



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:15 PM UTC

PDB ID : 5HAA / pdb_00005haa
Title : Crystal structure of mpy-RNase J, an archaeal RNase J from Methanobolus psychrophilus R15
Authors : Feng, N.; Li, D.F.
Deposited on : 2015-12-30
Resolution : 2.90 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

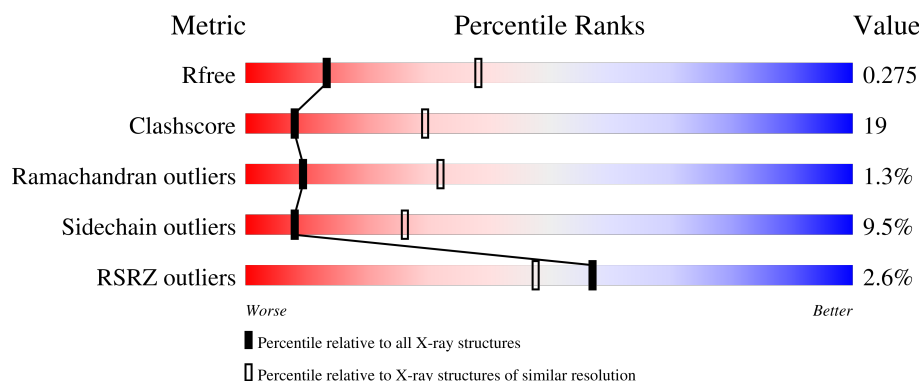
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

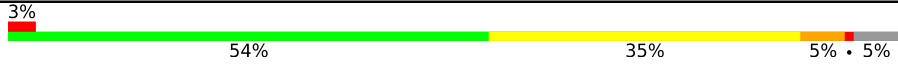
The reported resolution of this entry is 2.90 Å.

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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	470	
1	B	470	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	506	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7113 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 Ribonuclease J.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3482	2192	608	662	20			
1	B	460	Total	C	N	O	S	0	0	0
			3580	2249	630	681	20			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP K4MAF9
A	-20	GLY	-	expression tag	UNP K4MAF9
A	-19	SER	-	expression tag	UNP K4MAF9
A	-18	SER	-	expression tag	UNP K4MAF9
A	-17	HIS	-	expression tag	UNP K4MAF9
A	-16	HIS	-	expression tag	UNP K4MAF9
A	-15	HIS	-	expression tag	UNP K4MAF9
A	-14	HIS	-	expression tag	UNP K4MAF9
A	-13	HIS	-	expression tag	UNP K4MAF9
A	-12	HIS	-	expression tag	UNP K4MAF9
A	-11	SER	-	expression tag	UNP K4MAF9
A	-10	SER	-	expression tag	UNP K4MAF9
A	-9	GLY	-	expression tag	UNP K4MAF9
A	-8	LEU	-	expression tag	UNP K4MAF9
A	-7	VAL	-	expression tag	UNP K4MAF9
A	-6	PRO	-	expression tag	UNP K4MAF9
A	-5	ARG	-	expression tag	UNP K4MAF9
A	-4	GLY	-	expression tag	UNP K4MAF9
A	-3	SER	-	expression tag	UNP K4MAF9
A	-2	HIS	-	expression tag	UNP K4MAF9
A	-1	MET	-	expression tag	UNP K4MAF9
A	0	ALA	-	expression tag	UNP K4MAF9
A	1	SER	-	expression tag	UNP K4MAF9
B	-21	MET	-	initiating methionine	UNP K4MAF9
B	-20	GLY	-	expression tag	UNP K4MAF9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	SER	-	expression tag	UNP K4MAF9
B	-18	SER	-	expression tag	UNP K4MAF9
B	-17	HIS	-	expression tag	UNP K4MAF9
B	-16	HIS	-	expression tag	UNP K4MAF9
B	-15	HIS	-	expression tag	UNP K4MAF9
B	-14	HIS	-	expression tag	UNP K4MAF9
B	-13	HIS	-	expression tag	UNP K4MAF9
B	-12	HIS	-	expression tag	UNP K4MAF9
B	-11	SER	-	expression tag	UNP K4MAF9
B	-10	SER	-	expression tag	UNP K4MAF9
B	-9	GLY	-	expression tag	UNP K4MAF9
B	-8	LEU	-	expression tag	UNP K4MAF9
B	-7	VAL	-	expression tag	UNP K4MAF9
B	-6	PRO	-	expression tag	UNP K4MAF9
B	-5	ARG	-	expression tag	UNP K4MAF9
B	-4	GLY	-	expression tag	UNP K4MAF9
B	-3	SER	-	expression tag	UNP K4MAF9
B	-2	HIS	-	expression tag	UNP K4MAF9
B	-1	MET	-	expression tag	UNP K4MAF9
B	0	ALA	-	expression tag	UNP K4MAF9
B	1	SER	-	expression tag	UNP K4MAF9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Zn 2 2	0	0
2	B	2	Total Zn 2 2	0	0

