



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2016 – 04:41 PM EDT

PDB ID : 5ANH
Title : CRYSTAL STRUCTURE OF LACCASE FROM BASIDIOMYCETE PM1
(CECT 2971)
Authors : Medrano, F.J.; Romero, A.
Deposited on : 2015-09-07
Resolution : 2.49 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027939

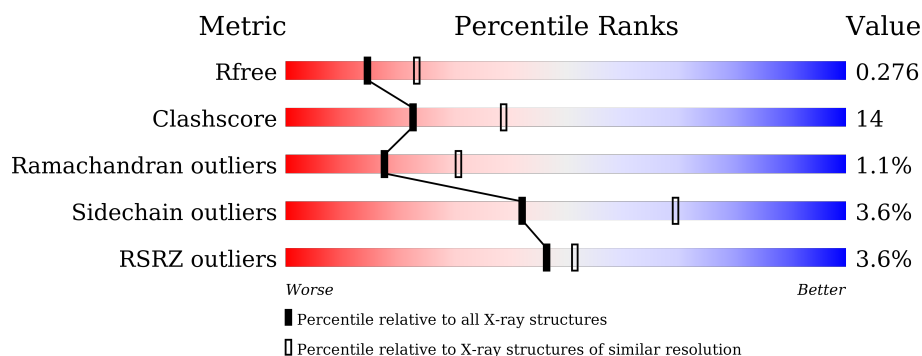
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	496	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>32%</div> <div>.</div> </div> </div>
1	B	496	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>27%</div> <div>.</div> </div> </div>
1	C	496	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>30%</div> <div>.</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11875 atoms, of which 6 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 LACCASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	496	Total	C	H	N	O	S	0	0	0
			3767	2385	2	639	732	9			
1	B	496	Total	C	H	N	O	S	0	0	0
			3767	2385	2	639	732	9			
1	C	496	Total	C	H	N	O	S	0	0	0
			3767	2385	2	639	732	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	178	ASP	ASN	CONFLICT	UNP Q12571
A	470	GLU	ASP	CONFLICT	UNP Q12571
B	178	ASP	ASN	CONFLICT	UNP Q12571
B	470	GLU	ASP	CONFLICT	UNP Q12571
C	178	ASP	ASN	CONFLICT	UNP Q12571
C	470	GLU	ASP	CONFLICT	UNP Q12571

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	4	Total	Cu	0	0
			4	4		
2	A	4	Total	Cu	0	0
			4	4		
2	C	4	Total	Cu	0	0
			4	4		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

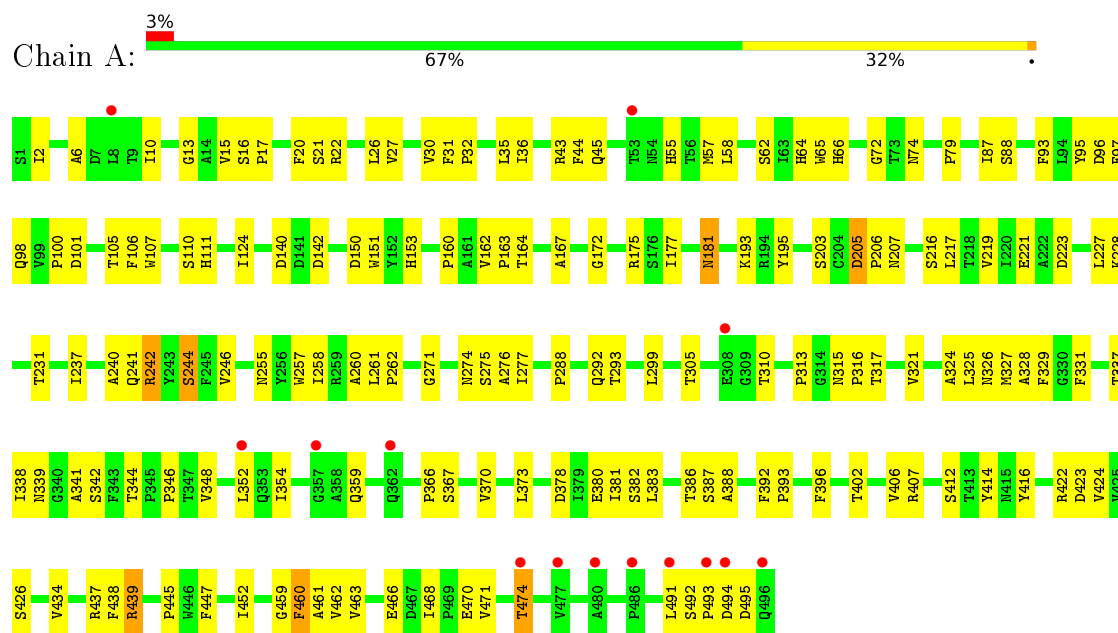
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	164	Total	O	0	0
			164	164		
4	C	174	Total	O	0	0
			174	174		

