



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 11:09 PM UTC

PDB ID : 2E7Y / pdb_00002e7y
Title : High resolution structure of T. maritima tRNase Z
Authors : Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-01-15
Resolution : 1.97 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

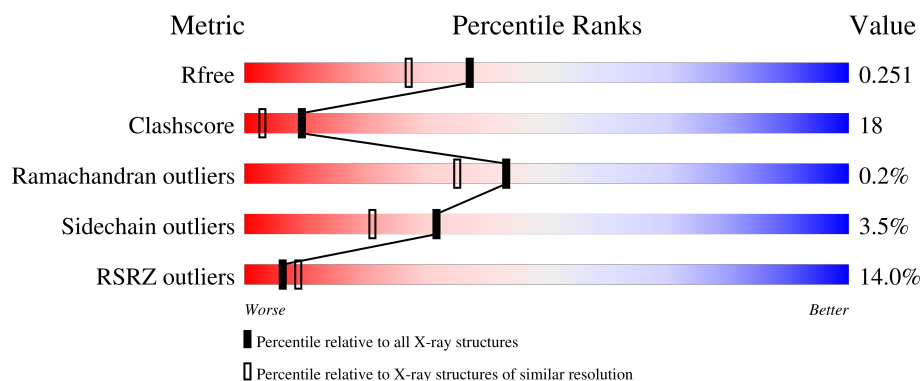
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	280	9% 70% 25% • •
1	B	280	18% 63% 29% • •

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4820 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 tRNase Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2234	1440	386	401	7			
1	B	269	Total	C	N	O	S	0	0	0
			2227	1437	387	397	6			

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

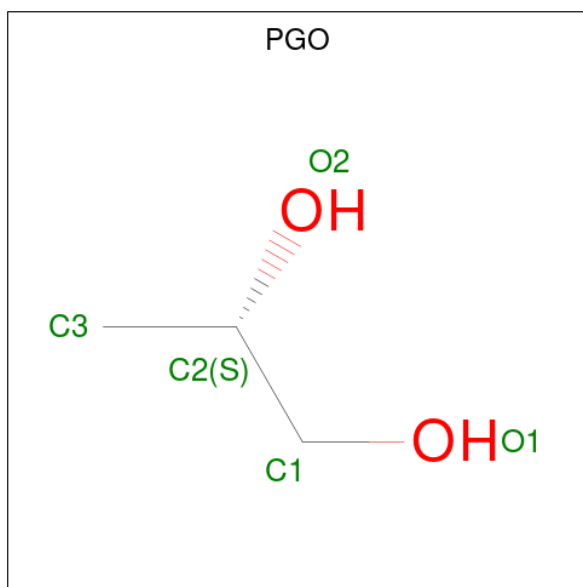
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: $C_3H_8O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0
4	A	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0
4	B	1	Total C O 5 3 2	0	0

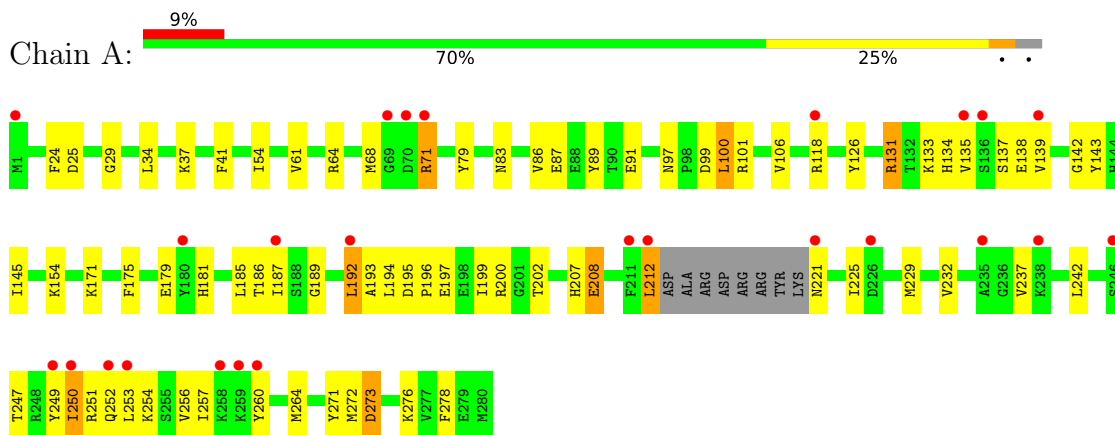
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	195	Total O 195 195	0	0
5	B	130	Total O 130 130	0	0