- Molecule 3 is SULFATE ION (CCD ID: 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	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	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.51Å 162.51Å 180.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.03 – 2.90 39.03 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.1 (39.03-2.90) 98.1 (39.03-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.90Å)	Xtriage
Refinement program	PHENIX dev_1980	Depositor
R, R_{free}	0.237 , 0.274 0.240 , 0.275	Depositor DCC
R_{free} test set	1998 reflections (6.43%)	wwPDB-VP
Wilson B-factor (Å ²)	92.8	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7113	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3398e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: SO4, ZN

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	0/3544	0.92	2/4798 (0.0%)
1	B	0.46	0/3645	0.97	8/4932 (0.2%)
All	All	0.43	0/7189	0.95	10/9730 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	VAL	N-CA-C	-7.76	96.90	108.85
1	B	303	ASN	N-CA-C	7.33	119.35	111.36
1	B	283	LEU	N-CA-C	-6.43	105.06	113.17
1	A	283	LEU	N-CA-C	-6.01	105.60	113.17
1	B	236	SER	N-CA-C	5.71	117.31	111.14
1	A	320	MET	N-CA-C	5.69	116.59	108.74
1	B	264	ARG	CA-C-N	-5.36	118.73	122.59
1	B	264	ARG	C-N-CA	-5.36	118.73	122.59
1	B	158	VAL	N-CA-C	5.14	116.06	108.45
1	B	124	VAL	CG1-CB-CG2	5.05	121.91	110.80

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	3482	0	3488	155	0
1	B	3580	0	3577	129	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	20	0	0	4	0
3	B	25	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	7113	0	7065	276	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 19.