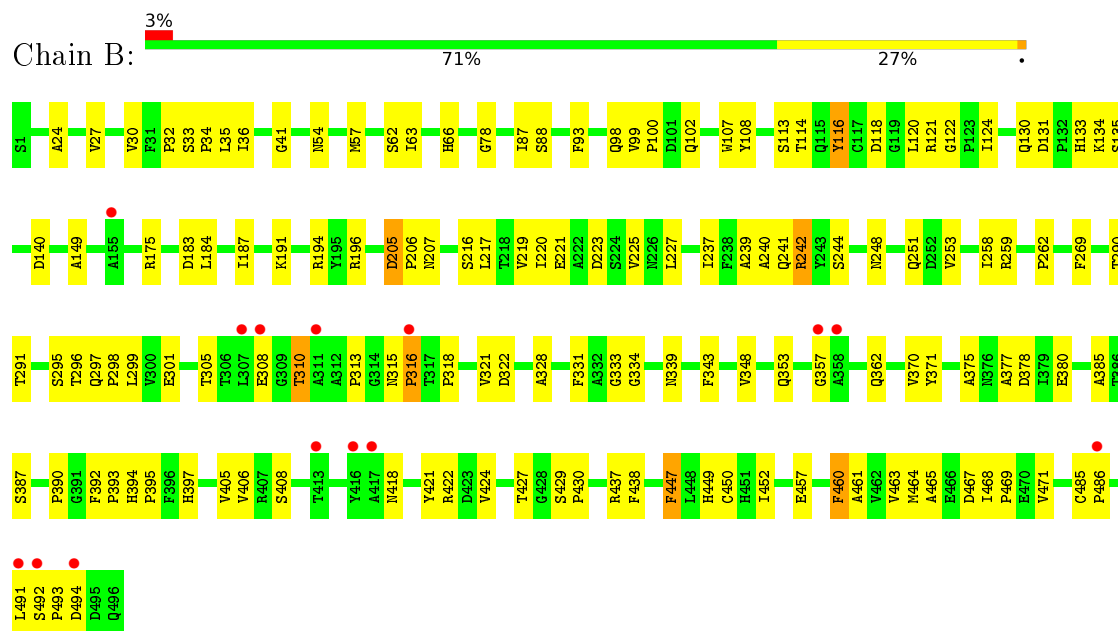
3 Residue-property plots

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 ($\text{RSRZ} > 2$). 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.

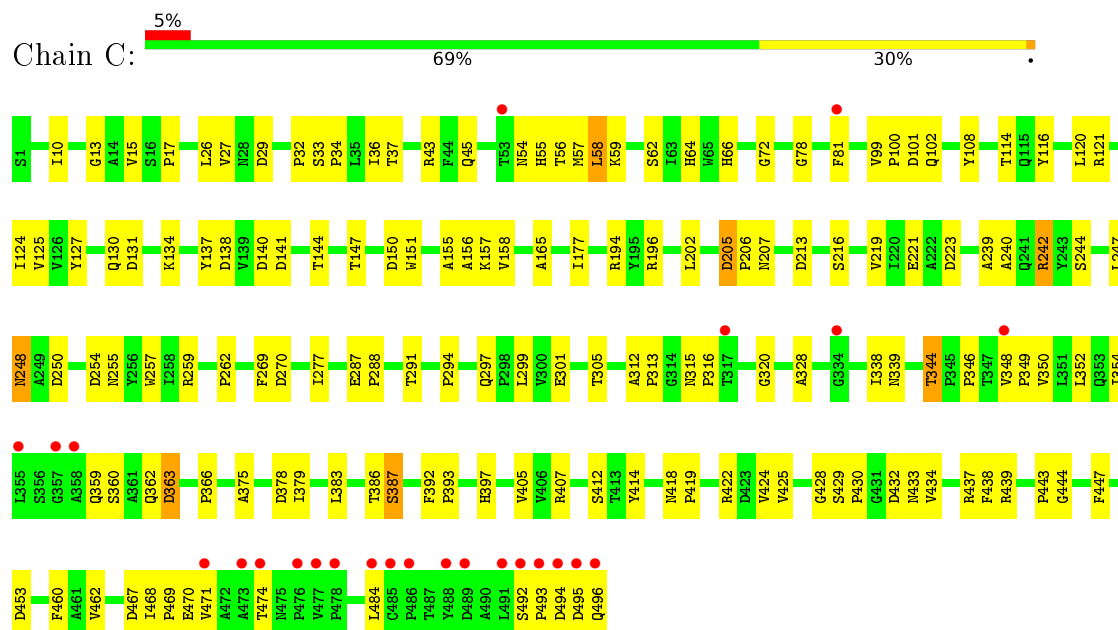
• Molecule 1: LACCASE



• Molecule 1: LACCASE



• Molecule 1: LACCASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	101.44Å 175.66Å 103.70Å 90.00° 104.16° 90.00°	Depositor
Resolution (Å)	49.18 – 2.49 49.18 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (49.18-2.49) 92.4 (49.18-2.49)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.48Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.273 0.193 , 0.276	Depositor DCC
R_{free} test set	2842 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 56.0	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	0.92	EDS
Total number of atoms	11875	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.80% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CU

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	0.44	0/3876	0.60	0/5324
1	B	0.42	0/3876	0.58	0/5324
1	C	0.43	0/3876	0.60	0/5324
All	All	0.43	0/11628	0.60	0/15972

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3765	2	3579	102	1
1	B	3765	2	3579	99	0
1	C	3765	2	3579	108	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
4	A	199	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	164	0	0	5	0
4	C	174	0	0	14	0
All	All	11869	6	10737	301	1

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 14.