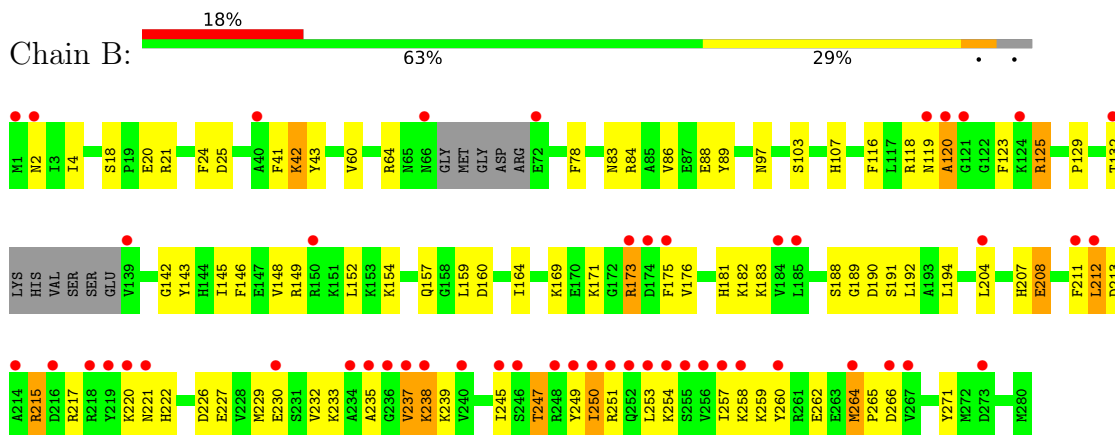
3 Residue-property plots

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: tRNase Z



• Molecule 1: tRNase Z



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	150.30Å 172.69Å 64.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.44 – 1.97 37.44 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.44-1.97) 97.5 (37.44-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.97Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.204 , 0.249 0.204 , 0.251	Depositor DCC
R_{free} test set	2950 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4820	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: ZN, SO4, PGO

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	0.58	0/2286	1.01	10/3072 (0.3%)
1	B	0.53	0/2278	1.02	14/3060 (0.5%)
All	All	0.56	0/4564	1.02	24/6132 (0.4%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	GLY	N-CA-C	-8.14	97.28	112.10
1	B	142	GLY	N-CA-C	-7.78	97.93	112.10
1	B	237	VAL	N-CA-C	6.83	118.15	108.93
1	B	145	ILE	N-CA-C	-6.82	98.63	108.17
1	B	189	GLY	N-CA-C	-6.40	100.65	112.62
1	B	250	ILE	N-CA-C	6.15	116.82	110.36
1	B	42	LYS	N-CA-C	-5.84	106.70	113.88
1	B	264	MET	CA-C-N	5.75	125.45	119.82
1	B	264	MET	C-N-CA	5.75	125.45	119.82
1	A	264	MET	CA-C-N	5.70	125.55	119.28
1	A	264	MET	C-N-CA	5.70	125.55	119.28
1	A	189	GLY	N-CA-C	-5.69	101.98	112.62
1	B	4	ILE	N-CA-C	-5.54	99.58	107.77
1	B	212	LEU	N-CA-C	-5.54	106.57	113.38
1	B	188	SER	N-CA-C	5.47	117.32	111.36
1	B	120	ALA	N-CA-C	-5.47	106.49	112.72
1	A	225	ILE	N-CA-C	5.35	116.72	110.62
1	B	215	ARG	CA-C-N	-5.30	115.69	122.79
1	B	215	ARG	C-N-CA	-5.30	115.69	122.79
1	A	54	ILE	N-CA-C	5.25	118.70	113.71
1	A	145	ILE	N-CA-C	-5.14	100.35	107.80
1	A	273	ASP	CA-C-N	5.11	124.83	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ASP	C-N-CA	5.11	124.83	119.82
1	A	139	VAL	N-CA-C	5.02	115.57	109.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2234	0	2239	68	0
1	B	2227	0	2235	91	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	10	0	0	0	0
4	A	10	0	16	5	0
4	B	10	0	16	2	0
5	A	195	0	0	4	1
5	B	130	0	0	7	0
All	All	4820	0	4506	161	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 18.