All (276) 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:39:ARG:HA	1:A:42:ILE:HD13	1.56	0.85
1:B:305:LEU:HA	1:B:308:ILE:HG22	1.60	0.84
1:B:305:LEU:HD21	1:B:341:PHE:H	1.46	0.81
1:A:179:ARG:NH1	1:B:232:GLY:O	2.15	0.80
1:B:76:ARG:NH1	1:B:139:ILE:O	2.16	0.78
1:B:16:GLY:HA2	1:B:86:ASP:HB2	1.64	0.78
1:B:152:HIS:HB3	1:B:157:THR:HG21	1.64	0.77
1:A:332:GLY:O	1:A:336:ASN:ND2	2.18	0.77
1:A:320:MET:HE1	1:A:334:ILE:HD12	1.65	0.76
1:A:56:LEU:O	1:A:60:GLY:N	2.15	0.75
1:A:151:GLN:NE2	1:A:185:GLU:O	2.20	0.74
1:A:348:ARG:NH2	1:B:396:GLU:OE1	2.22	0.73
1:A:28:ILE:HB	1:A:75:VAL:HA	1.70	0.72
1:B:343:VAL:HG13	1:B:375:LYS:HG2	1.72	0.71
1:A:334:ILE:HG12	1:A:339:THR:HG21	1.70	0.71
1:A:365:ARG:NH2	1:A:381:ASP:OD1	2.22	0.70
1:B:38:ASP:OD1	1:B:358:ASN:ND2	2.24	0.70
1:A:298:ARG:NH2	3:A:506:SO4:O4	2.26	0.69
1:A:7:ILE:HG23	1:A:21:ALA:HB3	1.75	0.69
1:B:7:ILE:HD13	1:B:442:GLU:HG3	1.73	0.68
1:A:171:TYR:HE1	1:A:173:CYS:HB2	1.59	0.68
1:A:185:GLU:N	1:A:185:GLU:OE1	2.26	0.68
1:B:142:ASP:HB3	1:B:165:PRO:HD3	1.73	0.68
1:B:140:THR:O	1:B:142:ASP:N	2.27	0.67
1:B:183:LEU:HD12	1:B:250:ALA:HA	1.74	0.67
1:B:332:GLY:O	1:B:336:ASN:ND2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:HB2	1:A:124:VAL:HG23	1.77	0.67
1:B:306:LYS:HD3	1:B:340:PRO:HB3	1.76	0.67
1:B:365:ARG:NH2	1:B:381:ASP:OD1	2.28	0.66
1:A:271:ARG:NH2	3:A:506:SO4:O1	2.29	0.65
1:A:151:GLN:OE1	1:A:187:PRO:HD3	1.97	0.65
1:A:297:SER:OG	1:A:300:ASP:OD2	2.13	0.65
1:A:23:ARG:HH21	1:A:444:TYR:HE1	1.45	0.65
1:A:124:VAL:H	1:A:125:LYS:HD2	1.61	0.65
1:A:187:PRO:HG2	1:A:189:PHE:CE1	2.32	0.64
1:B:398:LEU:HD22	1:B:422:MET:HE1	1.79	0.64
1:B:420:ILE:HG12	1:B:434:LEU:HD21	1.80	0.64
1:A:23:ARG:HB2	1:A:28:ILE:HD13	1.79	0.64
1:B:47:ASP:HB3	1:B:51:MET:HE3	1.80	0.63
1:A:228:ASP:O	1:B:215:LYS:NZ	2.31	0.63
1:A:354:ASN:HB3	1:A:384:HIS:HD2	1.63	0.63
1:B:52:HIS:HA	1:B:93:LYS:HZ1	1.64	0.63
1:B:324:GLN:NE2	1:B:361:THR:OG1	2.29	0.63
1:B:15:MET:HG2	1:B:411:GLY:HA2	1.81	0.63
1:B:56:LEU:O	1:B:60:GLY:N	2.23	0.62
1:B:395:TRP:HA	1:B:422:MET:HE3	1.80	0.62
1:B:356:ILE:HB	1:B:361:THR:HG21	1.81	0.62
1:A:273:MET:O	1:A:277:VAL:HG22	2.00	0.62
1:A:120:ARG:NH2	1:A:123:GLY:O	2.32	0.62
1:A:19:MET:HE1	1:A:65:ASP:HB3	1.82	0.61
1:A:183:LEU:HD12	1:A:250:ALA:HA	1.81	0.61
1:A:44:GLU:CD	1:A:44:GLU:H	2.07	0.61
1:A:123:GLY:HA3	1:A:125:LYS:HD3	1.82	0.61
1:A:240:MET:HE1	1:A:262:MET:HE1	1.82	0.60
1:A:142:ASP:HB2	1:A:165:PRO:HD3	1.82	0.60
1:A:142:ASP:OD2	1:A:142:ASP:N	2.25	0.60
1:B:6:ILE:HB	1:B:443:LEU:HD23	1.83	0.60
1:A:251:ARG:HD3	1:A:352:SER:OG	2.01	0.59
1:B:110:ALA:HA	1:B:113:LYS:HE2	1.84	0.59
1:A:272:SER:HB2	1:A:321:THR:HG21	1.85	0.59
1:B:25:ASN:CG	1:B:26:GLU:H	2.05	0.58
1:B:109:THR:O	1:B:113:LYS:HG2	2.03	0.58
1:B:267:VAL:HG22	1:B:293:GLU:HB2	1.86	0.58
1:A:111:LEU:HD11	1:A:276:TYR:CE1	2.39	0.58
1:A:101:PRO:HB3	1:A:127:ASN:ND2	2.18	0.58
1:A:258:PHE:O	1:A:262:MET:HG2	2.04	0.58
1:B:437:LEU:HD11	1:B:443:LEU:HD22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:SER:O	1:A:154:ILE:HD13	2.04	0.57
1:B:226:LEU:HB3	1:B:258:PHE:HE2	1.68	0.57
1:A:405:HIS:HD2	1:A:435:HIS:NE2	2.03	0.57