All (301) 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:B:406:VAL:HG21	1:B:437:ARG:HD2	1.49	0.95
1:B:221:GLU:HB3	1:B:244:SER:HB2	1.55	0.87
1:C:43:ARG:NH1	1:C:45:GLN:OE1	2.08	0.86
1:A:205:ASP:HB3	1:A:206:PRO:HD3	1.58	0.86
1:A:181:ASN:ND2	4:A:2093:HOH:O	2.11	0.83
1:B:397:HIS:HB2	1:B:424:VAL:HG22	1.63	0.79
1:A:337:THR:HG22	1:A:342:SER:HB2	1.66	0.76
1:B:333:GLY:N	4:B:2134:HOH:O	2.13	0.76
1:B:205:ASP:HB3	1:B:206:PRO:HD3	1.69	0.75
1:A:10:ILE:HD12	1:A:27:VAL:HG22	1.69	0.74
1:C:221:GLU:HB3	1:C:244:SER:HB2	1.70	0.73
1:B:387:SER:HB3	1:C:339:ASN:OD1	1.89	0.72
1:C:101:ASP:O	4:C:2048:HOH:O	2.09	0.71
1:B:205:ASP:HB3	1:B:206:PRO:CD	2.21	0.69
1:C:54:ASN:ND2	4:C:2013:HOH:O	2.17	0.69
1:A:88:SER:HB3	1:A:491:LEU:HD11	1.75	0.68
1:C:492:SER:HB3	1:C:493:PRO:HD2	1.75	0.68
1:C:157:LYS:HE2	4:C:2055:HOH:O	1.94	0.67
1:C:66:HIS:CE1	1:C:240:ALA:HB1	2.29	0.66
1:B:308:GLU:HB2	1:B:310:THR:HG22	1.77	0.66
1:C:121:ARG:HD2	1:C:202:LEU:HB3	1.76	0.66
1:C:10:ILE:HD12	1:C:27:VAL:HG22	1.76	0.66
1:C:32:PRO:HB2	4:C:2019:HOH:O	1.95	0.66
1:C:363:ASP:OD1	1:C:363:ASP:N	2.26	0.66
1:C:205:ASP:HB3	1:C:206:PRO:HD3	1.79	0.65
1:C:305:THR:CG2	1:C:418:ASN:HB2	2.26	0.65
1:B:301:GLU:OE2	1:B:405:VAL:HG11	1.96	0.64
1:C:338:ILE:HD12	1:C:462:VAL:HG13	1.79	0.63
1:C:360:SER:HB2	4:C:2150:HOH:O	1.98	0.63
1:C:155:ALA:HB3	1:C:158:VAL:HG23	1.80	0.63
1:A:348:VAL:HG13	1:A:352:LEU:HD23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HG3	1:B:184:LEU:HD21	1.81	0.62
1:C:130:GLN:NE2	4:C:2059:HOH:O	2.29	0.62
1:A:17:PRO:HG3	1:A:31:PHE:CE1	2.34	0.62
1:B:187:ILE:HD12	1:B:258:ILE:CD1	2.29	0.62
1:C:360:SER:OG	1:C:363:ASP:OD1	2.12	0.62
1:A:387:SER:HB3	1:B:339:ASN:OD1	1.99	0.62
1:B:88:SER:OG	1:B:491:LEU:HD11	1.98	0.62
1:C:141:ASP:H	1:C:144:THR:HG23	1.65	0.61
1:A:221:GLU:HB3	1:A:244:SER:CB	2.31	0.60
1:A:223:ASP:OD2	1:A:422:ARG:HB2	2.01	0.60
1:A:339:ASN:OD1	1:C:387:SER:HB3	2.01	0.60
1:C:407:ARG:O	1:C:434:VAL:HA	2.01	0.60
1:A:338:ILE:HD12	1:A:462:VAL:HG13	1.83	0.60
1:C:131:ASP:O	1:C:134:LYS:HB2	2.02	0.60
1:A:468:ILE:HA	1:A:471:VAL:HG23	1.84	0.59
1:A:321:VAL:HG21	1:A:380:GLU:HB3	1.85	0.59
1:B:387:SER:HB2	1:C:328:ALA:HB2	1.84	0.59
1:C:114:THR:HA	1:C:453:ASP:OD2	2.03	0.59
1:C:305:THR:HG23	1:C:418:ASN:HB2	1.84	0.59
1:C:407:ARG:NH1	1:C:433:ASN:HB3	2.18	0.58
1:C:55:HIS:NE2	1:C:494:ASP:HA	2.18	0.58
1:C:207:ASN:O	1:C:262:PRO:HA	2.03	0.58
1:C:407:ARG:HD2	1:C:414:TYR:CZ	2.38	0.58
1:A:426:SER:O	1:A:434:VAL:HG21	2.04	0.58
1:B:465:ALA:CB	1:B:468:ILE:HD11	2.33	0.57
1:C:254:ASP:OD1	1:C:255:ASN:N	2.35	0.57
1:B:194:ARG:HG2	1:B:248:ASN:OD1	2.04	0.57
1:B:392:PHE:HB2	1:B:393:PRO:HA	1.85	0.57
1:C:205:ASP:HB3	1:C:206:PRO:CD	2.34	0.57
1:B:225:VAL:HG11	1:B:421:TYR:HB2	1.87	0.57
1:B:291:THR:HG22	4:B:2036:HOH:O	2.04	0.57
1:C:297:GLN:NE2	4:C:2142:HOH:O	2.26	0.57
1:A:221:GLU:HB3	1:A:244:SER:HB3	1.87	0.56
1:A:72:GLY:HA2	1:A:474:THR:O	2.05	0.56
1:B:313:PRO:HG2	1:B:438:PHE:HA	1.86	0.56
1:A:392:PHE:HB2	1:A:393:PRO:HA	1.88	0.56
1:B:371:TYR:HB2	1:B:464:MET:HE2	1.88	0.56
1:B:191:LYS:HE2	1:B:251:GLN:O	2.06	0.55
1:A:193:LYS:HE2	4:A:2028:HOH:O	2.06	0.55
1:C:81:PHE:O	1:C:349:PRO:HA	2.06	0.55
1:A:17:PRO:HB3	1:A:172:GLY:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:MET:HB2	1:A:383:LEU:HD23	1.89	0.55
1:B:296:THR:C	1:B:298:PRO:HD3	2.27	0.55
1:A:167:ALA:HA	4:A:2078:HOH:O	2.07	0.55
1:A:195:TYR:O	1:A:246:VAL:HA	2.07	0.55
1:B:406:VAL:CG2	1:B:437:ARG:HD2	2.30	0.55
1:B:465:ALA:HB1	1:B:468:ILE:HD11	1.89	0.55
1:A:359:GLN:N	1:A:359:GLN:OE1	2.40	0.54
1:C:219:VAL:HG21	1:C:299:LEU:HD12	1.89	0.54
1:C:397:HIS:HB2	1:C:424:VAL:HG22	1.89	0.54
1:B:33:SER:HB3	1:B:108:TYR:OH	2.07	0.54
1:A:346:PRO:HD3	1:A:366:PRO:HD3	1.89	0.54
1:B:239:ALA:O	1:B:240:ALA:HB3	2.08	0.54
1:B:348:VAL:HG12	1:B:353:GLN:HG3	1.90	0.54
1:B:375:ALA:HB2	1:B:467:ASP:CG	2.27	0.54
1:C:147:THR:HB	1:C:202:LEU:CD1	2.37	0.54
1:C:375:ALA:HB2	1:C:467:ASP:CG	2.29	0.53
1:C:138:ASP:OD1	1:C:194:ARG:NH2	2.36	0.53
1:C:223:ASP:OD2	1:C:422:ARG:HB2	2.08	0.53
1:C:338:ILE:CD1	1:C:462:VAL:HG13	2.38	0.53
1:A:142:ASP:OD2	4:A:2001:HOH:O	2.18	0.53
1:A:62:SER:O	1:A:110:SER:HA	2.09	0.53
1:C:15:VAL:HG23	1:C:17:PRO:HD3	1.90	0.53
1:A:205:ASP:HA	1:A:452:ILE:HG23	1.91	0.53
1:A:328:ALA:HB2	1:C:387:SER:HB2	1.89	0.53
1:C:470:GLU:HG2	4:C:2167:HOH:O	2.08	0.53
1:A:79:PRO:HA	1:A:111:HIS:HB3	1.91	0.52
1:C:10:ILE:CD1	1:C:27:VAL:HG22	2.38	0.52
