



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:39 AM UTC

PDB ID : 3OKG / pdb_00003okg
Title : Crystal structure of HsdS subunit from Thermoanaerobacter tengcongensis
Authors : Liang, D.; Gao, P.; Tang, Q.; An, X.; Yan, X.
Deposited on : 2010-08-24
Resolution : 1.95 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

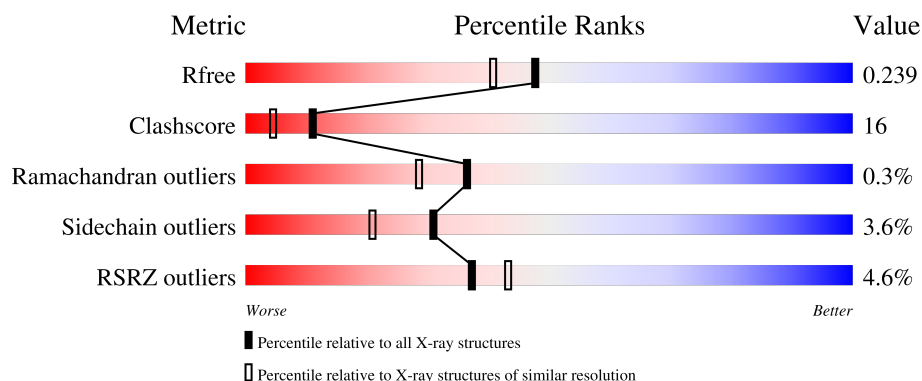
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	412	3% 72% 19% • 5%
1	B	412	5% 72% 21% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7061 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 Restriction endonuclease S subunits.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	1	0	0
			3096	1973	550	560	13			
1	B	391	Total	C	N	O	S	1	0	0
			3104	1978	551	561	14			

There are 28 discrepancies between the modelled and reference sequences:

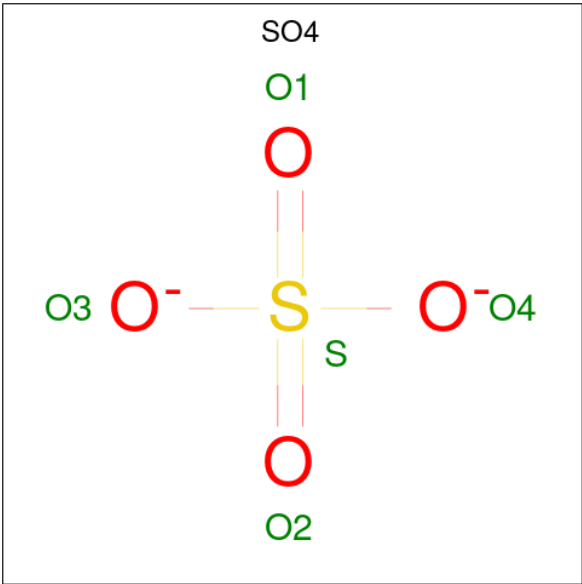
Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	expression tag	UNP Q8R9Q6
A	-12	SER	-	expression tag	UNP Q8R9Q6
A	-11	HIS	-	expression tag	UNP Q8R9Q6
A	-10	HIS	-	expression tag	UNP Q8R9Q6
A	-9	HIS	-	expression tag	UNP Q8R9Q6
A	-8	HIS	-	expression tag	UNP Q8R9Q6
A	-7	HIS	-	expression tag	UNP Q8R9Q6
A	-6	HIS	-	expression tag	UNP Q8R9Q6
A	-5	SER	-	expression tag	UNP Q8R9Q6
A	-4	MET	-	expression tag	UNP Q8R9Q6
A	-3	ASP	-	expression tag	UNP Q8R9Q6
A	-2	ILE	-	expression tag	UNP Q8R9Q6
A	-1	GLU	-	expression tag	UNP Q8R9Q6
A	0	PHE	-	expression tag	UNP Q8R9Q6
B	-13	MET	-	expression tag	UNP Q8R9Q6
B	-12	SER	-	expression tag	UNP Q8R9Q6
B	-11	HIS	-	expression tag	UNP Q8R9Q6
B	-10	HIS	-	expression tag	UNP Q8R9Q6
B	-9	HIS	-	expression tag	UNP Q8R9Q6
B	-8	HIS	-	expression tag	UNP Q8R9Q6
B	-7	HIS	-	expression tag	UNP Q8R9Q6
B	-6	HIS	-	expression tag	UNP Q8R9Q6
B	-5	SER	-	expression tag	UNP Q8R9Q6
B	-4	MET	-	expression tag	UNP Q8R9Q6
B	-3	ASP	-	expression tag	UNP Q8R9Q6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	ILE	-	expression tag	UNP Q8R9Q6
B	-1	GLU	-	expression tag	UNP Q8R9Q6
B	0	PHE	-	expression tag	UNP Q8R9Q6

