	118.26	111.85
1	C	54	ARG	CA-C-N	5.57	124.76	118.97
1	C	54	ARG	C-N-CA	5.57	124.76	118.97
1	C	396	VAL	N-CA-C	5.25	115.67	108.12
1	A	282	GLY	N-CA-C	5.06	117.21	111.85
1	A	54	ARG	CA-C-N	5.02	124.62	119.05
1	A	54	ARG	C-N-CA	5.02	124.62	119.05

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	43	0
1	C	4376	0	4163	66	0
1	D	4376	0	4163	36	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	177	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 (177) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:ARG:HG3	1:C:384:ARG:HH11	1.48	0.79
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:B:126:GLY:C	5:B:2274:HOH:O	2.48	0.57
1:C:517:ASP:OD1	1:C:519:SER:OG	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:69:ASP:CG	1:B:414:ASN:HB2	2.35	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:D:231:ASN:CG	1:D:232:PRO:HA	2.37	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:231:ASN:CG	1:A:232:PRO:HA	2.38	0.49
1:A:421:LEU:HD13	1:A:486:LEU:CD1	2.43	0.49
1:C:69:ASP:CG	1:C:414:ASN:HB2	2.38	0.49
1:C:231:ASN:CG	1:C:232:PRO:HA	2.38	0.48
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:D:69:ASP:CG	1:D:414:ASN:HB2	2.39	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:D:210:ASN:HD22	1:D:237:TRP:CD1	2.33	0.47
1:A:147:ASP:O	1:A:154:PRO:HA	2.14	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:69:ASP:CG	1:A:414:ASN:HB2	2.41	0.45
1:C:462:TYR:HB2	1:C:477:SER:HB3	1.97	0.45
1:A:25:TYR:OH	1:A:256:HIS:HD2	2.00	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:C:147:ASP:O	1:C:154:PRO:HA	2.17	0.44
1:B:265:LEU:C	1:B:265:LEU:HD12	2.41	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:C:272:ARG:O	1:C:273:GLU:C	2.60	0.44
1:D:44:LYS:HB2	1:D:322:VAL:HB	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:147:ASP:O	1:B:154:PRO:HA	2.18	0.43
1:C:40:ILE:HB	1:C:53:ALA:HB3	1.99	0.43
1:C:206:GLY:C	1:C:208:ARG:H	2.27	0.43
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: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:193:LYS:C	1:C:194:ILE:HG13	2.45	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: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%)	21	10
1	B	531/535 (99%)	506 (95%)	23 (4%)	2 (0%)	30	18
1	C	531/535 (99%)	495 (93%)	32 (6%)	4 (1%)	16	5
1	D	531/535 (99%)	503 (95%)	25 (5%)	3 (1%)	21	10
All	All	2124/2140 (99%)	2006 (94%)	106 (5%)	12 (1%)	21	10

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%)	36	19
1	B	469/471 (100%)	459 (98%)	10 (2%)	47	32
1	C	469/471 (100%)	457 (97%)	12 (3%)	40	24
1	D	469/471 (100%)	462 (98%)	7 (2%)	57	46
All	All	1876/1884 (100%)	1833 (98%)	43 (2%)	44	29

