



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:15 AM UTC

PDB ID : 1ESJ / pdb_00001esj
Title : CRYSTAL STRUCTURE OF THIAZOLE KINASE MUTANT (C198S)
Authors : Campobasso, N.; Mathews, I.I.; Begley, T.P.; Ealick, S.E.
Deposited on : 2000-04-10
Resolution : 1.80 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

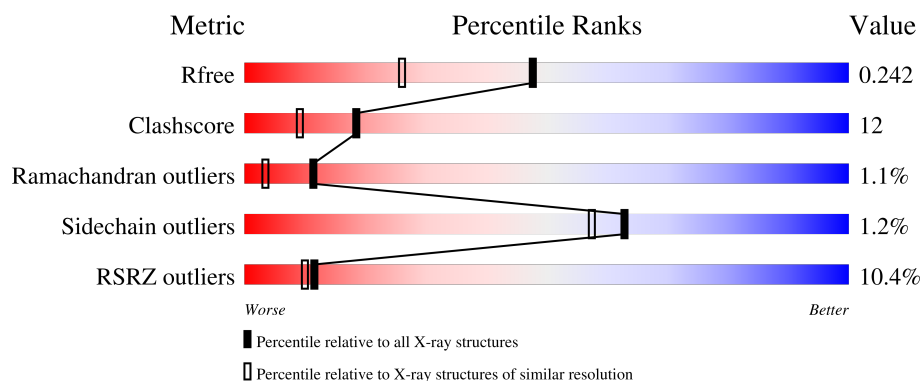
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	284	11% 77% 22% .
1	B	284	12% 80% 18% .
1	C	284	8% 77% 22% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6592 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 HYDROXYETHYLTHIAZOLE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	45	0	0
			2080	1297	374	402	7			
1	B	284	Total	C	N	O	S	62	0	0
			2080	1297	374	402	7			
1	C	284	Total	C	N	O	S	38	0	0
			2080	1297	374	402	7			

There are 39 discrepancies between the modelled and reference sequences:

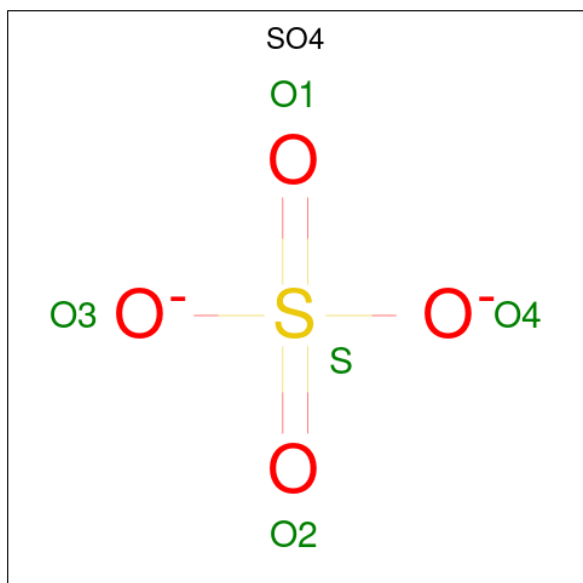
Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P39593
A	-10	ARG	-	expression tag	UNP P39593
A	-9	GLY	-	expression tag	UNP P39593
A	-8	SER	-	expression tag	UNP P39593
A	-7	HIS	-	expression tag	UNP P39593
A	-6	HIS	-	expression tag	UNP P39593
A	-5	HIS	-	expression tag	UNP P39593
A	-4	HIS	-	expression tag	UNP P39593
A	-3	HIS	-	expression tag	UNP P39593
A	-2	HIS	-	expression tag	UNP P39593
A	-1	GLY	-	expression tag	UNP P39593
A	0	SER	-	expression tag	UNP P39593
A	198	SER	CYS	engineered mutation	UNP P39593
B	-11	MET	-	expression tag	UNP P39593
B	-10	ARG	-	expression tag	UNP P39593
B	-9	GLY	-	expression tag	UNP P39593
B	-8	SER	-	expression tag	UNP P39593
B	-7	HIS	-	expression tag	UNP P39593
B	-6	HIS	-	expression tag	UNP P39593
B	-5	HIS	-	expression tag	UNP P39593
B	-4	HIS	-	expression tag	UNP P39593
B	-3	HIS	-	expression tag	UNP P39593
B	-2	HIS	-	expression tag	UNP P39593

