



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 4GIJ / pdb_00004gij
Title : Crystal Structure of Pseudouridine Monophosphate Glycosidase Complexed with Sulfate
Authors : Huang, S.; Mahanta, N.; Begley, T.P.; Ealick, S.E.
Deposited on : 2012-08-08
Resolution : 1.94 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

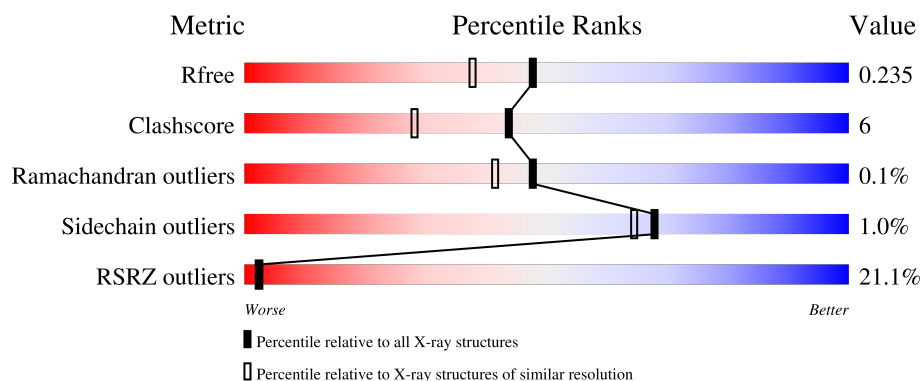
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	335	16% 79% 10% 9%
1	B	335	16% 80% 10% 9%
1	C	335	26% 78% 12% 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6787 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 Pseudouridine-5'-phosphate glycosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2157	1366	371	413	7			
1	B	304	Total	C	N	O	S	0	0	0
			2161	1371	366	418	6			
1	C	302	Total	C	N	O	S	0	0	0
			2086	1322	358	399	7			

There are 69 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP P33025
A	-21	GLY	-	expression tag	UNP P33025
A	-20	SER	-	expression tag	UNP P33025
A	-19	ASP	-	expression tag	UNP P33025
A	-18	LYS	-	expression tag	UNP P33025
A	-17	ILE	-	expression tag	UNP P33025
A	-16	HIS	-	expression tag	UNP P33025
A	-15	HIS	-	expression tag	UNP P33025
A	-14	HIS	-	expression tag	UNP P33025
A	-13	HIS	-	expression tag	UNP P33025
A	-12	HIS	-	expression tag	UNP P33025
A	-11	HIS	-	expression tag	UNP P33025
A	-10	SER	-	expression tag	UNP P33025
A	-9	SER	-	expression tag	UNP P33025
A	-8	GLY	-	expression tag	UNP P33025
A	-7	GLU	-	expression tag	UNP P33025
A	-6	ASN	-	expression tag	UNP P33025
A	-5	LEU	-	expression tag	UNP P33025
A	-4	TYR	-	expression tag	UNP P33025
A	-3	PHE	-	expression tag	UNP P33025
A	-2	GLN	-	expression tag	UNP P33025
A	-1	GLY	-	expression tag	UNP P33025
A	0	HIS	-	expression tag	UNP P33025