All (161) 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:135:VAL:HG13	1:A:137:SER:H	1.36	0.90
1:B:103:SER:HB2	5:B:2357:HOH:O	1.71	0.88
1:B:217:ARG:HH11	1:B:220:LYS:HG2	1.37	0.88
1:B:217:ARG:HD3	1:B:220:LYS:HA	1.55	0.86
1:B:42:LYS:HE3	1:B:118:ARG:HD3	1.58	0.85
1:B:266:ASP:HB2	5:B:2388:HOH:O	1.78	0.84
1:B:212:LEU:HD12	1:B:249:TYR:HB3	1.60	0.82
1:A:194:LEU:H	1:A:207:HIS:HE1	1.28	0.82
1:B:116:PHE:O	5:B:2375:HOH:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HG3	1:B:119:ASN:H	1.47	0.79
1:B:84:ARG:NH1	1:B:84:ARG:HB3	1.98	0.78
1:A:253:LEU:O	1:A:257:ILE:HG12	1.84	0.78
1:B:232:VAL:HG13	1:B:237:VAL:HB	1.65	0.78
1:B:245:ILE:HG21	1:B:253:LEU:HD21	1.67	0.76
1:B:119:ASN:CG	1:B:120:ALA:H	1.94	0.76
1:B:169:LYS:HB2	5:B:2343:HOH:O	1.86	0.75
1:A:185:LEU:HD21	1:A:187:ILE:HG23	1.67	0.75
1:B:173:ARG:CB	1:B:173:ARG:HH11	1.99	0.74
1:A:247:THR:O	1:A:250:ILE:HG13	1.89	0.73
1:A:250:ILE:CD1	1:A:251:ARG:H	2.02	0.72
1:B:41:PHE:O	1:B:64:ARG:NH2	2.23	0.72
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.55	0.70
1:B:247:THR:O	1:B:250:ILE:HB	1.92	0.70
1:A:194:LEU:H	1:A:207:HIS:CE1	2.10	0.69
1:B:217:ARG:NH1	1:B:220:LYS:HG2	2.08	0.69
1:A:232:VAL:HG13	1:A:237:VAL:HB	1.74	0.69
1:A:254:LYS:HE2	1:A:271:TYR:OH	1.93	0.68
1:A:249:TYR:HB3	1:A:253:LEU:HD23	1.75	0.68
1:A:71:ARG:HD2	1:A:71:ARG:H	1.59	0.67
1:A:61:VAL:HG12	1:A:100:LEU:HG	1.77	0.67
1:A:29:GLY:HA3	4:A:601:PGO:H11	1.78	0.66
1:B:194:LEU:H	1:B:207:HIS:HE1	1.42	0.66
1:A:41:PHE:O	1:A:64:ARG:NH2	2.29	0.66
1:B:173:ARG:HH11	1:B:173:ARG:HB2	1.59	0.66
1:B:212:LEU:HB2	1:B:249:TYR:CD2	2.31	0.65
1:B:132:THR:HB	1:B:191:SER:HB3	1.78	0.65
1:A:126:TYR:OH	1:A:181:HIS:HD2	1.80	0.64
1:A:272:MET:HE3	1:A:278:PHE:HB3	1.81	0.63
1:A:29:GLY:HA3	4:A:601:PGO:C1	2.29	0.62
1:A:171:LYS:HD3	1:A:175:PHE:CE2	2.35	0.62
1:B:83:ASN:HD22	1:B:86:VAL:H	1.47	0.62
4:A:604:PGO:H12	5:A:1354:HOH:O	2.00	0.61
1:B:118:ARG:HG3	1:B:119:ASN:N	2.15	0.61
1:A:250:ILE:HD12	1:A:251:ARG:H	1.64	0.61
1:A:143:TYR:HD1	1:A:187:ILE:HD11	1.66	0.61
1:A:135:VAL:HG13	1:A:137:SER:N	2.13	0.60
1:A:179:GLU:H	4:A:604:PGO:H31	1.64	0.60
1:A:212:LEU:HD23	1:A:253:LEU:HD22	1.81	0.60
1:A:252:GLN:O	1:A:256:VAL:HG23	2.00	0.60
1:A:79:TYR:CE2	1:A:106:VAL:HG12	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:O	1:B:119:ASN:HB3	2.01	0.60
1:A:118:ARG:HG3	5:A:1432:HOH:O	2.01	0.60
1:A:135:VAL:C	1:A:137:SER:H	2.07	0.60
1:B:42:LYS:CE	1:B:118:ARG:HD3	2.29	0.60