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP P39593
B	0	SER	-	expression tag	UNP P39593
B	198	SER	CYS	engineered mutation	UNP P39593
C	-11	MET	-	expression tag	UNP P39593
C	-10	ARG	-	expression tag	UNP P39593
C	-9	GLY	-	expression tag	UNP P39593
C	-8	SER	-	expression tag	UNP P39593
C	-7	HIS	-	expression tag	UNP P39593
C	-6	HIS	-	expression tag	UNP P39593
C	-5	HIS	-	expression tag	UNP P39593
C	-4	HIS	-	expression tag	UNP P39593
C	-3	HIS	-	expression tag	UNP P39593
C	-2	HIS	-	expression tag	UNP P39593
C	-1	GLY	-	expression tag	UNP P39593
C	0	SER	-	expression tag	UNP P39593
C	198	SER	CYS	engineered mutation	UNP P39593

- 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	C	1	Total	O	S	0	0
			5	4	1		

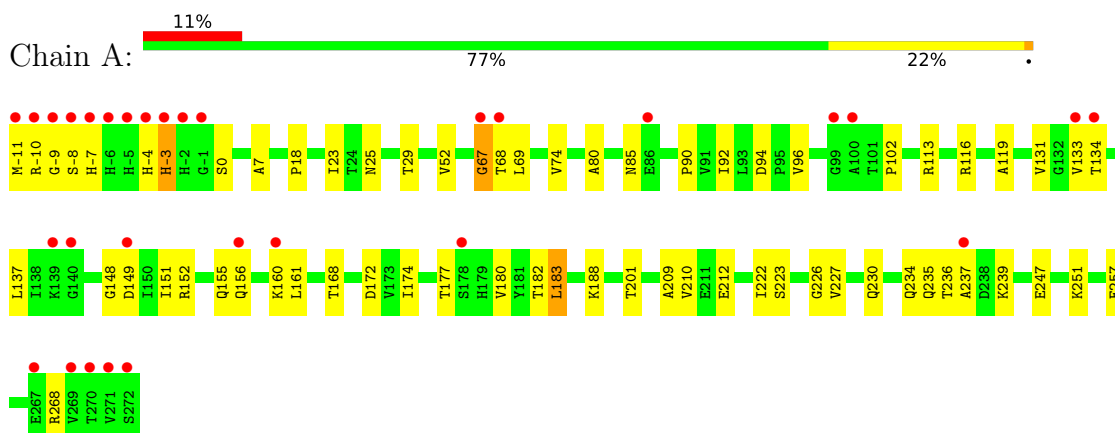
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total 99	O 99	0	0
3	B	100	Total 100	O 100	0	0
3	C	143	Total 143	O 143	0	0

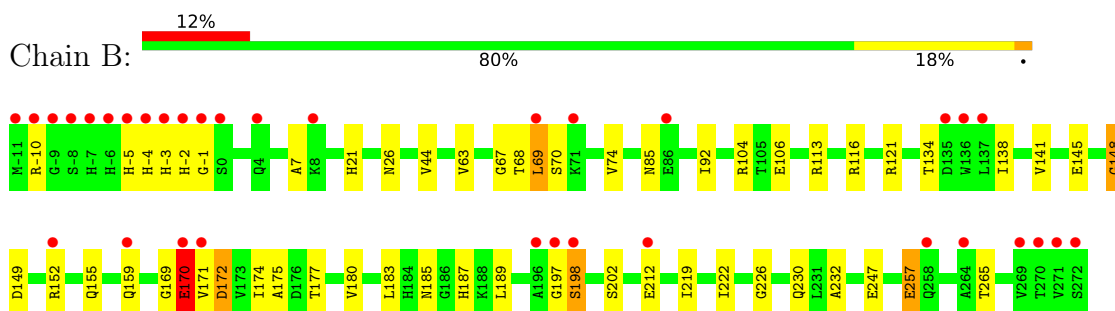
3 Residue-property plots [i](#)

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.