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	LEU
1	A	90	THR
1	A	100	LYS
1	A	135	GLU
1	A	149	ARG
1	A	268	ARG
1	A	273	GLU
1	A	333	ASP
1	A	338	THR
1	A	383	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	447	LEU
1	B	501	LYS
1	B	531	LEU
1	C	3	LYS
1	C	26	TYR
1	C	65	ILE
1	C	84	LYS
1	C	149	ARG
1	C	173	GLU
1	C	195	ASN
1	C	366	LEU
1	C	386	GLN

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Mol	Chain	Res	Type
1	C	396	VAL
1	C	433	LEU
1	C	447	LEU
1	D	59	LEU
1	D	149	ARG
1	D	333	ASP
1	D	366	LEU
1	D	383	ARG
1	D	447	LEU
1	D	495	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	HIS
1	A	98	GLN
1	A	210	ASN
1	A	256	HIS
1	A	275	GLN
1	A	389	HIS
1	A	422	GLN
1	A	522	ASN
1	B	77	HIS
1	B	98	GLN
1	B	104	ASN
1	B	152	HIS
1	B	210	ASN
1	C	61	GLN
1	C	77	HIS
1	C	195	ASN
1	C	210	ASN
1	C	249	HIS
1	C	389	HIS
1	C	468	GLN
1	C	521	GLN
1	D	77	HIS
1	D	195	ASN
1	D	256	HIS
1	D	280	HIS
1	D	422	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

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	GOL	C	2010	-	5,5,5	0.40	0	5,5,5	0.35	0
3	MES	D	2007	-	12,12,12	1.74	2 (16%)	15,16,16	8.56	9 (60%)
4	GOL	D	2011	-	5,5,5	0.42	0	5,5,5	0.35	0
4	GOL	B	2009	-	5,5,5	0.37	0	5,5,5	0.51	0
3	MES	A	2005	-	12,12,12	1.67	3 (25%)	15,16,16	5.87	8 (53%)
3	MES	B	2006	-	12,12,12	2.56	4 (33%)	15,16,16	6.12	8 (53%)
4	GOL	A	2008	-	5,5,5	0.33	0	5,5,5	0.71	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	GOL	C	2010	-	-	2/4/4/4	-
3	MES	D	2007	-	-	3/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	2011	-	-	0/4/4/4	-
4	GOL	B	2009	-	-	3/4/4/4	-
3	MES	A	2005	-	-	3/6/14/14	0/1/1/1
3	MES	B	2006	-	-	2/6/14/14	0/1/1/1
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	5.89	1.85	1.77
3	D	2007	MES	C8-S	4.88	1.84	1.77
3	B	2006	MES	O1S-S	4.79	1.58	1.45
3	A	2005	MES	C8-S	4.45	1.83	1.77
3	B	2006	MES	O2S-S	3.10	1.53	1.45
3	B	2006	MES	O3S-S	2.59	1.56	1.47
3	A	2005	MES	O2S-S	2.37	1.51	1.45
3	A	2005	MES	O1S-S	2.18	1.51	1.45
3	D	2007	MES	O1S-S	2.10	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2007	MES	O1S-S-C8	-15.63	83.11	106.73
3	D	2007	MES	O2S-S-C8	-15.19	83.77	106.73
3	D	2007	MES	O3S-S-O2S	-14.02	76.32	111.40
3	D	2007	MES	O3S-S-O1S	-13.24	78.26	111.40
3	D	2007	MES	O3S-S-C8	13.02	131.47	106.00
3	B	2006	MES	O3S-S-C8	-11.90	82.72	106.00
3	A	2005	MES	O3S-S-O2S	-11.43	82.81	111.40
3	B	2006	MES	O3S-S-O1S	-11.36	82.98	111.40
3	B	2006	MES	O3S-S-O2S	-11.07	83.71	111.40
3	A	2005	MES	O3S-S-O1S	-11.01	83.86	111.40
3	A	2005	MES	O3S-S-C8	-9.64	87.14	106.00
3	B	2006	MES	O1S-S-C8	8.12	118.99	106.73
3	A	2005	MES	C5-N4-C3	7.42	124.81	108.84