1:B:119:ASN:ND2	1:B:120:ALA:H	2.00	0.59
1:A:197:GLU:OE2	1:A:200:ARG:NH1	2.34	0.59
1:B:84:ARG:HB3	1:B:84:ARG:HH11	1.67	0.59
1:A:185:LEU:HD23	1:A:186:THR:N	2.18	0.58
1:B:149:ARG:NH1	1:B:182:LYS:HG2	2.18	0.58
1:A:87:GLU:O	1:A:91:GLU:HG3	2.03	0.58
1:A:131:ARG:HG3	1:A:131:ARG:NH1	2.18	0.58
1:A:249:TYR:O	1:A:253:LEU:HD23	2.03	0.58
1:A:250:ILE:HD13	1:A:251:ARG:HG3	1.84	0.58
1:B:207:HIS:HD2	1:B:208:GLU:O	1.87	0.57
1:A:79:TYR:HE2	1:A:106:VAL:HG12	1.69	0.56
1:A:187:ILE:HG13	1:A:187:ILE:O	2.06	0.56
1:B:254:LYS:O	1:B:258:LYS:HG2	2.06	0.56
1:A:135:VAL:C	1:A:137:SER:N	2.64	0.56
1:B:119:ASN:CG	1:B:120:ALA:N	2.64	0.55
1:A:249:TYR:HB3	1:A:253:LEU:CD2	2.36	0.55
1:B:116:PHE:HB3	1:B:123:PHE:HD2	1.72	0.55
1:A:194:LEU:HG	1:A:207:HIS:CE1	2.42	0.55
1:A:68:MET:O	1:A:71:ARG:HG2	2.06	0.55
1:B:254:LYS:HG3	1:B:258:LYS:HE2	1.88	0.54
1:B:238:LYS:HG2	1:B:239:LYS:N	2.23	0.54
1:B:20:GLU:OE1	1:B:125:ARG:HD3	2.08	0.54
1:B:43:TYR:OH	1:B:118:ARG:HG2	2.08	0.53
1:B:249:TYR:O	1:B:253:LEU:HG	2.09	0.53
1:B:259:LYS:O	1:B:262:GLU:HB3	2.09	0.53
1:B:148:VAL:HG22	1:B:181:HIS:CD2	2.44	0.52
1:B:211:PHE:HE1	1:B:222:HIS:HB2	1.73	0.52
1:A:212:LEU:HB2	1:A:253:LEU:HD21	1.91	0.52
1:B:212:LEU:CD1	1:B:249:TYR:HB3	2.38	0.52
1:A:99:ASP:HB2	5:A:1325:HOH:O	2.10	0.52
1:B:217:ARG:HH22	1:B:227:GLU:CD	2.17	0.52
1:A:83:ASN:HD22	1:A:86:VAL:H	1.58	0.52
1:A:185:LEU:HD23	1:A:185:LEU:C	2.35	0.52
1:A:71:ARG:HD2	1:A:71:ARG:N	2.25	0.51
1:B:119:ASN:ND2	1:B:120:ALA:N	2.58	0.51
1:B:192:LEU:HD21	1:B:220:LYS:C	2.35	0.51
1:B:125:ARG:HA	1:B:146:PHE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ARG:NH2	1:B:227:GLU:OE1	2.44	0.51
1:A:185:LEU:CD2	1:A:187:ILE:HG23	2.37	0.50
1:A:133:LYS:O	1:A:192:LEU:HD13	2.10	0.50
4:A:601:PGO:H33	4:B:602:PGO:H2	1.94	0.50
1:B:171:LYS:HG2	1:B:175:PHE:CD2	2.47	0.50
1:B:250:ILE:HG23	1:B:251:ARG:N	2.27	0.49
1:A:194:LEU:N	1:A:207:HIS:HE1	2.05	0.49
1:B:154:LYS:O	1:B:157:GLN:HG3	2.12	0.49
1:B:173:ARG:CB	1:B:173:ARG:NH1	2.72	0.49
1:A:229:MET:N	1:A:229:MET:HE2	2.28	0.48
1:A:212:LEU:C	1:A:212:LEU:HD13	2.38	0.48
1:B:229:MET:HE2	1:B:229:MET:HA	1.95	0.48
1:A:207:HIS:HD2	1:A:208:GLU:O	1.96	0.48
1:A:195:ASP:OD2	1:A:196:PRO:HD2	2.14	0.47
1:B:2:ASN:HA	1:B:18:SER:OG	2.13	0.47
1:B:84:ARG:HB3	1:B:84:ARG:CZ	2.44	0.47
1:B:251:ARG:C	1:B:253:LEU:N	2.71	0.46
1:A:89:TYR:OH	5:A:1363:HOH:O	2.09	0.46
1:B:132:THR:HB	1:B:191:SER:CB	2.44	0.46
1:B:190:ASP:O	1:B:191:SER:HB3	2.14	0.46
1:B:250:ILE:CG2	1:B:251:ARG:N	2.78	0.45