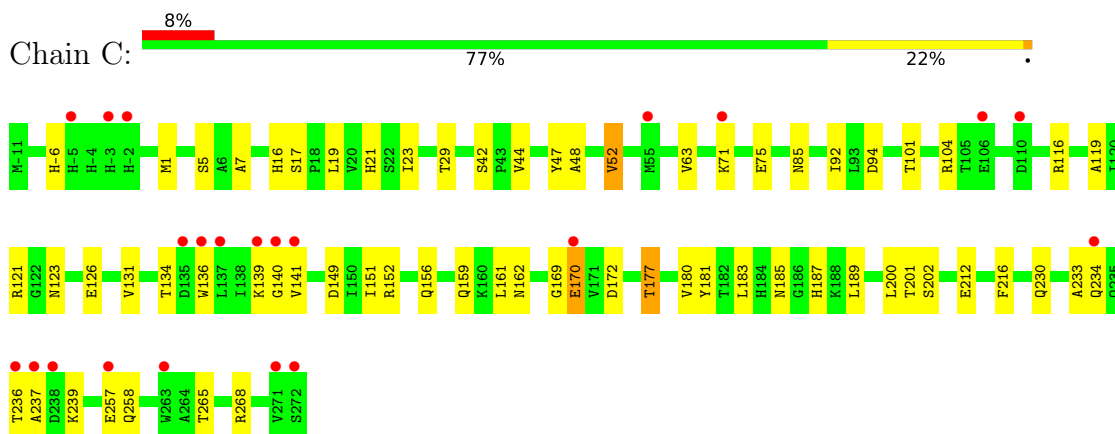
• Molecule 1: HYDROXYETHYLTHIAZOLE KINASE



• Molecule 1: HYDROXYETHYLTHIAZOLE KINASE



• Molecule 1: HYDROXYETHYLTHIAZOLE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.06Å 100.89Å 73.07Å 90.00° 96.02° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 20.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.8 (20.00-1.80) 98.9 (20.00-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.253 0.242 , 0.242	Depositor DCC
R_{free} test set	4175 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	19.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6592	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: 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	0.37	0/2111	0.85	3/2870 (0.1%)
1	B	0.38	0/2111	0.87	1/2870 (0.0%)
1	C	0.39	0/2111	0.88	5/2870 (0.2%)
All	All	0.38	0/6333	0.87	9/8610 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	-3	HIS	N-CA-C	-7.70	102.99	112.38
1	A	149	ASP	N-CA-C	-6.85	103.88	111.82
1	C	170	GLU	N-CA-C	-5.87	104.07	111.11
1	A	23	ILE	N-CA-C	-5.74	98.87	107.37
1	C	52	VAL	N-CA-C	5.51	116.24	110.62
1	C	23	ILE	N-CA-C	-5.43	98.05	109.34
1	C	212	GLU	N-CA-C	5.28	117.03	111.28
1	A	148	GLY	N-CA-C	-5.19	106.21	112.49
1	C	177	THR	N-CA-C	5.13	117.61	111.71

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	2080	0	2100	50	0
1	B	2080	0	2100	47	0
1	C	2080	0	2100	52	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0
3	A	99	0	0	3	0
3	B	100	0	0	3	0
3	C	143	0	0	0	0
All	All	6592	0	6300	147	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 12.