1:C:444:GLY:HA2	1:C:471:VAL:HG22	1.91	0.52
1:B:183:ASP:O	1:B:184:LEU:HD23	2.09	0.52
1:B:485:CYS:HB2	1:B:486:PRO:HD3	1.91	0.52
1:A:423:ASP:OD1	1:A:424:VAL:HG23	2.08	0.52
1:A:100:PRO:HG2	1:A:101:ASP:OD1	2.09	0.52
1:A:74:ASN:OD1	1:A:445:PRO:HD2	2.10	0.52
1:C:147:THR:HG21	1:C:202:LEU:HD11	1.92	0.52
1:B:113:SER:OG	1:B:114:THR:N	2.42	0.52
1:B:87:ILE:CD1	1:B:93:PHE:HB3	2.40	0.52
1:C:259:ARG:HB3	1:C:269:PHE:CE1	2.44	0.52
1:C:359:GLN:OE1	1:C:359:GLN:N	2.42	0.52
1:A:22:ARG:HD3	1:A:151:TRP:CZ2	2.46	0.51
1:C:248:ASN:O	1:C:250:ASP:N	2.42	0.51
1:A:325:LEU:HB2	1:A:381:ILE:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:HB3	1:A:244:SER:HB2	1.93	0.51
1:C:100:PRO:HG2	1:C:101:ASP:OD1	2.11	0.51
1:C:429:SER:HB2	1:C:430:PRO:HD2	1.91	0.51
1:C:470:GLU:HA	1:C:470:GLU:OE1	2.10	0.51
1:B:32:PRO:HB2	4:B:2016:HOH:O	2.11	0.51
1:C:58:LEU:HD22	1:C:496:GLN:OXT	2.11	0.51
1:A:221:GLU:OE1	1:A:244:SER:HB2	2.11	0.51
1:A:313:PRO:HG3	1:A:438:PHE:HA	1.92	0.50
1:C:301:GLU:OE2	1:C:405:VAL:HG11	2.10	0.50
1:C:150:ASP:N	1:C:150:ASP:OD1	2.40	0.50
1:A:87:ILE:CD1	1:A:93:PHE:HB3	2.41	0.50
1:A:370:VAL:HG22	1:A:463:VAL:HB	1.94	0.49
1:B:331:PHE:CZ	1:B:334:GLY:HA2	2.47	0.49
1:A:354:ILE:HG23	1:A:468:ILE:HG23	1.94	0.49
1:B:121:ARG:NH2	1:B:149:ALA:HB1	2.28	0.49
1:B:343:PHE:HB2	1:B:461:ALA:O	2.12	0.49
1:C:165:ALA:HB3	4:C:2127:HOH:O	2.12	0.49
1:A:470:GLU:HA	1:A:470:GLU:OE1	2.13	0.49
1:C:57:MET:O	1:C:58:LEU:HB2	2.12	0.49
1:C:468:ILE:HB	1:C:469:PRO:HD3	1.93	0.49
1:C:346:PRO:HD3	1:C:366:PRO:HD3	1.95	0.49
1:A:313:PRO:HG2	1:A:437:ARG:HB3	1.94	0.49
1:C:72:GLY:HA2	1:C:474:THR:O	2.11	0.49
1:B:63:ILE:CD1	1:B:120:LEU:HD21	2.43	0.49
1:A:414:TYR:HB3	1:A:416:TYR:CE2	2.48	0.48
1:B:223:ASP:OD2	1:B:422:ARG:HB2	2.12	0.48
1:B:241:GLN:C	1:B:242:ARG:HD3	2.34	0.48
1:B:485:CYS:HB2	1:B:486:PRO:CD	2.42	0.48
1:A:258:ILE:HB	1:A:276:ALA:HB3	1.94	0.48
1:A:150:ASP:N	1:A:150:ASP:OD1	2.30	0.48
1:B:30:VAL:HG12	1:B:32:PRO:O	2.14	0.48
1:B:394:HIS:HB3	1:B:450:CYS:SG	2.54	0.48
1:C:99:VAL:O	1:C:99:VAL:HG12	2.13	0.48
1:C:13:GLY:HA3	1:C:26:LEU:HD11	1.96	0.48
1:C:140:ASP:HA	1:C:144:THR:HG21	1.96	0.48
4:A:2167:HOH:O	1:C:392:PHE:HZ	1.96	0.48
1:A:162:VAL:HG11	4:A:2198:HOH:O	2.14	0.48
1:A:10:ILE:CD1	1:A:27:VAL:HG22	2.41	0.48
1:A:55:HIS:CD2	1:A:494:ASP:HA	2.49	0.48
1:A:216:SER:C	1:A:217:LEU:HD23	2.34	0.47
1:C:360:SER:OG	1:C:362:GLN:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD1	1:A:101:ASP:N	2.47	0.47
1:A:219:VAL:HG12	1:A:227:LEU:HD12	1.97	0.47
1:A:277:ILE:HG12	1:A:288:PRO:HD3	1.96	0.47
1:B:205:ASP:CB	1:B:206:PRO:CD	2.91	0.47
1:C:247:LEU:HD23	1:C:247:LEU:C	2.35	0.47
1:A:160:PRO:HD2	1:A:163:PRO:HB3	1.95	0.47
1:A:315:ASN:O	1:A:317:THR:N	2.45	0.47
1:A:324:ALA:O	1:A:325:LEU:HD23	2.15	0.47
1:A:43:ARG:HD2	1:A:98:GLN:HE21	1.80	0.47
1:C:108:TYR:HB3	1:C:124:ILE:HD11	1.95	0.47
1:B:301:GLU:HG2	1:B:408:SER:OG	2.14	0.47
1:C:379:ILE:O	1:C:437:ARG:HA	2.14	0.47
1:A:35:LEU:HD23	1:A:142:ASP:OD1	2.15	0.47
1:A:175:ARG:NH1	1:A:271:GLY:O	2.44	0.47
1:C:101:ASP:HA	4:C:2046:HOH:O	2.15	0.47
1:A:326:ASN:OD1	1:A:382:SER:OG	2.29	0.46
1:B:54:ASN:HB3	4:B:2005:HOH:O	2.14	0.46
1:B:187:ILE:HD12	1:B:258:ILE:HD12	1.96	0.46
1:B:322:ASP:HB2	1:B:377:ALA:HB1	1.97	0.46
1:A:140:ASP:HB3	4:A:2069:HOH:O	2.16	0.46
1:A:492:SER:HB2	1:A:495:ASP:OD1	2.16	0.46
1:C:64:HIS:NE2	1:C:66:HIS:HA	2.30	0.46
1:C:62:SER:OG	1:C:78:GLY:O	2.28	0.46
1:C:392:PHE:HB2	1:C:393:PRO:HA	1.96	0.46
1:C:312:ALA:HB2	1:C:419:PRO:HG3	1.98	0.46
1:C:155:ALA:HB3	1:C:158:VAL:CG2	2.44	0.46
1:B:27:VAL:HB	1:B:34:PRO:CD	2.46	0.46
1:A:255:ASN:HB3	1:A:288:PRO:HG3	1.97	0.46
1:B:62:SER:OG	1:B:78:GLY:O	2.30	0.46
1:A:164:THR:HG23	1:B:362:GLN:OE1	2.16	0.46
1:A:55:HIS:NE2	1:A:494:ASP:HA	2.30	0.46
1:C:348:VAL:CG1	1:C:352:LEU:HB3	2.46	0.46
1:A:13:GLY:HA3	1:A:26:LEU:HD11	1.98	0.45
1:B:395:PRO:HD2	1:B:452:ILE:HG13	1.98	0.45
1:C:100:PRO:HD2	4:C:2044:HOH:O	2.15	0.45
1:A:105:THR:HG22	1:A:242:ARG:HG2	1.98	0.45
1:A:337:THR:HA	1:A:341:ALA:O	2.16	0.45
1:B:63:ILE:HD11	1:B:120:LEU:HD21	1.98	0.45
1:B:41:GLY:HA2	1:B:100:PRO:HA	1.98	0.45
1:C:36:ILE:O	1:C:124:ILE:HA	2.16	0.45
1:A:387:SER:HB2	1:B:328:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:484:LEU:HD23	1:C:484:LEU:HA	1.69	0.45
1:B:305:THR:HG23	1:B:418:ASN:O	2.16	0.45
1:C:66:HIS:HE1	1:C:240:ALA:HB1	1.77	0.45
1:C:287:GLU:HG3	4:C:2141:HOH:O	2.17	0.45
1:A:257:TRP:CE3	1:A:275:SER:HB3	2.51	0.45