- 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		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	A	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		
2	B	1	Total	O	S	0	0
			5	4	1		
			Total	O	S		
			5	4	1		
			Total	O	S		

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

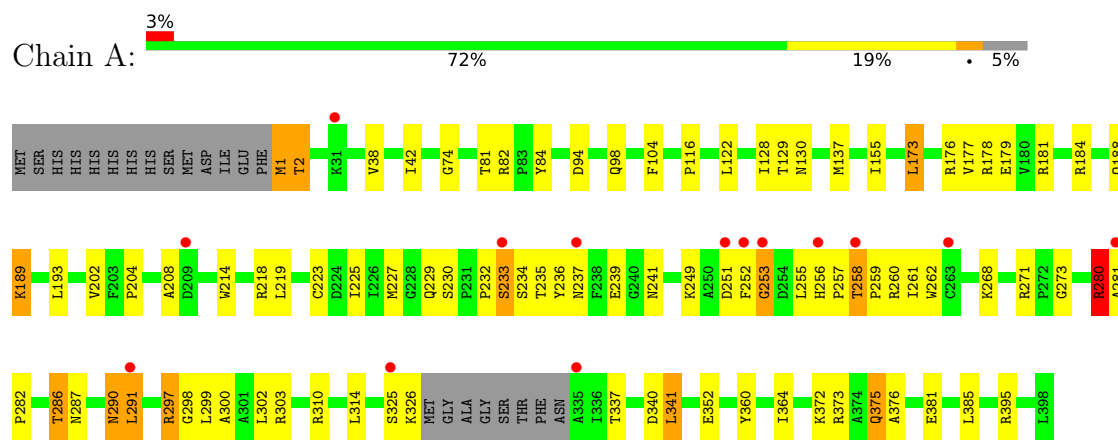
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	397	Total	O	0	0
			397	397		
3	B	389	Total	O	0	0
			389	389		

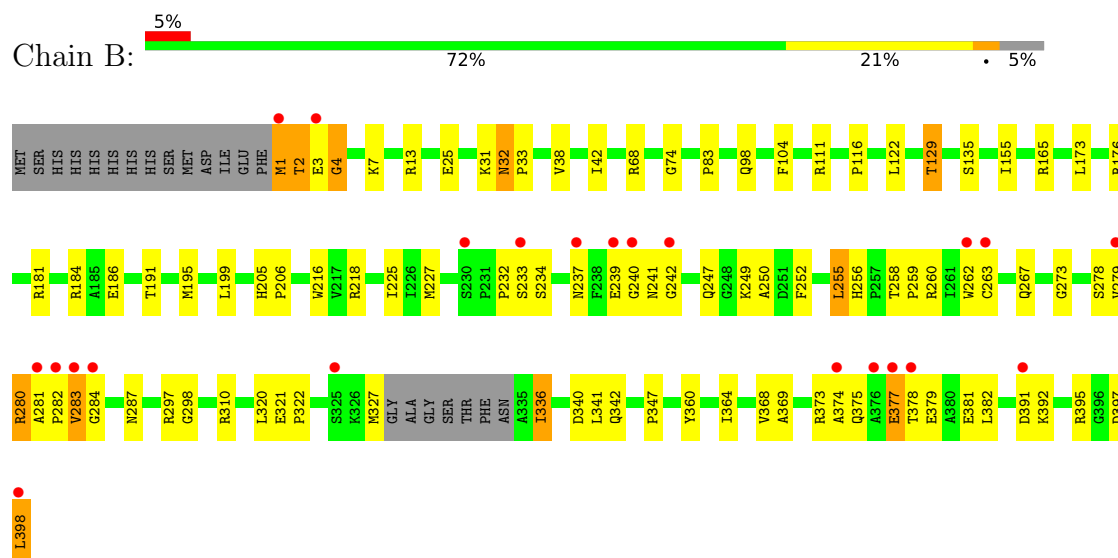
3 Residue-property plots

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: Restriction endonuclease S subunits



• Molecule 1: Restriction endonuclease S subunits



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	60.99Å 137.80Å 142.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.95 10.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-1.95) 98.9 (10.00-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.55 (at 1.95Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.197 , 0.240 0.206 , 0.239	Depositor DCC
R_{free} test set	4373 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7061	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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 66.19 % 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 6.2913e-06. 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