All (147) 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:7:ALA:HB1	1:C:257:GLU:HG3	1.30	1.12
1:B:185:ASN:HD21	1:B:265:THR:H	1.10	0.99
1:B:85:ASN:HD21	1:B:116:ARG:H	1.14	0.92
1:B:7:ALA:HB1	1:B:257:GLU:HG2	1.57	0.86
1:C:185:ASN:HD21	1:C:265:THR:H	1.22	0.85
1:C:159:GLN:HG2	1:C:177:THR:HG23	1.57	0.85
1:C:85:ASN:HD21	1:C:116:ARG:H	1.23	0.84
1:C:-6:HIS:HB3	1:C:1:MET:HE1	1.62	0.81
1:B:187:HIS:HD2	1:B:189:LEU:H	1.27	0.80
1:C:1:MET:HE3	1:C:216:PHE:CG	2.16	0.80
1:C:1:MET:HE3	1:C:216:PHE:CD2	2.17	0.80
3:A:670:HOH:O	1:C:71:LYS:HE2	1.83	0.78
1:A:133:VAL:HG23	1:A:134:THR:HG23	1.64	0.78
1:C:71:LYS:O	1:C:75:GLU:HG3	1.87	0.74
1:B:85:ASN:ND2	1:B:116:ARG:H	1.89	0.71
1:C:121:ARG:NH2	1:C:200:LEU:HD23	2.06	0.71
1:B:159:GLN:HG2	1:B:177:THR:HG23	1.72	0.71
1:B:69:LEU:HD22	1:B:104:ARG:NE	2.06	0.71
1:A:183:LEU:HD22	1:A:183:LEU:N	2.06	0.70
1:B:170:GLU:H	1:B:170:GLU:CD	2.00	0.69
1:A:92:ILE:HD12	1:A:119:ALA:HB3	1.77	0.67
1:A:85:ASN:HD21	1:A:116:ARG:H	1.41	0.65
1:C:21:HIS:HA	1:C:44:VAL:HG23	1.77	0.65
1:C:187:HIS:HD2	1:C:189:LEU:H	1.45	0.64
1:A:-8:SER:HB2	1:A:212:GLU:CD	2.23	0.64
1:B:174:ILE:HD11	1:B:222:ILE:HD12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ILE:HD11	1:A:222:ILE:HD12	1.80	0.62
1:B:69:LEU:HD22	1:B:104:ARG:HE	1.62	0.62
1:B:185:ASN:ND2	1:B:265:THR:H	1.92	0.62
1:B:187:HIS:CD2	1:B:189:LEU:H	2.15	0.61
1:C:131:VAL:HG12	1:C:161:LEU:HD11	1.82	0.61
1:A:96:VAL:HG22	3:A:502:HOH:O	2.00	0.61
1:C:-6:HIS:CB	1:C:1:MET:HE1	2.29	0.61
1:C:121:ARG:HH21	1:C:200:LEU:HD23	1.67	0.60
1:A:25:ASN:O	1:A:29:THR:HG23	2.02	0.59
1:B:198:SER:HB3	3:B:454:HOH:O	2.03	0.59
1:C:187:HIS:CD2	1:C:189:LEU:H	2.21	0.58
1:C:85:ASN:ND2	1:C:116:ARG:H	1.99	0.58
1:C:7:ALA:CB	1:C:257:GLU:HG3	2.19	0.58
1:A:226:GLY:O	1:A:230:GLN:HG3	2.05	0.57
1:C:92:ILE:HD12	1:C:119:ALA:HB3	1.86	0.56
1:B:-4:HIS:C	1:B:-2:HIS:N	2.62	0.56
1:A:69:LEU:CD2	1:A:69:LEU:H	2.19	0.56
1:B:148:GLY:O	1:B:152:ARG:HG3	2.05	0.56
1:A:-10:ARG:HD2	1:A:90:PRO:HD3	1.88	0.56
1:A:247:GLU:O	1:A:251:LYS:HG2	2.06	0.55
1:C:230:GLN:O	1:C:234:GLN:HG2	2.06	0.54
1:B:85:ASN:HD21	1:B:116:ARG:N	1.93	0.54
1:A:52:VAL:HB	1:A:80:ALA:HB2	1.89	0.53
1:B:121:ARG:HH12	1:B:197:GLY:CA	2.21	0.53
1:A:160:LYS:O	1:A:160:LYS:HD3	2.09	0.53
1:B:185:ASN:HD21	1:B:265:THR:N	1.94	0.53
1:A:223:SER:O	1:A:227:VAL:HG23	2.08	0.53