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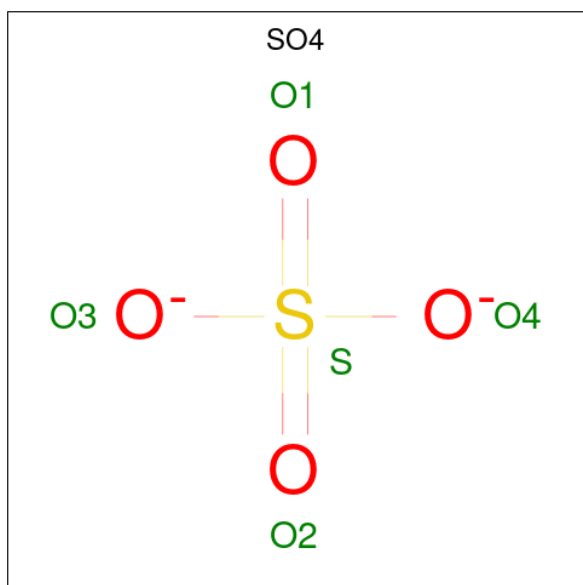
Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	expression tag	UNP P33025
B	-21	GLY	-	expression tag	UNP P33025
B	-20	SER	-	expression tag	UNP P33025
B	-19	ASP	-	expression tag	UNP P33025
B	-18	LYS	-	expression tag	UNP P33025
B	-17	ILE	-	expression tag	UNP P33025
B	-16	HIS	-	expression tag	UNP P33025
B	-15	HIS	-	expression tag	UNP P33025
B	-14	HIS	-	expression tag	UNP P33025
B	-13	HIS	-	expression tag	UNP P33025
B	-12	HIS	-	expression tag	UNP P33025
B	-11	HIS	-	expression tag	UNP P33025
B	-10	SER	-	expression tag	UNP P33025
B	-9	SER	-	expression tag	UNP P33025
B	-8	GLY	-	expression tag	UNP P33025
B	-7	GLU	-	expression tag	UNP P33025
B	-6	ASN	-	expression tag	UNP P33025
B	-5	LEU	-	expression tag	UNP P33025
B	-4	TYR	-	expression tag	UNP P33025
B	-3	PHE	-	expression tag	UNP P33025
B	-2	GLN	-	expression tag	UNP P33025
B	-1	GLY	-	expression tag	UNP P33025
B	0	HIS	-	expression tag	UNP P33025
C	-22	MET	-	expression tag	UNP P33025
C	-21	GLY	-	expression tag	UNP P33025
C	-20	SER	-	expression tag	UNP P33025
C	-19	ASP	-	expression tag	UNP P33025
C	-18	LYS	-	expression tag	UNP P33025
C	-17	ILE	-	expression tag	UNP P33025
C	-16	HIS	-	expression tag	UNP P33025
C	-15	HIS	-	expression tag	UNP P33025
C	-14	HIS	-	expression tag	UNP P33025
C	-13	HIS	-	expression tag	UNP P33025
C	-12	HIS	-	expression tag	UNP P33025
C	-11	HIS	-	expression tag	UNP P33025
C	-10	SER	-	expression tag	UNP P33025
C	-9	SER	-	expression tag	UNP P33025
C	-8	GLY	-	expression tag	UNP P33025
C	-7	GLU	-	expression tag	UNP P33025
C	-6	ASN	-	expression tag	UNP P33025
C	-5	LEU	-	expression tag	UNP P33025
C	-4	TYR	-	expression tag	UNP P33025

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	PHE	-	expression tag	UNP P33025
C	-2	GLN	-	expression tag	UNP P33025
C	-1	GLY	-	expression tag	UNP P33025
C	0	HIS	-	expression tag	UNP P33025

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

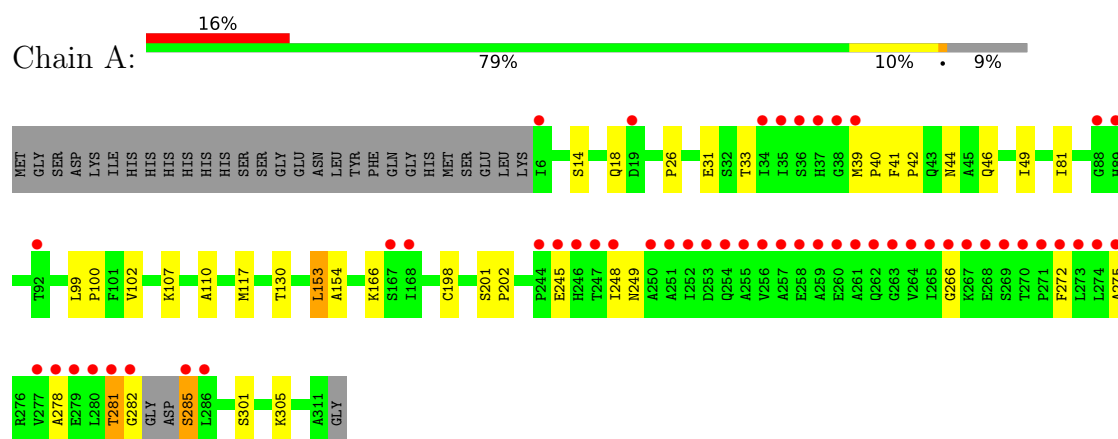
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	170	Total 170	O 170	0	0
4	B	109	Total 109	O 109	0	0
4	C	86	Total 86	O 86	0	0