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	0.61	0/3170	0.90	7/4309 (0.2%)
1	B	0.59	0/3178	0.86	6/4319 (0.1%)
All	All	0.60	0/6348	0.88	13/8628 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	280	ARG	N-CA-C	8.64	122.73	108.48
1	A	253	GLY	N-CA-C	-6.77	103.46	112.81
1	B	280	ARG	N-CA-C	6.42	119.07	108.48
1	B	2	THR	N-CA-C	-5.98	105.99	113.28
1	A	258	THR	CA-C-N	5.90	126.21	119.83
1	A	258	THR	C-N-CA	5.90	126.21	119.83
1	A	235	THR	N-CA-C	-5.83	104.87	113.61
1	B	378	THR	N-CA-C	-5.77	104.42	113.02
1	B	283	VAL	N-CA-C	5.71	121.22	109.34
1	A	129	THR	CB-CA-C	-5.48	101.64	110.74
1	B	32	ASN	CA-C-N	5.47	125.30	119.28
1	B	32	ASN	C-N-CA	5.47	125.30	119.28
1	A	214	TRP	N-CA-C	-5.02	103.78	110.55

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	3096	0	3131	110	0
1	B	3104	0	3140	109	0
2	A	35	0	0	2	0
2	B	40	0	0	1	0
3	A	397	0	0	9	0
3	B	389	0	0	15	0
All	All	7061	0	6271	205	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 16.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ALA:HB3	1:B:282:PRO:CD	1.73	1.18
1:B:281:ALA:CB	1:B:282:PRO:HD3	1.71	1.18
1:A:281:ALA:HB3	1:A:282:PRO:HD3	1.30	1.12
1:A:281:ALA:CB	1:A:282:PRO:HD3	1.81	1.10
1:A:130:ASN:HB3	3:A:567:HOH:O	1.50	1.08
1:A:280:ARG:HH11	1:A:280:ARG:CG	1.68	1.07
1:A:280:ARG:HG3	1:A:280:ARG:NH1	1.64	1.05
1:A:281:ALA:HB3	1:A:282:PRO:CD	1.87	1.04
1:B:165:ARG:HH12	1:B:398:LEU:HD11	1.22	1.02
1:B:283:VAL:HG21	1:B:336:ILE:HG22	1.39	1.01
1:B:281:ALA:HB3	1:B:282:PRO:HD3	1.30	1.00
1:B:165:ARG:HH22	1:B:398:LEU:HD21	1.21	0.98
1:A:280:ARG:HH11	1:A:280:ARG:HG3	0.83	0.97
1:B:279:VAL:HG13	1:B:336:ILE:HG23	1.46	0.94
1:B:321:GLU:HB3	1:B:322:PRO:HD3	1.49	0.93
1:B:283:VAL:CG2	1:B:336:ILE:HG22	2.01	0.89
1:B:281:ALA:HB3	1:B:282:PRO:HD2	1.57	0.84
1:B:281:ALA:HB1	1:B:282:PRO:HD3	1.58	0.83
1:B:281:ALA:CB	1:B:282:PRO:CD	2.33	0.82
1:A:234:SER:HB2	1:B:234:SER:HB2	1.59	0.82
1:A:237:ASN:HD22	1:A:239:GLU:H	1.24	0.80
1:A:81:THR:HG23	2:A:399:SO4:O3	1.82	0.80
1:A:280:ARG:NH2	1:A:297:ARG:HD3	1.97	0.79
1:B:165:ARG:HH22	1:B:398:LEU:CD2	1.95	0.79
1:B:369:ALA:O	1:B:373:ARG:HD3	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLY:HA3	1:B:263:CYS:O	1.82	0.78
1:B:280:ARG:HG3	1:B:298:GLY:HA2	1.66	0.78
1:B:283:VAL:O	1:B:283:VAL:HG22	1.83	0.77
1:A:376:ALA:HB2	1:B:374:ALA:HB2	1.66	0.77
1:A:122:LEU:HD21	1:A:155:ILE:HB	1.65	0.77