3	A	2005	MES	O1S-S-C8	7.00	117.31	106.73
3	B	2006	MES	O2S-S-C8	6.91	117.17	106.73
3	A	2005	MES	O2S-S-C8	6.32	116.27	106.73
3	D	2007	MES	C5-N4-C3	5.80	121.34	108.84
3	B	2006	MES	C5-N4-C3	5.56	120.81	108.84
3	D	2007	MES	O2S-S-O1S	5.43	131.50	113.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2006	MES	C7-N4-C3	3.29	119.99	111.24
3	D	2007	MES	C7-N4-C3	3.22	119.83	111.24
3	A	2005	MES	O2S-S-O1S	3.04	123.73	113.82
3	B	2006	MES	C7-N4-C5	2.98	119.18	111.24
3	A	2005	MES	C7-N4-C5	2.94	119.08	111.24
3	D	2007	MES	C7-N4-C5	2.85	118.83	111.24

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	C7-C8-S-O3S
4	A	2008	GOL	O1-C1-C2-C3
3	A	2005	MES	C7-C8-S-O3S
4	B	2009	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-C3
3	D	2007	MES	N4-C7-C8-S
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 ⓘ

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, 95th 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%)	0.43	18 (3%) 48 53	16, 29, 43, 49	0
1	B	533/535 (99%)	0.46	30 (5%) 30 32	16, 29, 43, 48	0
1	C	533/535 (99%)	2.11	274 (51%) 0 0	26, 46, 59, 66	0
1	D	533/535 (99%)	0.65	23 (4%) 40 43	17, 32, 46, 51	0
All	All	2132/2140 (99%)	0.91	345 (16%) 4 5	16, 34, 54, 66	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	85	PHE	5.8
1	C	314	ILE	5.5
1	C	4	ILE	5.0
1	C	458	ILE	5.0
1	C	324	TRP	4.9
1	C	21	VAL	4.8
1	C	25	TYR	4.7
1	C	343	PHE	4.7
1	C	357	LEU	4.4
1	C	364	LEU	4.4
1	C	461	VAL	4.3
1	C	290	THR	4.3
1	C	260	TRP	4.3
1	C	319	VAL	4.2
1	C	334	PHE	4.2
1	C	467	VAL	4.2
1	C	460	TYR	4.2
1	C	483	TRP	4.1
1	C	454	VAL	4.1
1	C	40	ILE	4.0
1	C	519	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	529	TYR	4.0
1	C	385	TRP	4.0
1	C	261	PHE	4.0
1	A	151	ASP	3.9
1	C	247	ALA	3.9
1	C	116	TRP	3.9
1	C	17	SER	3.9
1	C	292	ILE	3.9
1	C	527	PHE	3.9
1	C	112	ILE	3.8
1	C	43	SER	3.8
1	C	234	LEU	3.8
1	C	317	PRO	3.8
1	C	255	THR	3.8
1	D	314	ILE	3.8
1	C	53	ALA	3.7
1	C	213	ALA	3.7
1	C	469	ALA	3.7
1	C	8	ILE	3.7
1	C	9	LEU	3.7
1	C	478	PHE	3.7
1	C	328	TYR	3.7
1	A	195	ASN	3.6
1	B	126	GLY	3.6
1	C	202	THR	3.6
1	C	38	VAL	3.6
1	C	339	LEU	3.6
1	C	41	TYR	3.5
1	C	222	TYR	3.5
1	C	256	HIS	3.5
1	C	396	VAL	3.5
1	C	200	LEU	3.5
1	C	265	LEU	3.5
1	C	16	PRO	3.5
1	C	257	THR	3.5
1	C	322	VAL	3.5
1	C	248	GLY	3.5
1	C	49	TRP	3.5
1	C	11	GLY	3.5
1	C	80	TYR	3.4
1	C	18	ILE	3.4
1	C	252	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	465	VAL	3.4
1	C	338	THR	3.4
1	C	26	TYR	3.4
1	C	137	GLY	3.4
1	D	319	VAL	3.4
1	C	530	PHE	3.4
1	C	284	CYS	3.3
1	C	77	HIS	3.3
1	D	453	VAL	3.3
1	C	531	LEU	3.3
1	C	235	THR	3.3
1	C	86	TRP	3.3
1	C	19	CYS	3.3
1	C	532	TYR	3.3
1	C	120	ILE	3.3