1:B:129:PRO:HB3	1:B:143:TYR:CE2	2.51	0.45
1:A:143:TYR:CD1	1:A:187:ILE:HD11	2.48	0.45
1:A:256:VAL:HG12	1:A:260:TYR:CD1	2.52	0.45
1:B:78:PHE:CD2	1:B:107:HIS:HB2	2.52	0.45
1:B:89:TYR:OH	5:B:2306:HOH:O	2.06	0.45
1:B:194:LEU:H	1:B:207:HIS:CE1	2.29	0.45
1:B:213:ASP:OD1	1:B:215:ARG:HB2	2.16	0.44
1:B:230:GLU:O	1:B:233:LYS:HB3	2.17	0.44
1:A:71:ARG:HH11	1:A:71:ARG:HG3	1.82	0.44
1:A:134:HIS:O	1:A:221:ASN:N	2.51	0.44
1:B:146:PHE:CE2	1:B:183:LYS:HG3	2.52	0.44
1:B:154:LYS:HA	1:B:157:GLN:OE1	2.16	0.44
1:A:250:ILE:HD13	1:A:251:ARG:H	1.77	0.44
1:B:262:GLU:O	1:B:265:PRO:HG3	2.17	0.44
1:B:60:VAL:O	1:B:64:ARG:HG3	2.18	0.44
1:A:199:ILE:O	1:A:202:THR:HG22	2.18	0.44
1:A:273:ASP:HB3	1:A:276:LYS:HG2	1.99	0.43
1:B:229:MET:HG3	1:B:260:TYR:CD2	2.53	0.43
1:B:24:PHE:O	1:B:25:ASP:HB2	2.17	0.43
1:B:97:ASN:ND2	5:B:2328:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:HD23	1:B:157:GLN:HA	1.99	0.43
1:B:217:ARG:NH2	1:B:227:GLU:CD	2.76	0.43
1:B:217:ARG:NH2	1:B:227:GLU:OE2	2.47	0.43
1:A:192:LEU:O	1:A:193:ALA:C	2.62	0.43
1:B:226:ASP:OD2	1:B:227:GLU:N	2.51	0.43
1:B:84:ARG:HH12	1:B:88:GLU:CD	2.26	0.43
1:B:254:LYS:NZ	4:B:603:PGO:H31	2.32	0.43
1:B:257:ILE:HD13	1:B:271:TYR:CD2	2.54	0.43
1:B:212:LEU:HD23	1:B:212:LEU:HA	1.84	0.43
1:B:226:ASP:HB3	1:B:260:TYR:OH	2.19	0.43
1:B:233:LYS:O	1:B:235:ALA:O	2.37	0.43
1:B:21:ARG:HB2	1:B:42:LYS:HD3	2.00	0.43
1:B:262:GLU:O	1:B:265:PRO:HD3	2.19	0.42
1:B:227:GLU:O	1:B:230:GLU:HB3	2.19	0.42
1:A:135:VAL:O	1:A:135:VAL:HG22	2.20	0.42
1:A:24:PHE:O	1:A:25:ASP:HB2	2.20	0.42
1:B:160:ASP:OD1	1:B:160:ASP:C	2.62	0.41
1:B:191:SER:HB2	5:B:2415:HOH:O	2.19	0.41
1:A:135:VAL:CG1	1:A:138:GLU:H	2.34	0.41
1:A:192:LEU:N	1:A:192:LEU:CD1	2.83	0.41
1:B:164:ILE:HD11	1:B:176:VAL:HG11	2.02	0.41
1:A:37:LYS:HE3	1:A:37:LYS:HB2	1.84	0.41
1:B:173:ARG:NH1	1:B:173:ARG:HB3	2.36	0.41
1:B:264:MET:N	1:B:265:PRO:HD3	2.36	0.41
1:B:173:ARG:HH11	1:B:173:ARG:HB3	1.82	0.41
1:A:34:LEU:HD22	1:A:37:LYS:HD2	2.02	0.40
1:A:97:ASN:HB2	1:A:100:LEU:HD22	2.03	0.40
1:B:233:LYS:HB2	1:B:233:LYS:HE3	1.88	0.40
1:B:84:ARG:CZ	1:B:84:ARG:CB	3.00	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)
5:A:1484:HOH:O	5:A:1484:HOH:O[3_655]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/280 (96%)	254 (95%)	14 (5%)	0	100	100
1	B	263/280 (94%)	244 (93%)	18 (7%)	1 (0%)	30	20
All	All	531/560 (95%)	498 (94%)	32 (6%)	1 (0%)	43	35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	238	LYS