1:A:280:ARG:HG2	1:A:298:GLY:HA2	1.66	0.77
1:B:397:ASP:O	1:B:398:LEU:HB2	1.83	0.76
1:A:179:GLU:HG2	3:A:767:HOH:O	1.84	0.76
1:A:249:LYS:HD3	1:A:282:PRO:HB2	1.65	0.76
1:B:205:HIS:CD2	1:B:206:PRO:HD2	2.20	0.76
1:A:225:ILE:HD13	1:A:341:LEU:HB3	1.69	0.74
1:A:271:ARG:HG3	1:A:303:ARG:NH2	2.03	0.74
1:A:281:ALA:CB	1:A:282:PRO:CD	2.51	0.74
1:B:283:VAL:CG2	1:B:336:ILE:CG2	2.67	0.73
1:B:255:LEU:HD22	1:B:256:HIS:CE1	2.23	0.73
1:B:279:VAL:HA	1:B:283:VAL:HG23	1.70	0.73
1:A:184:ARG:HG2	1:A:375:GLN:HG2	1.71	0.72
1:A:237:ASN:HD21	1:A:241:ASN:H	1.35	0.72
1:A:188:GLN:NE2	1:A:372:LYS:HA	2.04	0.72
1:A:337:THR:HG22	1:A:340:ASP:CG	2.14	0.72
1:A:337:THR:HG23	1:A:340:ASP:H	1.55	0.70
1:B:395:ARG:HD3	3:B:614:HOH:O	1.91	0.70
1:A:234:SER:CB	1:B:234:SER:HB2	2.22	0.69
1:A:286:THR:HG21	1:A:314:LEU:HD11	1.73	0.69
1:A:273:GLY:O	1:A:310:ARG:HD2	1.93	0.69
1:B:4:GLY:N	3:B:781:HOH:O	2.24	0.68
1:B:68:ARG:NE	3:B:787:HOH:O	2.26	0.68
1:A:225:ILE:HG22	1:A:227:MET:HE3	1.74	0.68
1:B:237:ASN:ND2	1:B:241:ASN:HB3	2.09	0.68
1:A:184:ARG:HD3	1:B:381:GLU:OE1	1.95	0.66
1:B:181:ARG:HD2	1:B:382:LEU:HD21	1.77	0.66
1:B:283:VAL:HG21	1:B:336:ILE:CG2	2.23	0.65
1:B:360:TYR:CZ	1:B:364:ILE:HD11	2.31	0.65
1:B:165:ARG:NH2	1:B:398:LEU:HD21	2.04	0.65
1:B:38:VAL:H	1:B:98:GLN:NE2	1.94	0.64
1:A:42:ILE:HG12	2:A:400:SO4:O2	1.97	0.64
1:A:280:ARG:HH22	1:A:297:ARG:HH11	1.43	0.64
1:A:337:THR:CG2	1:A:340:ASP:H	2.10	0.64
1:B:3:GLU:HG3	3:B:781:HOH:O	1.98	0.64
1:A:42:ILE:HD13	1:A:104:PHE:CZ	2.33	0.63
1:B:237:ASN:ND2	1:B:239:GLU:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:GLN:HE21	1:A:372:LYS:HA	1.61	0.63
1:A:230:SER:HB3	3:A:665:HOH:O	1.99	0.62
1:B:129:THR:HG23	3:B:790:HOH:O	2.00	0.62
1:B:195:MET:HE2	3:B:601:HOH:O	1.99	0.62
1:B:377:GLU:CG	1:B:377:GLU:O	2.47	0.61
1:A:178:ARG:NH1	3:A:490:HOH:O	2.34	0.60
1:A:286:THR:CG2	1:A:314:LEU:HD11	2.31	0.60
1:B:38:VAL:H	1:B:98:GLN:HE21	1.50	0.60
1:B:68:ARG:CZ	3:B:787:HOH:O	2.50	0.59
1:B:278:SER:O	1:B:283:VAL:HA	2.03	0.59
1:B:249:LYS:CD	1:B:282:PRO:HG2	2.33	0.59
1:B:232:PRO:HD3	1:B:267:GLN:NE2	2.18	0.58
1:A:202:VAL:C	1:A:204:PRO:HD3	2.29	0.58
1:B:321:GLU:HB3	1:B:322:PRO:CD	2.28	0.58
1:B:195:MET:HE3	1:B:199:LEU:HG	1.85	0.58
1:B:184:ARG:CZ	1:B:374:ALA:HB1	2.34	0.57
1:B:165:ARG:NH1	1:B:398:LEU:HD11	2.06	0.57
1:B:184:ARG:HG2	1:B:375:GLN:HG3	1.87	0.57