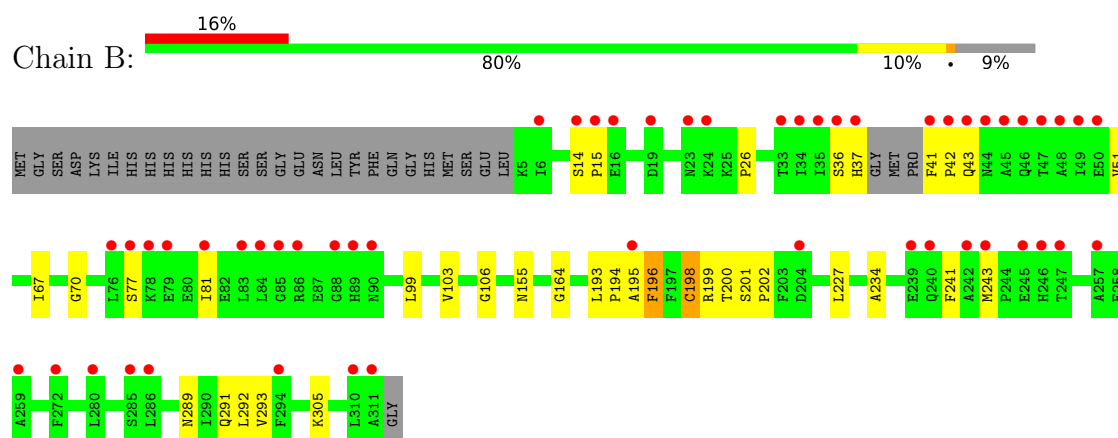
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

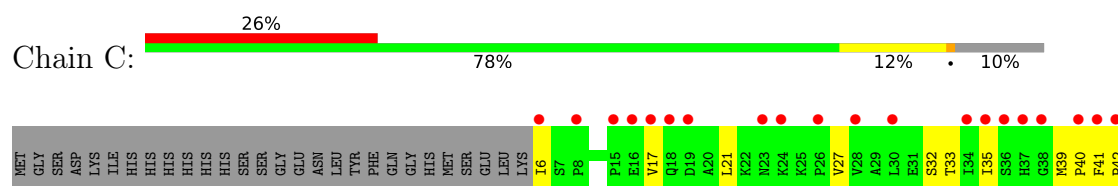
- Molecule 1: Pseudouridine-5'-phosphate glycosidase

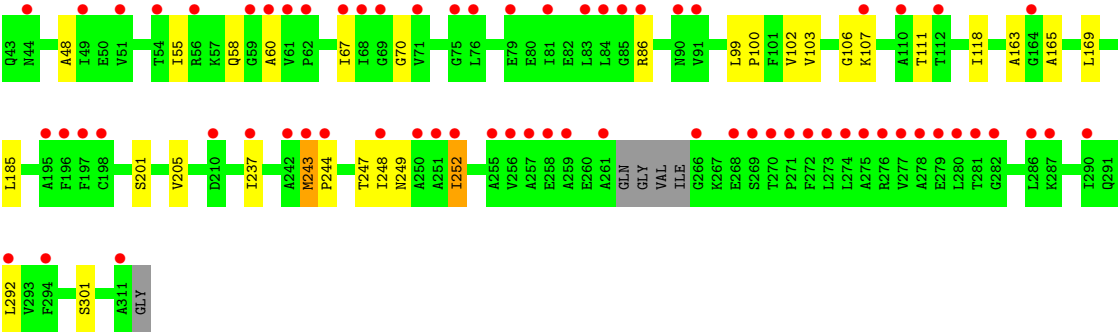


- Molecule 1: Pseudouridine-5'-phosphate glycosidase



- Molecule 1: Pseudouridine-5'-phosphate glycosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.10Å 115.40Å 132.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.44 – 1.94 43.44 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.44-1.94) 99.7 (43.44-1.94)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 1.94Å)	Xtriage
Refinement program	PHENIX 1.7.1 _743	Depositor
R, R_{free}	0.185 , 0.220 0.213 , 0.235	Depositor DCC
R_{free} test set	3572 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6787	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 5.13% 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: MN, SO4