1:B:67:GLY:O	1:B:68:THR:C	2.51	0.52
1:B:171:VAL:O	1:B:183:LEU:O	2.27	0.52
1:B:26:ASN:HD21	1:C:29:THR:HG21	1.75	0.52
1:A:174:ILE:CD1	1:A:222:ILE:HD12	2.39	0.52
1:A:183:LEU:HB3	3:A:517:HOH:O	2.09	0.52
1:C:134:THR:HG21	1:C:136:TRP:NE1	2.25	0.52
1:A:-11:MET:HG3	1:A:209:ALA:O	2.10	0.52
1:A:151:ILE:HG23	1:A:180:VAL:HG11	1.91	0.52
1:B:21:HIS:HA	1:B:44:VAL:CG1	2.40	0.52
1:B:169:GLY:C	1:B:171:VAL:H	2.17	0.52
1:C:63:VAL:HG21	1:C:202:SER:HA	1.91	0.52
1:B:63:VAL:HG21	1:B:202:SER:HA	1.93	0.51
1:B:21:HIS:HA	1:B:44:VAL:HG13	1.92	0.51
1:B:149:ASP:HA	1:B:152:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:GLN:HB3	1:A:247:GLU:HG2	1.92	0.51
1:C:-6:HIS:HD2	1:C:5:SER:OG	1.93	0.51
1:A:69:LEU:HD12	1:A:74:VAL:CG2	2.41	0.51
1:A:151:ILE:O	1:A:155:GLN:HG3	2.11	0.50
1:C:185:ASN:ND2	1:C:265:THR:H	2.00	0.50
1:C:19:LEU:HD23	1:C:42:SER:HB2	1.93	0.50
1:B:155:GLN:O	1:B:159:GLN:HG3	2.12	0.49
1:A:69:LEU:H	1:A:69:LEU:HD23	1.78	0.49
1:C:94:ASP:HB2	1:C:201:THR:HG21	1.93	0.49
1:B:92:ILE:HD12	1:B:92:ILE:N	2.26	0.49
1:C:233:ALA:O	1:C:237:ALA:HB2	2.13	0.49
1:B:172:ASP:HB2	1:B:183:LEU:HB2	1.95	0.49
1:C:139:LYS:C	1:C:141:VAL:H	2.21	0.48
1:B:121:ARG:HH12	1:B:197:GLY:HA2	1.78	0.48
1:A:-7:HIS:HE1	1:A:210:VAL:O	1.95	0.48
1:C:101:THR:OG1	1:C:104:ARG:HG3	2.13	0.48
1:A:69:LEU:HD23	1:A:69:LEU:N	2.29	0.48
1:C:258:GLN:N	1:C:258:GLN:CD	2.72	0.48
1:A:230:GLN:O	1:A:234:GLN:HG3	2.13	0.48
1:A:94:ASP:HB2	1:A:201:THR:HG21	1.96	0.47
1:C:-6:HIS:CG	1:C:1:MET:HE1	2.49	0.47
1:B:171:VAL:O	1:B:172:ASP:O	2.32	0.47
1:B:-10:ARG:HH11	1:B:-10:ARG:HG2	1.80	0.47
1:B:174:ILE:CD1	1:B:183:LEU:HD11	2.44	0.47
1:A:183:LEU:N	1:A:183:LEU:CD2	2.77	0.47
1:C:1:MET:CE	1:C:216:PHE:CG	2.96	0.47
1:C:151:ILE:HG23	1:C:180:VAL:HG11	1.97	0.47
1:A:131:VAL:HG22	1:A:161:LEU:HD11	1.96	0.47
1:A:25:ASN:HB2	1:A:68:THR:OG1	2.15	0.46
1:B:226:GLY:O	1:B:230:GLN:HG3	2.14	0.46
1:A:-4:HIS:O	1:A:-3:HIS:HB2	2.15	0.46
1:A:-9:GLY:O	1:A:212:GLU:N	2.41	0.46
1:B:-4:HIS:C	1:B:-2:HIS:H	2.23	0.46
1:A:182:THR:C	1:A:183:LEU:HD22	2.40	0.46
1:B:68:THR:HB	1:C:47:TYR:CE2	2.51	0.46
1:B:69:LEU:CD2	1:B:104:ARG:HE	2.27	0.46
1:C:185:ASN:HD21	1:C:265:THR:N	2.03	0.46
1:A:152:ARG:O	1:A:156:GLN:HG3	2.16	0.45
1:C:236:THR:HG22	1:C:239:LYS:HD2	1.98	0.45
1:A:85:ASN:ND2	1:A:116:ARG:H	2.10	0.45