1:A:30:VAL:HG12	1:A:32:PRO:O	2.17	0.45
1:B:315:ASN:HA	1:B:316:PRO:HD3	1.78	0.45
1:A:459:GLY:O	1:A:461:ALA:N	2.49	0.45
1:C:213:ASP:OD2	1:C:257:TRP:HB2	2.18	0.44
1:A:16:SER:HB3	1:A:21:SER:HA	1.99	0.44
1:A:328:ALA:HB2	1:C:387:SER:CB	2.47	0.44
1:B:207:ASN:O	1:B:262:PRO:HA	2.17	0.44
1:B:242:ARG:N	1:B:242:ARG:HD3	2.32	0.44
1:C:350:VAL:O	1:C:354:ILE:HG13	2.17	0.44
1:A:260:ALA:O	1:A:274:ASN:HB3	2.18	0.44
1:B:321:VAL:HB	1:B:378:ASP:O	2.18	0.44
1:C:259:ARG:HB3	1:C:269:PHE:CZ	2.52	0.44
1:B:87:ILE:HD13	1:B:93:PHE:HB3	2.00	0.44
1:A:2:ILE:O	1:A:36:ILE:HA	2.17	0.44
1:B:296:THR:O	1:B:296:THR:HG22	2.18	0.44
1:B:348:VAL:HG12	1:B:353:GLN:CG	2.48	0.44
1:B:449:HIS:HB3	1:B:461:ALA:CB	2.48	0.44
1:C:348:VAL:HG13	1:C:352:LEU:HB3	2.00	0.44
1:B:133:HIS:CD2	1:B:220:ILE:HB	2.52	0.44
1:B:107:TRP:HB2	1:B:122:GLY:O	2.18	0.43
1:B:370:VAL:HG22	1:B:463:VAL:HB	1.99	0.43
1:C:239:ALA:O	1:C:240:ALA:HB3	2.18	0.43
1:C:305:THR:HG21	1:C:418:ASN:HB2	2.00	0.43
1:A:207:ASN:O	1:A:262:PRO:HA	2.18	0.43
1:C:58:LEU:HG	1:C:157:LYS:HE3	2.00	0.43
1:B:290:THR:O	4:B:2110:HOH:O	2.21	0.43
1:B:457:GLU:O	1:B:457:GLU:HG3	2.18	0.43
1:C:156:ALA:HA	4:C:2071:HOH:O	2.18	0.43
1:A:329:PHE:HB2	1:A:386:THR:CG2	2.49	0.43
1:A:44:PHE:N	1:A:97:PHE:O	2.39	0.43
1:B:297:GLN:N	1:B:298:PRO:HD3	2.33	0.43
1:C:27:VAL:HB	1:C:34:PRO:HD2	1.99	0.43
1:A:45:GLN:HG2	1:A:96:ASP:OD1	2.19	0.43
1:B:183:ASP:C	1:B:184:LEU:HD23	2.39	0.43
1:C:407:ARG:HD2	1:C:414:TYR:CE1	2.54	0.43
1:B:99:VAL:CG1	1:B:102:GLN:HB2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:VAL:HG11	1:B:380:GLU:HB2	2.00	0.43
1:B:449:HIS:HB3	1:B:461:ALA:HB2	2.01	0.43
1:A:407:ARG:O	1:A:434:VAL:HA	2.19	0.43
1:B:57:MET:HB2	1:B:57:MET:HE2	1.88	0.43
1:B:27:VAL:HB	1:B:34:PRO:HD2	2.00	0.42
1:A:228:LYS:HD2	1:A:305:THR:CG2	2.49	0.42
1:A:6:ALA:HA	4:A:2003:HOH:O	2.19	0.42
1:B:24:ALA:HB1	1:B:118:ASP:O	2.18	0.42
1:A:406:VAL:HG21	1:A:437:ARG:HD2	2.01	0.42
1:A:64:HIS:NE2	1:A:66:HIS:HA	2.34	0.42
1:B:392:PHE:CE2	1:B:430:PRO:HD3	2.55	0.42
1:B:447:PHE:HD1	1:B:447:PHE:HA	1.69	0.42
1:B:468:ILE:HA	1:B:471:VAL:HG23	2.02	0.42
1:C:108:TYR:HD1	1:C:124:ILE:HG13	1.84	0.42
1:A:106:PHE:HB2	1:A:124:ILE:HB	2.01	0.42
1:B:390:PRO:O	1:B:394:HIS:HE1	2.03	0.42
1:B:99:VAL:HG13	1:B:102:GLN:HB2	2.01	0.42
1:C:277:ILE:HG12	1:C:288:PRO:HD3	2.00	0.42
1:C:137:TYR:CG	1:C:196:ARG:HB2	2.54	0.42
1:C:59:LYS:NZ	1:C:495:ASP:OD1	2.52	0.42
1:B:465:ALA:HB3	1:B:468:ILE:HD11	2.02	0.42
1:C:17:PRO:HG2	1:C:151:TRP:CE2	2.55	0.42
1:A:87:ILE:HD13	1:A:93:PHE:HB3	2.02	0.42
1:A:57:MET:HE3	1:A:57:MET:HB2	1.71	0.41
1:B:219:VAL:HG12	1:B:227:LEU:HD12	2.02	0.41
1:C:443:PRO:HG3	1:C:467:ASP:OD2	2.20	0.41
1:C:378:ASP:OD1	1:C:439:ARG:HG2	2.19	0.41
1:C:242:ARG:N	1:C:242:ARG:HD3	2.35	0.41
1:A:15:VAL:HG23	1:A:17:PRO:HD3	2.02	0.41
1:A:237:ILE:HG13	1:A:241:GLN:HB2	2.02	0.41
1:A:380:GLU:OE1	1:A:437:ARG:NE	2.52	0.41
1:B:130:GLN:HA	1:B:130:GLN:OE1	2.20	0.41
1:B:140:ASP:CG	1:B:196:ARG:HD3	2.41	0.41
1:B:460:PHE:HD1	1:B:460:PHE:HA	1.77	0.41
1:A:107:TRP:HZ2	1:A:240:ALA:CB	2.34	0.41
1:A:150:ASP:OD1	1:A:203:SER:HA	2.20	0.41
1:A:378:ASP:OD1	1:A:439:ARG:HD2	2.20	0.41
1:A:20:PHE:CD2	1:A:153:HIS:CD2	3.08	0.41
1:A:261:LEU:HD12	1:A:262:PRO:HD2	2.02	0.41
1:A:292:GLN:HG2	1:A:293:THR:N	2.36	0.41
1:B:216:SER:O	1:B:217:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:373:LEU:HB2	1:A:466:GLU:HA	2.01	0.41
1:A:492:SER:HB3	1:A:493:PRO:HD2	2.02	0.41
1:B:385:ALA:HB2	1:B:427:THR:O	2.21	0.41
1:C:315:ASN:HB3	1:C:316:PRO:HD2	2.02	0.41
1:C:125:VAL:HG11	1:C:127:TYR:CZ	2.56	0.41
1:C:43:ARG:HD2	4:C:2045:HOH:O	2.19	0.41
1:A:65:TRP:HZ2	1:A:95:TYR:CD2	2.39	0.41
1:A:98:GLN:C	1:A:100:PRO:HD3	2.42	0.41
1:B:468:ILE:N	1:B:469:PRO:CD	2.84	0.41
1:C:428:GLY:HA3	1:C:432:ASP:OD2	2.21	0.41
1:B:116:TYR:O	1:B:121:ARG:HD3	2.20	0.40
1:B:299:LEU:HD23	1:B:299:LEU:C	2.42	0.40
1:B:492:SER:O	1:B:494:ASP:N	2.54	0.40
1:C:99:VAL:HG13	1:C:102:GLN:HB2	2.03	0.40
1:C:344:THR:O	1:C:366:PRO:HG3	2.21	0.40
1:B:66:HIS:CE1	1:B:240:ALA:HB1	2.56	0.40
1:B:237:ILE:HD11	1:B:241:GLN:O	2.22	0.40
1:C:313:PRO:HG2	1:C:438:PHE:HA	2.03	0.40
1:B:36:ILE:O	1:B:124:ILE:HA	2.22	0.40
1:B:131:ASP:O	1:B:134:LYS:HB2	2.22	0.40
1:A:321:VAL:HB	1:A:378:ASP:O	2.22	0.40
1:B:259:ARG:HB3	1:B:269:PHE:CE1	2.57	0.40
1:B:429:SER:HB2	1:B:430:PRO:CD	2.52	0.40
1:C:37:THR:HA	1:C:125:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASP:OD2	1:C:56:THR:OG1[2_555]	2.17	0.03