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	0.66	2/2188 (0.1%)	0.85	1/2979 (0.0%)
1	B	0.68	5/2190 (0.2%)	0.90	6/2987 (0.2%)
1	C	0.64	1/2117 (0.0%)	0.85	0/2895
All	All	0.66	8/6495 (0.1%)	0.87	7/8861 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	LEU	C-O	-6.86	1.16	1.24
1	B	201	SER	C-N	6.47	1.40	1.34
1	A	154	ALA	C-O	-6.13	1.16	1.24
1	B	199	ARG	C-O	-5.56	1.17	1.24
1	B	42	PRO	N-CD	5.33	1.55	1.47
1	B	155	ASN	C-O	-5.17	1.17	1.24
1	C	201	SER	C-O	-5.17	1.17	1.24
1	B	202	PRO	N-CD	5.05	1.54	1.47

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	51	VAL	N-CA-C	-5.63	105.04	110.72
1	B	41	PHE	C-N-CD	5.60	132.92	120.60
1	B	164	GLY	N-CA-C	-5.59	103.78	112.45
1	B	201	SER	CA-C-N	-5.51	114.00	120.12
1	B	201	SER	C-N-CA	-5.51	114.00	120.12
1	B	198	CYS	N-CA-C	5.15	118.13	109.95
1	A	281	THR	N-CA-C	5.08	116.63	111.14

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	2157	0	2109	25	0
1	B	2161	0	2139	19	0
1	C	2086	0	1987	34	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	170	0	0	2	0
4	B	109	0	0	0	0
4	C	86	0	0	0	0
All	All	6787	0	6235	77	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 6.