1	C	42	HIS	3.3
1	C	312	LEU	3.3
1	C	508	GLY	3.3
1	C	476	TYR	3.2
1	C	291	ALA	3.2
1	C	199	TYR	3.2
1	C	520	GLY	3.2
1	C	264	HIS	3.2
1	C	159	VAL	3.2
1	A	316	GLY	3.2
1	C	172	GLY	3.2
1	C	333	ASP	3.2
1	C	462	TYR	3.1
1	C	366	LEU	3.1
1	C	212	ALA	3.1
1	C	55	PRO	3.1
1	C	283	TYR	3.1
1	C	29	VAL	3.1
1	D	320	GLU	3.1
1	C	224	PRO	3.1
1	C	251	SER	3.1
1	C	88	ILE	3.1
1	C	463	LEU	3.1
1	C	455	PRO	3.1
1	C	191	LEU	3.0
1	C	303	TYR	3.0
1	C	228	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	196	GLY	3.0
1	C	196	GLY	3.0
1	C	115	ALA	3.0
1	C	392	ALA	3.0
1	C	78	LEU	3.0
1	C	233	LEU	3.0
1	C	350	LEU	3.0
1	B	197	TYR	3.0
1	B	198	TYR	3.0
1	C	301	TRP	3.0
1	D	22	GLY	3.0
1	C	468	GLN	3.0
1	C	308	ASN	3.0
1	C	140	TYR	3.0
1	D	483	TRP	3.0
1	B	223	GLY	2.9
1	C	250	ALA	2.9
1	C	354	ILE	2.9
1	C	39	ARG	2.9
1	C	466	THR	2.9
1	C	237	TRP	2.9
1	C	249	HIS	2.9
1	B	151	ASP	2.9
1	C	323	SER	2.9
1	C	484	ILE	2.9
1	B	171	VAL	2.9
1	C	10	THR	2.9
1	C	524	TYR	2.9
1	C	32	PHE	2.9
1	C	201	LEU	2.9
1	C	221	LEU	2.9
1	C	295	LEU	2.9
1	C	108	THR	2.8
1	C	227	VAL	2.8
1	B	174	PRO	2.8
1	B	173	GLU	2.8
1	C	482	ASN	2.8
1	D	484	ILE	2.8
1	D	257	THR	2.8
1	C	13	HIS	2.8
1	C	381	VAL	2.8
1	C	198	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	28	ALA	2.8
1	C	510	PHE	2.8
1	C	304	VAL	2.8
1	C	225	TYR	2.8
1	C	481	MET	2.8
1	C	448	ARG	2.8
1	C	254	HIS	2.8
1	C	363	HIS	2.8
1	C	219	THR	2.8
1	D	458	ILE	2.8
1	C	238	PRO	2.8
1	C	379	ALA	2.7
1	C	402	THR	2.7
1	B	535	LEU	2.7
1	C	400	PRO	2.7
1	C	305	VAL	2.7
1	C	386	GLN	2.7
1	C	84	LYS	2.7
1	C	474	TYR	2.7
1	C	109	CYS	2.7
1	C	388	PHE	2.7
1	C	46	LEU	2.7
1	C	486	LEU	2.7
1	C	236	SER	2.7
1	C	263	VAL	2.7
1	C	504	ALA	2.7
1	B	121	TYR	2.7
1	C	197	TYR	2.7
1	C	262	LEU	2.7
1	C	302	PRO	2.7
1	C	447	LEU	2.7
1	C	506	PHE	2.6
1	C	36	PRO	2.6
1	C	203	ALA	2.6
1	C	471	THR	2.6
1	B	218	SER	2.6
1	C	485	ASP	2.6
1	C	489	THR	2.6
1	C	398	PHE	2.6
1	A	312	LEU	2.6
1	C	27	ILE	2.6
1	C	215	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	315	ASP	2.6
1	C	332	ASP	2.6
1	C	316	GLY	2.6
1	C	395	LYS	2.6
1	D	3	LYS	2.6
1	C	453	VAL	2.6
1	B	119	PRO	2.5
1	C	229	PRO	2.5
1	C	310	PRO	2.5
1	C	515	CYS	2.5
1	C	132	PHE	2.5
1	C	277	LEU	2.5
1	B	157	GLY	2.5
1	C	52	VAL	2.5
1	C	50	ARG	2.5
1	C	293	GLN	2.5
1	C	521	GLN	2.5
1	C	361	PRO	2.5
1	C	311	SER	2.5
1	C	216	ALA	2.5
1	C	355	ALA	2.5
1	C	390	PHE	2.5
1	C	340	ASN	2.5
1	A	503	ARG	2.5
1	C	24	ASP	2.5
1	C	14	PRO	2.5
1	A	239	TYR	2.4
1	B	156	TYR	2.4
1	C	380	PHE	2.4
1	B	164	SER	2.4
1	C	394	THR	2.4
1	C	407	ALA	2.4
1	B	137	GLY	2.4
1	C	83	GLY	2.4
1	C	81	SER	2.4
1	C	192	TYR	2.4
1	A	182	ASP	2.4
1	C	511	VAL	2.4
1	C	433	LEU	2.4
1	A	197	TYR	2.4
1	C	258	ASP	2.4