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	494/496 (100%)	457 (92%)	31 (6%)	6 (1%)	16	29
1	B	494/496 (100%)	462 (94%)	26 (5%)	6 (1%)	16	29
1	C	494/496 (100%)	459 (93%)	31 (6%)	4 (1%)	24	41
All	All	1482/1488 (100%)	1378 (93%)	88 (6%)	16 (1%)	17	31

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	205	ASP
1	A	460	PHE
1	C	205	ASP
1	A	205	ASP
1	A	388	ALA
1	B	357	GLY
1	C	294	PRO
1	A	316	PRO
1	C	58	LEU
1	A	58	LEU
1	A	331	PHE
1	C	320	GLY
1	B	493	PRO
1	B	253	VAL
1	B	316	PRO
1	B	318	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	411/411 (100%)	395 (96%)	16 (4%)	39	66
1	B	411/411 (100%)	402 (98%)	9 (2%)	60	84
1	C	411/411 (100%)	392 (95%)	19 (5%)	33	57
All	All	1233/1233 (100%)	1189 (96%)	44 (4%)	42	69

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ILE
1	A	181	ASN
1	A	231	THR
1	A	242	ARG
1	A	244	SER
1	A	299	LEU
1	A	310	THR
1	A	344	THR
1	A	367	SER
1	A	396	PHE
1	A	402	THR
1	A	412	SER
1	A	439	ARG
1	A	447	PHE
1	A	460	PHE
1	A	474	THR
1	B	35	LEU
1	B	98	GLN
1	B	116	TYR
1	B	135	SER
1	B	242	ARG
1	B	295	SER
1	B	310	THR
1	B	447	PHE
1	B	460	PHE
1	C	29	ASP
1	C	33	SER
1	C	116	TYR
1	C	120	LEU
1	C	177	ILE
1	C	216	SER
1	C	242	ARG
1	C	248	ASN
1	C	270	ASP
1	C	291	THR
1	C	344	THR
1	C	363	ASP
1	C	383	LEU
1	C	386	THR
1	C	387	SER
1	C	412	SER
1	C	425	VAL