All (77) 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:C:41:PHE:CE1	1:C:86:ARG:HG3	1.95	1.02
1:B:195:ALA:HB3	1:B:198:CYS:HB2	1.54	0.88
1:C:41:PHE:CE1	1:C:86:ARG:CG	2.64	0.81
1:C:244:PRO:HB2	1:C:247:THR:HG23	1.72	0.70
1:A:266:GLY:O	4:A:529:HOH:O	2.09	0.70
1:C:33:THR:HG23	1:C:111:THR:O	1.94	0.67
1:A:281:THR:N	1:A:282:GLY:HA2	2.08	0.67
1:C:99:LEU:HB3	1:C:100:PRO:HD3	1.76	0.66
1:C:67:ILE:HD11	1:C:99:LEU:CD1	2.26	0.66
1:A:39:MET:HB2	1:A:40:PRO:HD2	1.76	0.66
1:A:278:ALA:O	1:A:282:GLY:HA2	1.96	0.66
1:C:41:PHE:HE1	1:C:86:ARG:HG3	1.61	0.65
1:A:198:CYS:SG	1:A:248:ILE:HG21	2.37	0.65
1:B:77:SER:O	1:B:81:ILE:HG13	1.99	0.61
1:C:163:ALA:HB2	1:C:292:LEU:HD22	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLU:OE1	1:A:130:THR:OG1	2.14	0.60
1:C:70:GLY:HA3	1:C:106:GLY:HA2	1.82	0.59
1:B:26:PRO:HG3	1:B:305:LYS:HG2	1.83	0.59
1:C:237:ILE:HB	1:C:292:LEU:HD21	1.84	0.59
1:B:243:MET:HE2	1:B:243:MET:HA	1.84	0.58
1:C:41:PHE:CD2	1:C:42:PRO:CA	2.88	0.57
1:A:33:THR:HA	1:A:110:ALA:HB1	1.87	0.56
1:C:21:LEU:CD1	1:C:27:VAL:HG21	2.35	0.56
1:C:41:PHE:CG	1:C:42:PRO:HA	2.40	0.56
1:C:21:LEU:HD12	1:C:27:VAL:HG21	1.88	0.55
1:C:249:ASN:HA	1:C:252:ILE:HG22	1.88	0.55
1:A:201:SER:HB2	1:A:202:PRO:HD2	1.88	0.54
1:C:17:VAL:O	1:C:21:LEU:HD13	2.09	0.53
1:C:41:PHE:CD2	1:C:42:PRO:HA	2.44	0.53
1:C:165:ALA:HB1	1:C:169:LEU:HD12	1.91	0.52
1:B:70:GLY:HA3	1:B:106:GLY:HA2	1.92	0.51
1:B:67:ILE:HD11	1:B:99:LEU:CD1	2.41	0.50
1:A:281:THR:CB	1:A:285:SER:HB3	2.42	0.49
1:A:281:THR:CB	1:A:285:SER:CB	2.90	0.49
1:B:241:PHE:CG	1:B:291:GLN:HG3	2.48	0.48
1:C:249:ASN:HA	1:C:252:ILE:CG2	2.43	0.48
1:C:41:PHE:CD2	1:C:41:PHE:C	2.90	0.48
1:B:227:LEU:HD21	1:C:118:ILE:HG21	1.95	0.48
1:A:26:PRO:HG3	1:A:305:LYS:HG2	1.95	0.47
1:A:301:SER:O	1:A:305:LYS:HG3	2.13	0.47
1:B:14:SER:HB2	1:B:15:PRO:HD2	1.96	0.47
1:B:289:ASN:O	1:B:292:LEU:HG	2.14	0.47
1:B:195:ALA:HB2	1:B:200:THR:O	2.15	0.47
1:C:41:PHE:CE1	1:C:86:ARG:HG2	2.48	0.47
1:B:195:ALA:O	1:B:196:PHE:HB3	2.15	0.46
1:C:243:MET:HE3	1:C:243:MET:HB2	1.84	0.46
1:C:243:MET:HG3	1:C:244:PRO:HD2	1.96	0.46
1:B:292:LEU:HD12	1:B:292:LEU:C	2.41	0.46
1:A:41:PHE:CD1	1:A:42:PRO:HA	2.50	0.46
1:A:49:ILE:CD1	1:A:81:ILE:HG21	2.46	0.45
1:A:99:LEU:HB3	1:A:100:PRO:HD3	1.99	0.45
1:A:39:MET:CB	1:A:40:PRO:HD2	2.45	0.45
1:C:55:ILE:HG23	1:C:60:ALA:HB3	1.98	0.45
1:C:58:GLN:HG2	1:C:301:SER:HB2	1.99	0.45
1:C:70:GLY:O	1:C:103:VAL:HG13	2.18	0.44
1:A:272:PHE:O	1:A:275:ALA:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:PRO:O	1:A:46:GLN:HG3	2.17	0.44
1:A:102:VAL:HG13	1:A:107:LYS:HB2	2.00	0.44
1:B:193:LEU:HD12	1:B:194:PRO:HD2	2.00	0.43
1:A:39:MET:HG2	1:A:44:ASN:HB3	2.00	0.43
1:A:41:PHE:CG	1:A:42:PRO:HA	2.54	0.42
1:C:39:MET:HE3	1:C:40:PRO:HD2	2.02	0.42
1:C:41:PHE:CD2	1:C:42:PRO:N	2.87	0.42
1:C:102:VAL:HG13	1:C:107:LYS:HB2	2.00	0.42
1:B:292:LEU:HD12	1:B:293:VAL:N	2.35	0.42
1:A:117:MET:HE1	1:A:153:LEU:HA	2.02	0.41
1:C:185:LEU:O	1:C:205:VAL:HB	2.21	0.41
1:C:248:ILE:O	1:C:252:ILE:HG22	2.21	0.41
1:A:14:SER:O	1:A:18:GLN:HG3	2.20	0.41
1:A:166:LYS:NZ	4:A:629:HOH:O	2.53	0.40
1:A:245:GLU:O	1:A:249:ASN:HB2	2.20	0.40
1:C:35:ILE:HG12	1:C:48:ALA:HB2	2.02	0.40
1:B:194:PRO:HD2	1:B:234:ALA:HB1	2.03	0.40
1:B:36:SER:O	1:B:37:HIS:CB	2.70	0.40
1:B:67:ILE:HD11	1:B:99:LEU:HD13	2.04	0.40
1:B:70:GLY:O	1:B:103:VAL:HG13	2.21	0.40
1:C:252:ILE:HD12	1:C:252:ILE:O	2.22	0.40

There are no symmetry-related clashes.