1:A:113:ARG:HH11	1:A:113:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ALA:O	1:C:52:VAL:HG13	2.17	0.45
1:A:0:SER:HB3	1:A:268:ARG:HH11	1.82	0.45
1:B:175:ALA:CB	1:B:180:VAL:HG22	2.47	0.44
1:C:16:HIS:O	1:C:17:SER:C	2.61	0.44
1:C:181:TYR:CZ	1:C:268:ARG:HD3	2.53	0.44
1:C:169:GLY:O	1:C:170:GLU:C	2.61	0.44
1:C:139:LYS:O	1:C:141:VAL:N	2.47	0.44
1:A:-10:ARG:CB	1:A:-10:ARG:NH1	2.81	0.43
1:A:-10:ARG:HH11	1:A:-10:ARG:HB2	1.83	0.43
1:A:25:ASN:ND2	1:A:67:GLY:HA3	2.32	0.43
1:A:168:THR:HA	1:A:172:ASP:OD1	2.19	0.43
1:B:70:SER:O	1:B:74:VAL:HG23	2.18	0.43
1:C:152:ARG:HH11	1:C:152:ARG:HG3	1.83	0.43
1:B:-5:HIS:O	1:B:-2:HIS:HB2	2.19	0.43
1:B:121:ARG:NH1	1:B:197:GLY:O	2.52	0.43
1:A:236:THR:O	1:A:237:ALA:HB3	2.19	0.42
1:A:102:PRO:HG2	3:B:455:HOH:O	2.19	0.42
1:B:-2:HIS:N	1:B:-2:HIS:CD2	2.86	0.42
1:C:172:ASP:HB2	1:C:183:LEU:HB2	2.00	0.42
1:B:-10:ARG:NH2	1:B:212:GLU:HA	2.34	0.42
1:A:-11:MET:SD	1:A:18:PRO:HB3	2.60	0.42
1:B:134:THR:HG22	3:B:662:HOH:O	2.20	0.41
1:A:94:ASP:OD1	1:A:96:VAL:CG2	2.68	0.41
1:C:258:GLN:CD	1:C:258:GLN:H	2.27	0.41
1:A:177:THR:O	1:A:177:THR:HG22	2.19	0.41
1:C:152:ARG:HG3	1:C:152:ARG:NH1	2.35	0.41
1:A:7:ALA:HB1	1:A:257:GLU:HG2	2.00	0.41
1:A:236:THR:O	1:A:239:LYS:HG3	2.20	0.41
1:C:19:LEU:HD23	1:C:42:SER:CB	2.51	0.41
1:A:25:ASN:CB	1:A:68:THR:OG1	2.69	0.41
1:B:106:GLU:OE2	1:B:113:ARG:NH2	2.53	0.41
1:B:232:ALA:HB1	1:B:247:GLU:HB3	2.03	0.41
1:C:152:ARG:O	1:C:156:GLN:HG3	2.21	0.41
1:B:174:ILE:HD12	1:B:219:ILE:HG12	2.03	0.40
1:C:161:LEU:O	1:C:162:ASN:C	2.64	0.40
1:A:94:ASP:OD1	1:A:96:VAL:HG23	2.20	0.40
1:C:123:ASN:OD1	1:C:126:GLU:HG3	2.20	0.40
1:C:149:ASP:OD1	1:C:149:ASP:N	2.55	0.40
1:C:-6:HIS:CD2	1:C:5:SER:OG	2.74	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	282/284 (99%)	267 (95%)	13 (5%)	2 (1%)	18	8
1	B	282/284 (99%)	261 (93%)	15 (5%)	6 (2%)	5	1
1	C	282/284 (99%)	266 (94%)	15 (5%)	1 (0%)	30	19
All	All	846/852 (99%)	794 (94%)	43 (5%)	9 (1%)	11	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	-3	HIS
1	B	172	ASP
1	B	-1	GLY
1	B	138	ILE
1	B	170	GLU
1	B	148	GLY
1	A	67	GLY
1	B	141	VAL
1	C	140	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/216 (100%)	213 (99%)	3 (1%)	59	52
1	B	216/216 (100%)	211 (98%)	5 (2%)	44	33
1	C	216/216 (100%)	216 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	648/648 (100%)	640 (99%)	8 (1%)	63	57