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Mol	Chain	Res	Type
1	C	447	PHE
1	C	460	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 12 are monoatomic - leaving 5 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	SO4	A	1497	-	4,4,4	0.23	0	6,6,6	0.35	0
3	SO4	A	1498	-	4,4,4	0.44	0	6,6,6	0.12	0
3	SO4	B	1497	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	B	1498	-	4,4,4	0.26	0	6,6,6	0.20	0
3	SO4	C	1497	-	4,4,4	0.18	0	6,6,6	0.28	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	SO4	A	1497	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1498	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1497	-	-	0/0/0/0	0/0/0/0
3	SO4	B	1498	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1497	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	496/496 (100%)	0.08	14 (2%) 56 61	13, 30, 60, 108	0
1	B	496/496 (100%)	0.16	14 (2%) 56 61	14, 32, 61, 134	0
1	C	496/496 (100%)	0.15	25 (5%) 32 37	16, 31, 61, 132	0
All	All	1488/1488 (100%)	0.13	53 (3%) 46 51	13, 31, 61, 134	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	494	ASP	7.2
1	C	494	ASP	6.9
1	B	491	LEU	4.2
1	B	492	SER	4.0
1	A	357	GLY	4.0
1	C	496	GLN	4.0
1	C	492	SER	3.8
1	B	357	GLY	3.8
1	B	494	ASP	3.8
1	C	477	VAL	3.8
1	B	316	PRO	3.7
1	B	416	TYR	3.6
1	C	355	LEU	3.6
1	C	491	LEU	3.5
1	C	474	THR	3.1
1	B	308	GLU	3.0
1	A	496	GLN	2.9
1	B	486	PRO	2.9
1	C	471	VAL	2.8
1	C	334	GLY	2.8
1	B	311	ALA	2.8
1	A	486	PRO	2.7
1	C	495	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	417	ALA	2.6
1	A	352	LEU	2.6
1	C	485	CYS	2.4
1	A	477	VAL	2.4
1	C	357	GLY	2.4
1	B	413	THR	2.4
1	B	155	ALA	2.4
1	A	491	LEU	2.4
1	C	473	ALA	2.3
1	C	358	ALA	2.3
1	B	358	ALA	2.3
1	B	307	LEU	2.3
1	C	478	PRO	2.2
1	A	493	PRO	2.2
1	C	488	TYR	2.2
1	C	484	LEU	2.2
1	A	474	THR	2.2
1	C	317	THR	2.2
1	C	493	PRO	2.2
1	C	348	VAL	2.2
1	C	476	PRO	2.2
1	C	489	ASP	2.1
1	A	308	GLU	2.1
1	A	53	THR	2.1
1	C	53	THR	2.1
1	A	480	ALA	2.1
1	C	81	PHE	2.1
1	A	8	LEU	2.0
1	C	486	PRO	2.0
1	A	362	GLN	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 carbohydrates in this entry.