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	300/335 (90%)	292 (97%)	8 (3%)	0	100	100
1	B	300/335 (90%)	297 (99%)	2 (1%)	1 (0%)	36	30
1	C	298/335 (89%)	295 (99%)	3 (1%)	0	100	100
All	All	898/1005 (89%)	884 (98%)	13 (1%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	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	209/266 (79%)	208 (100%)	1 (0%)	81	82
1	B	214/266 (80%)	213 (100%)	1 (0%)	81	82
1	C	193/266 (73%)	189 (98%)	4 (2%)	47	37
All	All	616/798 (77%)	610 (99%)	6 (1%)	68	64

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	285	SER
1	B	43	GLN
1	C	6	ILE
1	C	32	SER
1	C	243	MET
1	C	252	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	58	GLN
1	A	155	ASN
1	A	291	GLN
1	B	155	ASN
1	C	155	ASN
1	C	308	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\# Z > 2$
2	SO4	B	400	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	C	400	-	4,4,4	0.23	0	6,6,6	0.10	0
2	SO4	A	400	-	4,4,4	0.29	0	6,6,6	0.21	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 [i](#)

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	304/335 (90%)	0.58	52 (17%) 4 4	12, 23, 78, 110	0
1	B	304/335 (90%)	0.94	52 (17%) 4 4	15, 32, 58, 80	0
1	C	302/335 (90%)	1.43	88 (29%) 1 1	17, 40, 67, 90	0
All	All	910/1005 (90%)	0.98	192 (21%) 2 2	12, 32, 69, 110	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	255	ALA	7.9
1	C	41	PHE	6.7
1	A	256	VAL	6.4
1	A	261	ALA	6.3
1	C	197	PHE	6.2
1	B	41	PHE	6.1
1	A	265	ILE	6.0
1	A	247	THR	5.4
1	B	35	ILE	5.3
1	B	42	PRO	5.3
1	A	274	LEU	5.2
1	C	252	ILE	5.2
1	A	264	VAL	5.1
1	A	282	GLY	5.0
1	B	37	HIS	4.9
1	B	45	ALA	4.9
1	B	86	ARG	4.9
1	A	273	LEU	4.8
1	C	42	PRO	4.8
1	C	280	LEU	4.8
1	B	47	THR	4.8
1	A	277	VAL	4.7
1	A	34	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
1	C	274	LEU	4.7
1	B	48	ALA	4.5
1	B	311	ALA	4.4
1	B	49	ILE	4.3
1	A	281	THR	4.2
1	B	15	PRO	4.2
1	B	85	GLY	4.2
1	C	259	ALA	4.2
1	B	43	GLN	4.2
1	A	280	LEU	4.2
1	B	247	THR	4.1
1	B	34	ILE	4.1
1	C	272	PHE	4.0
1	C	286	LEU	4.0
1	A	275	ALA	4.0
1	C	34	ILE	4.0
1	A	244	PRO	4.0
1	A	267	LYS	4.0
1	A	271	PRO	4.0
1	C	258	GLU	4.0
1	A	252	ILE	4.0
1	C	49	ILE	3.9
1	A	270	THR	3.9
1	B	44	ASN	3.8
1	C	81	ILE	3.8
1	A	38	GLY	3.8
1	B	88	GLY	3.8
1	A	254	GLN	3.8
1	C	6	ILE	3.8
1	A	278	ALA	3.7
1	B	81	ILE	3.7
1	A	259	ALA	3.7
1	C	281	THR	3.7
1	A	272	PHE	3.7
1	A	167	SER	3.6
1	B	78	LYS	3.6
1	A	268	GLU	3.6
1	A	262	GLN	3.6
1	A	257	ALA	3.5
1	A	248	ILE	3.5
1	A	250	ALA	3.5
1	A	279	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	275	ALA	3.5