1	C	176	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	397	SER	2.4
1	C	425	TRP	2.4
1	C	526	ASP	2.3
1	C	270	LEU	2.3
1	D	312	LEU	2.3
1	A	25	TYR	2.3
1	C	472	TYR	2.3
1	C	420	THR	2.3
1	C	470	THR	2.3
1	C	7	PRO	2.3
1	C	107	VAL	2.3
1	C	142	VAL	2.3
1	C	259	GLU	2.3
1	C	382	ALA	2.3
1	C	194	ILE	2.3
1	C	452	ILE	2.3
1	B	224	PRO	2.3
1	C	3	LYS	2.3
1	C	117	SER	2.3
1	A	226	GLU	2.3
1	C	56	LEU	2.3
1	D	324	TRP	2.3
1	C	342	HIS	2.3
1	C	12	PHE	2.3
1	D	328	TYR	2.3
1	C	114	GLY	2.3
1	C	480	GLY	2.3
1	B	136	ASP	2.3
1	C	82	ASP	2.3
1	C	111	THR	2.3
1	C	331	LYS	2.3
1	C	441	LEU	2.3
1	C	206	GLY	2.2
1	C	269	PRO	2.2
1	C	525	ALA	2.2
1	C	79	SER	2.2
1	C	23	ASP	2.2
1	B	159	VAL	2.2
1	C	214	THR	2.2
1	D	50	ARG	2.2
1	D	219	THR	2.2
1	B	160	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	421	LEU	2.2
1	A	205	GLY	2.2
1	C	30	SER	2.2
1	C	174	PRO	2.2
1	C	318	SER	2.2
1	C	351	GLY	2.2
1	B	132	PHE	2.2
1	C	432	ILE	2.2
1	C	20	ARG	2.2
1	C	266	THR	2.2
1	D	466	THR	2.2
1	C	477	SER	2.2
1	C	209	TYR	2.2
1	D	151	ASP	2.2
1	B	170	LEU	2.2
1	C	435	LEU	2.2
1	C	119	PRO	2.2
1	C	360	ARG	2.2
1	C	35	PHE	2.1
1	A	303	TYR	2.1
1	B	140	TYR	2.1
1	D	273	GLU	2.1
1	A	158	ILE	2.1
1	B	297	TRP	2.1
1	C	165	VAL	2.1
1	C	130	SER	2.1
1	C	300	GLY	2.1
1	C	449	GLY	2.1
1	C	246	LYS	2.1
1	C	133	HIS	2.1
1	C	48	ASN	2.1
1	C	57	ASN	2.1
1	D	478	PHE	2.1
1	A	215	ILE	2.1
1	D	80	TYR	2.1
1	C	110	ASP	2.1
1	A	297	TRP	2.1
1	C	70	SER	2.1
1	C	356	THR	2.1
1	A	263	VAL	2.1
1	C	253	VAL	2.1
1	C	384	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	409	LEU	2.1
1	B	138	ARG	2.1
1	C	408	GLY	2.1
1	A	319	VAL	2.1
1	B	301	TRP	2.1
1	C	341	HIS	2.1
1	A	535	LEU	2.1
1	C	51	LEU	2.1
1	C	106	LEU	2.1
1	D	433	LEU	2.1
1	C	528	ASP	2.1
1	B	120	ILE	2.0
1	B	168	LYS	2.0
1	B	177	ILE	2.0
1	C	177	ILE	2.0
1	C	367	TYR	2.0
1	D	460	TYR	2.0
1	D	338	THR	2.0
1	C	242	ASN	2.0
1	C	410	VAL	2.0
1	C	446	PRO	2.0
1	C	297	TRP	2.0
1	C	495	LEU	2.0
1	C	513	MET	2.0
1	C	105	TYR	2.0
1	C	210	ASN	2.0
1	C	362	GLY	2.0
1	C	401	THR	2.0
1	C	294	ARG	2.0
1	C	391	VAL	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 ⓘ

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
3	MES	D	2007	12/12	0.65	0.23	96,97,97,98	0
3	MES	B	2006	12/12	0.68	0.25	76,77,78,78	0
2	CA	C	2003	1/1	0.85	0.12	61,61,61,61	0
4	GOL	B	2009	6/6	0.86	0.12	38,38,39,39	0
4	GOL	C	2010	6/6	0.90	0.07	33,36,36,37	0
4	GOL	A	2008	6/6	0.92	0.09	24,26,27,27	0
4	GOL	D	2011	6/6	0.93	0.08	24,26,28,29	0
3	MES	A	2005	12/12	0.94	0.09	29,33,34,34	0
2	CA	D	2004	1/1	0.97	0.04	35,35,35,35	0
2	CA	A	2001	1/1	0.98	0.04	27,27,27,27	0
2	CA	B	2002	1/1	0.99	0.03	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.