1:B:305:LEU:HG	1:B:341:PHE:HB2	1.86	0.57
1:A:148:ILE:HB	1:A:159:PHE:HB2	1.87	0.56
1:A:56:LEU:HD23	1:A:59:MET:HE2	1.86	0.56
1:A:269:LEU:HD13	1:A:301:ILE:HG23	1.87	0.56
1:A:53:SER:O	1:A:57:ILE:HD12	2.06	0.56
1:A:159:PHE:CZ	1:A:175:PHE:HD2	2.24	0.56
1:B:258:PHE:O	1:B:262:MET:HG2	2.06	0.56
1:A:84:HIS:NE2	1:A:154:ILE:HD11	2.21	0.56
1:A:366:TYR:O	1:A:370:THR:HG23	2.05	0.56
1:B:273:MET:O	1:B:277:VAL:HG22	2.05	0.56
1:A:79:VAL:HG11	1:A:160:VAL:HG21	1.86	0.55
1:B:366:TYR:O	1:B:370:THR:HG23	2.05	0.55
1:B:302:ASP:OD1	1:B:333:ARG:NH2	2.40	0.55
1:B:334:ILE:HG12	1:B:339:THR:HG21	1.87	0.55
1:B:354:ASN:HB3	1:B:384:HIS:HD2	1.72	0.55
1:B:24:VAL:HB	1:B:143:ILE:HD11	1.88	0.55
1:B:11:GLY:HA3	1:B:18:ASN:HD22	1.72	0.55
1:A:323:HIS:O	1:A:365:ARG:NH1	2.39	0.54
1:B:127:ASN:OD1	1:B:127:ASN:N	2.34	0.54
1:A:293:GLU:OE2	1:A:307:LYS:NZ	2.41	0.54
1:A:304:ALA:O	1:A:308:ILE:HB	2.07	0.54
1:A:53:SER:OG	1:A:93:LYS:O	2.25	0.54
1:A:289:PRO:O	1:A:292:VAL:HG13	2.08	0.54
1:A:325:GLY:HA2	1:A:368:LEU:HD22	1.89	0.54
1:B:334:ILE:HA	1:B:339:THR:HG21	1.88	0.54
1:A:396:GLU:O	1:A:400:MET:HG2	2.08	0.53
1:A:231:LEU:HD22	1:A:262:MET:HB3	1.88	0.53
1:A:391:ARG:HG3	1:A:422:MET:HG3	1.90	0.53
1:B:283:LEU:HD12	1:B:285:TYR:CE2	2.44	0.52
1:A:101:PRO:HB3	1:A:127:ASN:HD21	1.74	0.52
1:A:175:PHE:HE2	1:A:397:LEU:HD22	1.74	0.52
1:A:36:ARG:NE	1:A:38:ASP:OD2	2.39	0.52
1:B:330:VAL:O	1:B:334:ILE:HG13	2.09	0.52
1:B:207:SER:OG	1:B:416:HIS:HD2	1.93	0.52
1:A:389:ALA:HB1	1:A:393:ASP:HB2	1.91	0.52
1:B:122:PHE:HE1	1:B:125:LYS:HZ1	1.57	0.52
1:A:14:GLU:CD	1:A:17:ARG:HH21	2.17	0.51
1:A:273:MET:HG2	1:A:321:THR:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:CYS:SG	1:B:91:ILE:HD11	2.50	0.51
1:B:394:HIS:CD2	1:B:419:TYR:HE1	2.28	0.51
1:A:23:ARG:HB2	1:A:28:ILE:CD1	2.40	0.51
1:B:314:ASP:OD1	1:B:314:ASP:N	2.43	0.51
1:A:18:ASN:HD21	1:A:410:HIS:CG	2.29	0.51
1:A:175:PHE:CE2	1:A:397:LEU:HD22	2.45	0.51
1:A:189:PHE:CD2	1:B:234:GLU:HG3	2.46	0.51
1:A:271:ARG:NH2	3:A:506:SO4:S	2.74	0.51
1:A:342:LYS:HE3	1:A:375:LYS:HZ1	1.76	0.51
1:A:17:ARG:HB2	1:A:36:ARG:HB2	1.93	0.51
1:A:74:ASN:HB3	1:A:76:ARG:NH1	2.25	0.51
1:B:11:GLY:HA3	1:B:18:ASN:ND2	2.27	0.50
1:A:37:LEU:H	1:A:37:LEU:HD12	1.77	0.50
1:B:206:GLU:OE1	1:B:388:HIS:HD2	1.94	0.50
1:B:55:GLU:O	1:B:58:GLU:HG2	2.12	0.50
1:B:8:ALA:O	1:B:440:GLY:N	2.40	0.50
1:B:324:GLN:HE22	1:B:356:ILE:H	1.59	0.50
1:A:124:VAL:H	1:A:125:LYS:CD	2.24	0.50
1:B:132:LYS:HD3	1:B:133:ALA:H	1.77	0.49
1:B:193:LYS:O	1:B:197:LYS:HG3	2.12	0.49
1:B:304:ALA:O	1:B:307:LYS:HB3	2.12	0.49
1:B:28:ILE:HB	1:B:75:VAL:HA	1.94	0.49
1:B:119:GLU:OE1	1:B:120:ARG:N	2.44	0.49
1:A:283:LEU:HD12	1:A:285:TYR:CE2	2.47	0.49
1:B:428:TYR:HD1	1:B:433:THR:HG22	1.77	0.49
1:B:334:ILE:HA	1:B:339:THR:CG2	2.43	0.49
1:B:305:LEU:HD21	1:B:341:PHE:N	2.21	0.49
1:B:305:LEU:CG	1:B:341:PHE:HB2	2.42	0.49
1:A:242:VAL:HG11	1:A:255:ILE:HD13	1.95	0.49
1:B:355:VAL:HG22	1:B:365:ARG:HD3	1.94	0.49
1:A:109:THR:HG21	1:A:130:ALA:HA	1.94	0.49
1:A:392:GLU:OE1	1:B:378:ARG:HD2	2.13	0.49
1:A:420:ILE:HG23	1:A:434:LEU:HD21	1.94	0.49
1:A:7:ILE:CG2	1:A:21:ALA:HB3	2.42	0.49