1	B	89	HIS	3.5
1	C	255	ALA	3.4
1	A	269	SER	3.4
1	C	198	CYS	3.4
1	C	257	ALA	3.4
1	B	46	GLN	3.3
1	C	261	ALA	3.3
1	A	263	GLY	3.3
1	A	285	SER	3.3
1	A	246	HIS	3.3
1	C	294	PHE	3.3
1	A	266	GLY	3.3
1	C	248	ILE	3.2
1	C	256	VAL	3.2
1	C	271	PRO	3.2
1	C	196	PHE	3.2
1	B	23	ASN	3.2
1	C	269	SER	3.2
1	C	37	HIS	3.2
1	B	195	ALA	3.2
1	C	311	ALA	3.2
1	B	83	LEU	3.2
1	C	83	LEU	3.2
1	C	276	ARG	3.1
1	C	59	GLY	3.1
1	A	245	GLU	3.1
1	A	258	GLU	3.1
1	B	310	LEU	3.1
1	A	35	ILE	3.0
1	C	270	THR	3.0
1	C	266	GLY	3.0
1	A	251	ALA	3.0
1	B	242	ALA	3.0
1	B	36	SER	3.0
1	C	273	LEU	2.9
1	A	253	ASP	2.9
1	C	278	ALA	2.9
1	A	37	HIS	2.9
1	A	260	GLU	2.9
1	B	77	SER	2.8
1	B	50	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	79	GLU	2.8
1	C	277	VAL	2.8
1	A	39	MET	2.8
1	C	195	ALA	2.8
1	B	245	GLU	2.8
1	C	15	PRO	2.8
1	C	38	GLY	2.7
1	B	19	ASP	2.7
1	B	79	GLU	2.7
1	C	54	THR	2.7
1	C	290	ILE	2.7
1	C	91	VAL	2.7
1	B	84	LEU	2.6
1	C	75	GLY	2.6
1	C	243	MET	2.6
1	C	90	ASN	2.6
1	C	8	PRO	2.6
1	B	6	ILE	2.6
1	A	88	GLY	2.6
1	B	204	ASP	2.6
1	C	35	ILE	2.6
1	C	67	ILE	2.5
1	B	14	SER	2.5
1	C	71	VAL	2.5
1	C	60	ALA	2.5
1	C	86	ARG	2.4
1	B	246	HIS	2.4
1	A	6	ILE	2.4
1	C	242	ALA	2.4
1	C	268	GLU	2.4
1	B	240	GLN	2.4
1	C	76	LEU	2.4
1	C	18	GLN	2.4
1	C	40	PRO	2.4
1	C	84	LEU	2.3
1	B	239	GLU	2.3
1	C	164	GLY	2.3
1	B	76	LEU	2.3
1	C	24	LYS	2.3
1	C	287	LYS	2.3
1	B	259	ALA	2.3
1	C	85	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	36	SER	2.3
1	C	19	ASP	2.3
1	C	51	VAL	2.3
1	B	33	THR	2.3
1	C	61	VAL	2.2
1	B	90	ASN	2.2
1	C	17	VAL	2.2
1	A	92	THR	2.2
1	C	68	ILE	2.2
1	C	237	ILE	2.2
1	B	24	LYS	2.2
1	C	16	GLU	2.2
1	B	280	LEU	2.2
1	B	286	LEU	2.2
1	C	282	GLY	2.2
1	C	62	PRO	2.2
1	C	23	ASN	2.1
1	C	210	ASP	2.1
1	C	36	SER	2.1
1	C	44	ASN	2.1
1	C	110	ALA	2.1
1	C	251	ALA	2.1
1	C	28	VAL	2.1
1	C	69	GLY	2.1
1	C	107	LYS	2.1
1	A	89	HIS	2.1
1	A	286	LEU	2.1
1	C	292	LEU	2.1
1	B	294	PHE	2.1
1	C	56	ARG	2.1
1	C	26	PRO	2.1
1	C	244	PRO	2.1
1	B	257	ALA	2.1
1	A	19	ASP	2.1
1	A	168	ILE	2.0
1	B	16	GLU	2.0
1	B	272	PHE	2.0
1	B	285	SER	2.0
1	C	112	THR	2.0
1	C	30	LEU	2.0
1	C	250	ALA	2.0
1	C	279	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	243	MET	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(Å ²)	Q<0.9
2	SO4	C	400	5/5	0.82	0.11	90,91,92,93	0
2	SO4	A	400	5/5	0.91	0.11	47,51,57,59	0
2	SO4	B	400	5/5	0.96	0.10	36,36,43,49	0
3	MN	C	401	1/1	0.98	0.09	48,48,48,48	0
3	MN	A	401	1/1	0.99	0.05	33,33,33,33	0
3	MN	B	401	1/1	1.00	0.01	22,22,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.