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LEU
1	A	183	LEU
1	A	188	LYS
1	B	69	LEU
1	B	145	GLU
1	B	170	GLU
1	B	198	SER
1	B	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	234	GLN
1	A	235	GLN
1	A	261	GLN
1	B	-6	HIS
1	B	26	ASN
1	B	85	ASN
1	B	156	GLN
1	B	159	GLN
1	B	185	ASN
1	B	187	HIS
1	B	234	GLN
1	B	261	GLN
1	C	-6	HIS
1	C	85	ASN
1	C	159	GLN
1	C	185	ASN
1	C	187	HIS
1	C	234	GLN
1	C	235	GLN
1	C	261	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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	A	315	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	C	325	-	4,4,4	0.37	0	6,6,6	0.11	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	276/284 (97%)	0.82	30 (10%) 10 9	10, 19, 40, 57	0
1	B	274/284 (96%)	0.67	34 (12%) 8 6	9, 18, 37, 54	0
1	C	277/284 (97%)	0.35	22 (7%) 18 16	8, 15, 29, 43	0
All	All	827/852 (97%)	0.61	86 (10%) 11 10	8, 17, 35, 57	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	GLY	11.1
1	A	-9	GLY	7.9
1	A	-11	MET	7.7
1	A	-7	HIS	6.9
1	C	272	SER	6.8
1	A	-8	SER	6.8
1	A	-2	HIS	6.5
1	B	-2	HIS	6.2
1	B	271	VAL	6.2
1	B	137	LEU	5.9
1	B	171	VAL	5.9
1	A	272	SER	5.7
1	C	236	THR	5.6
1	B	-11	MET	5.4
1	C	237	ALA	5.4
1	A	-10	ARG	5.1
1	A	-3	HIS	4.9
1	A	-5	HIS	4.8
1	A	-1	GLY	4.8
1	C	141	VAL	4.4
1	B	-3	HIS	4.4
1	C	238	ASP	4.4
1	A	67	GLY	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	-4	HIS	4.1
1	B	-10	ARG	4.1
1	A	270	THR	3.9
1	C	135	ASP	3.9
1	B	-9	GLY	3.9
1	B	-1	GLY	3.8
1	C	271	VAL	3.8
1	B	272	SER	3.7
1	C	-3	HIS	3.7
1	A	68	THR	3.7
1	A	-6	HIS	3.6
1	B	-5	HIS	3.6
1	B	170	GLU	3.5
1	B	86	GLU	3.2
1	A	178	SER	3.2
1	C	140	GLY	3.1
1	C	139	LYS	3.1
1	B	69	LEU	3.0
1	A	271	VAL	3.0
1	B	198	SER	2.9
1	B	0	SER	2.9
1	B	197	GLY	2.9
1	A	237	ALA	2.9
1	A	149	ASP	2.9
1	C	136	TRP	2.8
1	C	263	TRP	2.8
1	A	133	VAL	2.8
1	B	-8	SER	2.7
1	B	71	LYS	2.7
1	C	-5	HIS	2.7
1	A	269	VAL	2.7
1	A	99	GLY	2.6
1	C	-2	HIS	2.6
1	A	139	LYS	2.6
1	B	196	ALA	2.6
1	B	-6	HIS	2.5
1	B	269	VAL	2.5
1	C	234	GLN	2.5
1	B	212	GLU	2.5
1	B	8	LYS	2.4
1	B	152	ARG	2.4
1	B	135	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	100	ALA	2.3
1	B	270	THR	2.3
1	A	134	THR	2.3
1	C	170	GLU	2.3
1	C	137	LEU	2.3
1	B	264	ALA	2.2
1	C	257	GLU	2.2
1	B	-4	HIS	2.2
1	A	160	LYS	2.2
1	C	71	LYS	2.2
1	C	106	GLU	2.2
1	C	110	ASP	2.2
1	A	86	GLU	2.2
1	A	267	GLU	2.1
1	B	136	TRP	2.1
1	B	-7	HIS	2.1
1	C	55	MET	2.1
1	B	159	GLN	2.1
1	A	156	GLN	2.1
1	B	258	GLN	2.0
1	B	4	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 oligosaccharides 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. 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
2	SO4	C	325	5/5	0.94	0.10	27,27,28,28	0
2	SO4	A	315	5/5	0.95	0.08	30,30,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.