1:B:264:ARG:HD3	1:B:316:TYR:O	2.13	0.49
1:A:12:TYR:CE1	1:A:409:ALA:HB1	2.48	0.48
1:A:55:GLU:O	1:A:58:GLU:HG3	2.12	0.48
1:A:313:LYS:HD2	1:A:341:PHE:CE1	2.48	0.48
1:B:255:ILE:HG21	1:B:319:VAL:HG11	1.94	0.48
1:B:309:MET:HG3	1:B:341:PHE:HA	1.94	0.48
1:A:171:TYR:CE1	1:A:173:CYS:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:LEU:O	1:A:308:ILE:HG22	2.12	0.48
1:B:271:ARG:NH1	1:B:297:SER:HA	2.28	0.48
1:A:19:MET:HE2	1:A:63:PRO:HG2	1.94	0.48
1:B:305:LEU:HD23	1:B:340:PRO:HB2	1.96	0.48
1:B:30:ILE:HB	1:B:78:ILE:HG12	1.94	0.48
1:B:111:LEU:HD11	1:B:276:TYR:CE1	2.49	0.48
1:A:80:CYS:SG	1:A:91:ILE:HD11	2.53	0.48
1:A:171:TYR:CD1	1:A:171:TYR:C	2.92	0.47
1:A:265:ILE:HG23	1:A:316:TYR:CD1	2.49	0.47
1:A:305:LEU:HA	1:A:308:ILE:HG22	1.95	0.47
1:A:234:GLU:HG2	1:B:179:ARG:HH21	1.79	0.47
1:B:119:GLU:CD	1:B:121:LYS:H	2.22	0.47
1:B:158:VAL:HG22	1:B:159:PHE:O	2.14	0.47
1:A:342:LYS:HG3	1:A:375:LYS:HE3	1.97	0.47
1:B:242:VAL:HG22	1:B:350:ILE:HB	1.95	0.47
1:B:305:LEU:HA	1:B:308:ILE:CG2	2.39	0.47
1:A:356:ILE:HA	1:A:357:PRO:HD3	1.75	0.47
1:B:76:ARG:HD3	1:B:140:THR:OG1	2.15	0.47
1:B:404:GLU:O	1:B:433:THR:HG23	2.15	0.47
1:A:271:ARG:NH2	3:A:506:SO4:O4	2.48	0.47
1:A:354:ASN:HB3	1:A:384:HIS:CD2	2.49	0.47
1:A:158:VAL:HG22	1:A:159:PHE:O	2.15	0.46
1:A:230:LEU:HD12	1:A:258:PHE:HD2	1.79	0.46
1:B:271:ARG:HH12	1:B:297:SER:HA	1.79	0.46
1:A:174:ASP:OD2	1:A:388:HIS:NE2	2.46	0.46
1:A:323:HIS:CD2	1:A:324:GLN:HG2	2.50	0.46
1:B:231:LEU:HD23	1:B:262:MET:HE3	1.97	0.46
1:B:311:ALA:O	1:B:315:LYS:NZ	2.49	0.46
1:B:19:MET:HE2	1:B:63:PRO:HG2	1.98	0.45
1:A:334:ILE:HA	1:A:339:THR:HG21	1.98	0.45
1:A:159:PHE:HZ	1:A:175:PHE:HD2	1.64	0.45
1:A:240:MET:HE2	1:A:264:ARG:CZ	2.47	0.45
1:B:405:HIS:HD2	1:B:435:HIS:NE2	2.14	0.45
1:A:56:LEU:CB	1:A:62:ILE:HG12	2.47	0.45
1:B:7:ILE:HB	1:B:21:ALA:HB3	1.99	0.45
1:A:314:ASP:OD2	1:A:314:ASP:N	2.48	0.45
1:B:151:GLN:HE21	1:B:181:PRO:HG2	1.82	0.45
1:A:35:ILE:CD1	1:A:89:GLY:HA3	2.47	0.44
1:B:174:ASP:HA	1:B:206:GLU:OE1	2.16	0.44
1:A:367:ALA:O	1:A:371:LYS:HG3	2.16	0.44
1:A:114:HIS:O	1:A:275:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:PHE:HE2	1:A:192:LEU:HD21	1.82	0.44
1:A:51:MET:SD	1:A:55:GLU:HG2	2.58	0.44
1:B:7:ILE:HG21	1:B:68:MET:HE2	2.00	0.44
1:B:147:PHE:HB3	1:B:158:VAL:HG21	1.99	0.44
1:A:35:ILE:HD12	1:A:85:LEU:HB3	2.00	0.44
1:A:80:CYS:SG	1:A:88:ILE:HG22	2.58	0.44
1:A:334:ILE:HA	1:A:339:THR:CG2	2.48	0.44
1:B:14:GLU:CD	1:B:17:ARG:HH21	2.26	0.44
1:B:106:PRO:O	1:B:109:THR:OG1	2.31	0.44
1:B:240:MET:HE2	1:B:264:ARG:CZ	2.47	0.44
1:A:96:HIS:O	1:A:124:VAL:HG21	2.17	0.44
1:A:222:ALA:HB2	1:A:385:VAL:HG13	1.99	0.44
1:A:268:LEU:HD12	1:A:277:VAL:HG21	1.99	0.44
1:B:159:PHE:HE2	1:B:192:LEU:HD11	1.83	0.44
1:A:241:ILE:HD11	1:A:341:PHE:CE2	2.52	0.43
1:A:323:HIS:HD2	1:A:324:GLN:HE21	1.64	0.43
1:B:15:MET:HE3	1:B:410:HIS:HE1	1.83	0.43
1:A:124:VAL:HB	1:A:125:LYS:HA	2.00	0.43
1:A:414:GLN:OE1	1:A:414:GLN:N	2.46	0.43
1:B:56:LEU:O	1:B:61:ALA:HB3	2.19	0.43
1:A:176:LYS:NZ	1:A:386:SER:O	2.52	0.43
1:A:7:ILE:HD12	1:A:8:ALA:N	2.34	0.43
1:A:383:VAL:O	1:A:383:VAL:HG22	2.19	0.43