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	241/248 (97%)	231 (96%)	10 (4%)	27	16
1	B	239/248 (96%)	232 (97%)	7 (3%)	37	28
All	All	480/496 (97%)	463 (96%)	17 (4%)	32	21

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	ARG
1	A	100	LEU
1	A	101	ARG
1	A	131	ARG
1	A	154	LYS

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Mol	Chain	Res	Type
1	A	192	LEU
1	A	208	GLU
1	A	212	LEU
1	A	242	LEU
1	A	250	ILE
1	B	125	ARG
1	B	159	LEU
1	B	173	ARG
1	B	204	LEU
1	B	208	GLU
1	B	221	ASN
1	B	247	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	HIS
1	A	83	ASN
1	A	134	HIS
1	A	181	HIS
1	A	207	HIS
1	B	2	ASN
1	B	65	ASN
1	B	83	ASN
1	B	97	ASN
1	B	119	ASN
1	B	207	HIS

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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	PGO	B	602	-	4,4,4	0.53	0	4,4,4	0.90	0
4	PGO	B	603	-	4,4,4	0.73	0	4,4,4	0.74	0
4	PGO	A	604	-	4,4,4	0.83	0	4,4,4	0.72	0
3	SO4	A	502	-	4,4,4	0.36	0	6,6,6	0.12	0
4	PGO	A	601	-	4,4,4	0.47	0	4,4,4	0.87	0
3	SO4	A	501	-	4,4,4	0.32	0	6,6,6	0.20	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	PGO	A	601	-	-	0/2/2/2	-
4	PGO	B	603	-	-	0/2/2/2	-
4	PGO	A	604	-	-	0/2/2/2	-
4	PGO	B	602	-	-	0/2/2/2	-