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	CU	B	602	1/1	0.98	0.15	0.98	35,35,35,35	0
3	SO4	A	1498	5/5	0.99	0.18	-0.53	22,28,33,35	0
2	CU	C	604	1/1	1.00	0.09	-2.45	34,34,34,34	0
2	CU	B	604	1/1	0.99	0.10	-2.48	30,30,30,30	0
2	CU	A	602	1/1	0.99	0.12	-2.56	34,34,34,34	0
2	CU	C	603	1/1	1.00	0.09	-2.57	33,33,33,33	0
2	CU	C	602	1/1	0.99	0.10	-2.70	43,43,43,43	0
2	CU	A	603	1/1	1.00	0.08	-3.57	38,38,38,38	0
2	CU	A	604	1/1	0.99	0.09	-3.70	27,27,27,27	0
2	CU	B	603	1/1	0.99	0.11	-3.72	32,32,32,32	0
3	SO4	A	1497	5/5	0.95	0.24	-	42,59,61,68	0
3	SO4	B	1497	5/5	0.96	0.21	-	43,58,61,64	0
3	SO4	C	1497	5/5	0.97	0.20	-	56,57,65,67	0
2	CU	C	601	1/1	0.98	0.07	-	48,48,48,48	0
3	SO4	B	1498	5/5	0.99	0.19	-	24,25,27,29	5
2	CU	A	601	1/1	0.99	0.10	-	46,46,46,46	0
2	CU	B	601	1/1	0.99	0.10	-	44,44,44,44	0

6.5 Other polymers

There are no such residues in this entry.