1:B:17:ARG:HB2	1:B:36:ARG:HB2	2.01	0.43
1:A:265:ILE:HA	1:A:266:PRO:HD2	1.76	0.43
1:B:36:ARG:HH12	1:B:39:ARG:NH2	2.17	0.43
1:A:265:ILE:HD13	1:A:291:ASN:HB2	2.00	0.42
1:A:308:ILE:HD13	1:A:318:PRO:HG3	2.01	0.42
1:B:7:ILE:HG13	1:B:21:ALA:HB3	2.01	0.42
1:B:29:ILE:HD12	1:B:77:ALA:HB3	2.02	0.42
1:B:242:VAL:O	1:B:319:VAL:HA	2.19	0.42
1:B:9:VAL:HG13	1:B:19:MET:HB3	2.01	0.42
1:A:31:ILE:HB	1:A:171:TYR:CE2	2.54	0.42
1:A:62:ILE:HD12	1:A:94:LEU:HD21	2.02	0.42
1:A:175:PHE:CE1	1:A:389:ALA:HB3	2.55	0.42
1:A:241:ILE:HD11	1:A:341:PHE:CZ	2.54	0.42
1:B:119:GLU:OE2	1:B:121:LYS:HB3	2.19	0.42
1:A:56:LEU:O	1:A:61:ALA:HB3	2.20	0.42
1:B:308:ILE:HD13	1:B:308:ILE:HG21	1.83	0.42
1:A:15:MET:HE1	1:A:208:THR:HG23	2.01	0.42
1:A:36:ARG:HH12	1:A:39:ARG:NH2	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:HH11	1:A:194:GLU:HG2	1.84	0.42
1:B:56:LEU:HD13	1:B:93:LYS:HE3	2.01	0.42
1:B:367:ALA:O	1:B:371:LYS:HG3	2.20	0.42
1:A:53:SER:C	1:A:57:ILE:HD12	2.45	0.42
1:A:93:LYS:HA	1:A:93:LYS:HD3	1.72	0.42
1:B:289:PRO:HB2	1:B:291:ASN:OD1	2.20	0.42
1:A:108:THR:O	1:A:112:ILE:HD12	2.19	0.42
1:A:305:LEU:HD22	1:A:341:PHE:HD2	1.84	0.42
1:A:341:PHE:CD1	1:A:341:PHE:C	2.98	0.42
1:B:164:THR:OG1	1:B:167:GLY:O	2.35	0.42
1:B:293:GLU:HB3	1:B:295:TYR:CZ	2.55	0.42
1:A:19:MET:HE2	1:A:63:PRO:CG	2.50	0.42
1:A:116:ILE:C	1:A:118:SER:H	2.27	0.42
1:B:230:LEU:HD12	1:B:258:PHE:HD2	1.85	0.42
1:A:45:ASP:OD1	1:A:45:ASP:N	2.52	0.41
1:A:396:GLU:OE2	1:B:348:ARG:NH2	2.53	0.41
1:A:378:ARG:NH1	1:B:392:GLU:OE2	2.47	0.41
1:B:174:ASP:OD2	1:B:410:HIS:NE2	2.53	0.41
1:B:82:HIS:NE2	1:B:84:HIS:HB2	2.35	0.41
1:B:148:ILE:HB	1:B:159:PHE:HB2	2.03	0.41
1:B:201:ILE:HD13	1:B:447:GLU:CD	2.45	0.41
1:B:299:ARG:HG3	1:B:300:ASP:OD2	2.21	0.41
1:B:337:GLY:C	1:B:339:THR:H	2.28	0.41
1:A:231:LEU:CD2	1:A:262:MET:HB3	2.51	0.41
1:A:251:ARG:O	1:A:255:ILE:HG13	2.19	0.41
1:B:7:ILE:HD13	1:B:442:GLU:CG	2.45	0.41
1:B:105:THR:OG1	1:B:106:PRO:HD2	2.21	0.41
1:B:268:LEU:HG	1:B:319:VAL:CG2	2.50	0.41
1:A:28:ILE:HB	1:A:75:VAL:CA	2.45	0.41
1:B:9:VAL:HG13	1:B:19:MET:O	2.20	0.41
1:B:56:LEU:HD22	1:B:93:LYS:HD3	2.03	0.41
1:A:100:ALA:O	1:A:126:ASN:HB3	2.20	0.41
1:A:153:SER:O	1:A:248:HIS:HA	2.21	0.41
1:A:171:TYR:HD1	1:A:172:ALA:N	2.18	0.41
1:B:53:SER:O	1:B:62:ILE:HD11	2.21	0.41
1:B:356:ILE:HA	1:B:357:PRO:HD3	1.84	0.40
1:A:230:LEU:HD12	1:A:258:PHE:CD2	2.56	0.40
1:A:320:MET:HB2	1:A:330:VAL:CG1	2.51	0.40
1:A:438:ARG:HA	1:A:438:ARG:HD2	1.95	0.40
1:A:56:LEU:HB2	1:A:62:ILE:HG12	2.03	0.40
1:A:154:ILE:HD12	1:A:247:SER:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HB2	1:B:62:ILE:HG12	2.04	0.40
1:A:175:PHE:C	1:A:175:PHE:CD1	3.00	0.40
1:A:268:LEU:HD22	1:A:319:VAL:HB	2.03	0.40
1:B:152:HIS:CG	1:B:153:SER:N	2.88	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	445/470 (95%)	411 (92%)	29 (6%)	5 (1%)	11	36
1	B	456/470 (97%)	417 (91%)	32 (7%)	7 (2%)	8	28
All	All	901/940 (96%)	828 (92%)	61 (7%)	12 (1%)	9	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	120	ARG
1	B	45	ASP
1	A	118	SER
1	A	45	ASP
1	B	32	ASP
1	B	118	SER
1	A	32	ASP
1	B	25	ASN
1	B	47	ASP
1	B	60	GLY
1	A	60	GLY
1	B	122	PHE