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.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	PGO	1	0
4	B	603	PGO	1	0
4	A	604	PGO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	PGO	3	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	272/280 (97%)	0.54	25 (9%) 14 20	22, 39, 84, 110	0
1	B	269/280 (96%)	1.06	51 (18%) 3 4	24, 50, 98, 125	0
All	All	541/560 (96%)	0.80	76 (14%) 6 9	22, 45, 91, 125	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ILE	7.8
1	A	69	GLY	5.3
1	B	255	SER	5.0
1	B	237	VAL	4.8
1	B	236	GLY	4.8
1	B	253	LEU	4.8
1	B	120	ALA	4.5
1	B	249	TYR	4.4
1	A	118	ARG	4.1
1	A	212	LEU	3.6
1	B	254	LYS	3.6
1	B	238	LYS	3.6
1	B	252	GLN	3.5
1	B	216	ASP	3.5
1	A	249	TYR	3.5
1	A	250	ILE	3.5
1	B	121	GLY	3.4
1	B	139	VAL	3.3
1	B	256	VAL	3.3
1	A	71	ARG	3.3
1	A	192	LEU	3.2
1	B	257	ILE	3.2
1	A	260	TYR	3.2
1	B	248	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	211	PHE	3.1
1	B	258	LYS	3.1
1	A	259	LYS	3.0
1	B	124	LYS	3.0
1	A	136	SER	2.9
1	A	139	VAL	2.8
1	A	235	ALA	2.8
1	B	2	ASN	2.8
1	A	226	ASP	2.8
1	B	219	TYR	2.8
1	A	135	VAL	2.7
1	B	1	MET	2.7
1	B	234	ALA	2.7
1	B	174	ASP	2.7
1	B	267	VAL	2.7
1	B	119	ASN	2.6
1	A	70	ASP	2.6
1	B	212	LEU	2.6
1	B	251	ARG	2.5
1	B	72	GLU	2.5
1	B	230	GLU	2.5
1	A	180	TYR	2.4
1	A	221	ASN	2.4
1	A	211	PHE	2.4
1	B	264	MET	2.4
1	B	246	SER	2.4
1	B	245	ILE	2.4
1	B	221	ASN	2.4
1	A	246	SER	2.4
1	A	238	LYS	2.4
1	A	258	LYS	2.4
1	B	235	ALA	2.3
1	B	173	ARG	2.3
1	A	187	ILE	2.3
1	B	240	VAL	2.3
1	B	273	ASP	2.3
1	B	266	ASP	2.2
1	B	184	VAL	2.2
1	B	214	ALA	2.2
1	A	253	LEU	2.2
1	B	175	PHE	2.1
1	B	150	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	132	THR	2.1
1	B	66	ASN	2.1
1	B	185	LEU	2.1
1	B	204	LEU	2.1
1	B	40	ALA	2.1
1	A	1	MET	2.1
1	A	252	GLN	2.1
1	B	220	LYS	2.0
1	B	260	TYR	2.0
1	B	218	ARG	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
4	PGO	A	604	5/5	0.81	0.16	36,47,88,93	0
4	PGO	B	603	5/5	0.82	0.18	62,77,80,88	0
3	SO4	A	502	5/5	0.83	0.12	96,99,114,122	0
4	PGO	B	602	5/5	0.91	0.16	42,45,58,91	0
3	SO4	A	501	5/5	0.92	0.11	59,59,67,85	0
4	PGO	A	601	5/5	0.93	0.15	38,59,79,83	0
2	ZN	B	2302	1/1	0.97	0.13	72,72,72,72	0
2	ZN	A	1302	1/1	0.99	0.17	64,64,64,64	0
2	ZN	B	2301	1/1	1.00	0.04	47,47,47,47	0
2	ZN	A	1301	1/1	1.00	0.03	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.