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	375/394 (95%)	339 (90%)	36 (10%)	8	26
1	B	386/394 (98%)	350 (91%)	36 (9%)	8	27
All	All	761/788 (97%)	689 (90%)	72 (10%)	8	26

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	9	VAL
1	A	23	ARG
1	A	35	ILE
1	A	37	LEU
1	A	38	ASP
1	A	45	ASP
1	A	46	VAL
1	A	55	GLU
1	A	58	GLU
1	A	71	VAL
1	A	75	VAL
1	A	108	THR
1	A	119	GLU
1	A	127	ASN
1	A	132	LYS
1	A	138	GLU
1	A	142	ASP
1	A	143	ILE
1	A	170	VAL
1	A	171	TYR
1	A	175	PHE
1	A	186	VAL
1	A	265	ILE
1	A	267	VAL
1	A	272	SER
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	292	VAL
1	A	315	LYS
1	A	320	MET
1	A	375	LYS
1	A	378	ARG
1	A	381	ASP
1	A	383	VAL
1	A	429	SER
1	A	443	LEU
1	B	7	ILE
1	B	9	VAL
1	B	15	MET
1	B	30	ILE
1	B	42	ILE
1	B	44	GLU
1	B	48	THR
1	B	54	LEU
1	B	58	GLU
1	B	75	VAL
1	B	85	LEU
1	B	119	GLU
1	B	122	PHE
1	B	124	VAL
1	B	127	ASN
1	B	132	LYS
1	B	139	ILE
1	B	143	ILE
1	B	157	THR
1	B	160	VAL
1	B	229	VAL
1	B	233	THR
1	B	247	SER
1	B	252	VAL
1	B	265	ILE
1	B	272	SER
1	B	283	LEU
1	B	287	ASP
1	B	303	ASN
1	B	307	LYS
1	B	385	VAL
1	B	406	VAL
1	B	434	LEU

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Mol	Chain	Res	Type
1	B	438	ARG
1	B	443	LEU
1	B	447	GLU

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	18	ASN
1	A	74	ASN
1	A	82	HIS
1	A	127	ASN
1	A	163	HIS
1	A	209	ASN
1	A	257	GLN
1	A	323	HIS
1	A	364	ASN
1	A	405	HIS
1	A	421	GLN
1	B	18	ASN
1	B	43	HIS
1	B	82	HIS
1	B	87	HIS
1	B	115	GLN
1	B	209	ASN
1	B	257	GLN
1	B	282	GLN
1	B	324	GLN
1	B	336	ASN
1	B	388	HIS
1	B	405	HIS
1	B	410	HIS
1	B	416	HIS
1	B	421	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	B	507	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	A	504	-	4,4,4	0.21	0	6,6,6	0.09	0
3	SO4	B	503	-	4,4,4	0.22	0	6,6,6	0.10	0
3	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	505	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	A	506	-	4,4,4	0.23	0	6,6,6	0.06	0
3	SO4	B	505	-	4,4,4	0.25	0	6,6,6	0.07	0
3	SO4	A	503	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SO4	B	506	-	4,4,4	0.23	0	6,6,6	0.09	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.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	SO4	4	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, 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	447/470 (95%)	0.26	13 (2%) 53 45	63, 101, 148, 208	0
1	B	460/470 (97%)	0.31	11 (2%) 59 50	63, 109, 168, 246	0
All	All	907/940 (96%)	0.29	24 (2%) 57 48	63, 105, 158, 246	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	124	VAL	5.8
1	B	123	GLY	3.8
1	A	61	ALA	3.6
1	A	37	LEU	3.2
1	B	122	PHE	2.9
1	A	201	ILE	2.9
1	A	35	ILE	2.6
1	B	42	ILE	2.6
1	A	86	ASP	2.5
1	A	7	ILE	2.4
1	A	173	CYS	2.4
1	A	39	ARG	2.4
1	B	245	PHE	2.4
1	B	40	VAL	2.3
1	B	67	ILE	2.3
1	A	175	PHE	2.2
1	B	119	GLU	2.2
1	A	119	GLU	2.2
1	A	161	ALA	2.2
1	A	40	VAL	2.1
1	B	-9	GLY	2.1
1	B	89	GLY	2.1
1	A	321	THR	2.0
1	B	77	ALA	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 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	SO4	B	507	5/5	0.19	0.22	428,428,430,431	0
3	SO4	B	506	5/5	0.54	0.09	187,187,187,187	0
3	SO4	A	506	5/5	0.59	0.10	130,163,169,170	0
3	SO4	A	504	5/5	0.66	0.14	137,159,165,165	0
3	SO4	B	504	5/5	0.75	0.10	167,167,168,168	0
3	SO4	B	505	5/5	0.80	0.10	128,148,152,153	0
3	SO4	A	505	5/5	0.86	0.11	108,123,132,132	0
2	ZN	A	501	1/1	0.93	0.15	152,152,152,152	0
3	SO4	B	503	5/5	0.93	0.10	76,87,97,104	0
3	SO4	A	503	5/5	0.94	0.10	67,78,83,88	0
2	ZN	B	501	1/1	0.97	0.10	139,139,139,139	0
2	ZN	A	502	1/1	0.97	0.04	93,93,93,93	0
2	ZN	B	502	1/1	0.98	0.07	114,114,114,114	0

6.5 Other polymers [i](#)

There are no such residues in this entry.