1:B:31:LYS:N	1:B:31:LYS:HD2	2.19	0.57
1:A:38:VAL:H	1:A:98:GLN:NE2	2.02	0.57
1:A:239:GLU:HB2	1:A:241:ASN:ND2	2.19	0.57
1:B:3:GLU:CD	1:B:7:LYS:HB2	2.30	0.56
1:A:271:ARG:HG3	1:A:303:ARG:HH21	1.68	0.56
1:A:286:THR:HG21	1:A:314:LEU:CD1	2.35	0.56
1:A:376:ALA:HB2	1:B:374:ALA:CB	2.34	0.56
1:B:379:GLU:HB2	3:B:659:HOH:O	2.05	0.56
1:A:290:ASN:HD22	1:A:290:ASN:H	1.52	0.56
1:B:239:GLU:HA	1:B:239:GLU:OE1	2.05	0.56
1:B:249:LYS:HD3	1:B:282:PRO:HG2	1.88	0.56
1:A:176:ARG:HD3	1:B:176:ARG:HD3	1.88	0.55
1:A:249:LYS:CD	1:A:282:PRO:HB2	2.36	0.55
1:A:375:GLN:HE21	1:A:375:GLN:HA	1.71	0.55
1:A:38:VAL:H	1:A:98:GLN:HE21	1.53	0.55
1:A:281:ALA:HB1	1:A:282:PRO:HD3	1.81	0.55
1:B:327:MET:HE1	1:B:336:ILE:HD12	1.88	0.55
1:B:336:ILE:HD11	1:B:341:LEU:HG	1.87	0.55
1:A:360:TYR:CZ	1:A:364:ILE:HD11	2.42	0.55
1:A:253:GLY:H	1:A:287:ASN:HD21	1.56	0.54
1:A:251:ASP:OD1	1:B:260:ARG:HG2	2.07	0.54
1:A:290:ASN:H	1:A:290:ASN:ND2	2.06	0.53
1:A:237:ASN:HD22	1:A:239:GLU:N	2.02	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:PHE:CZ	1:A:299:LEU:HD22	2.43	0.53
1:B:218:ARG:NH2	3:B:478:HOH:O	2.42	0.53
1:A:280:ARG:HH22	1:A:297:ARG:NH1	2.07	0.52
1:A:290:ASN:O	1:A:291:LEU:HD13	2.09	0.52
1:A:173:LEU:CD1	1:A:176:ARG:HH11	2.23	0.52
1:A:325:SER:O	1:A:326:LYS:C	2.53	0.52
1:B:392:LYS:HE3	3:B:712:HOH:O	2.09	0.52
1:A:1:MET:HE3	1:A:2:THR:H	1.74	0.52
1:A:395:ARG:HD2	3:A:797:HOH:O	2.10	0.52
1:A:251:ASP:O	1:A:257:PRO:HB3	2.11	0.51
1:A:325:SER:O	1:A:325:SER:OG	2.24	0.51
1:B:377:GLU:O	1:B:377:GLU:HG3	2.10	0.51
1:A:260:ARG:NH2	1:B:260:ARG:HH12	2.08	0.51
1:A:281:ALA:HB3	1:A:282:PRO:HD2	1.82	0.51
1:A:303:ARG:HD3	3:A:518:HOH:O	2.10	0.51
1:A:252:PHE:CZ	1:A:299:LEU:CD2	2.95	0.50
1:A:236:TYR:HB3	1:A:261:ILE:HD11	1.93	0.50
1:B:135:SER:HB2	3:B:694:HOH:O	2.12	0.49
1:B:247:GLN:NE2	1:B:297:ARG:HG2	2.28	0.49
1:A:381:GLU:O	1:A:385:LEU:HG	2.12	0.49
1:B:336:ILE:HG13	1:B:340:ASP:HB2	1.93	0.49
1:B:42:ILE:HD13	1:B:104:PHE:CZ	2.47	0.48
1:B:273:GLY:O	1:B:310:ARG:HD3	2.13	0.48
1:B:32:ASN:ND2	3:B:487:HOH:O	2.36	0.48
1:B:391:ASP:O	1:B:395:ARG:HG3	2.13	0.48
1:A:286:THR:HG22	3:A:720:HOH:O	2.13	0.48
1:B:184:ARG:HE	1:B:375:GLN:HE21	1.60	0.48
1:A:232:PRO:C	1:A:233:SER:O	2.53	0.48
1:B:284:GLY:O	1:B:321:GLU:OE2	2.32	0.48
1:B:122:LEU:HD21	1:B:155:ILE:HB	1.94	0.47
1:A:280:ARG:CG	1:A:280:ARG:NH1	2.40	0.47
1:B:3:GLU:OE1	1:B:7:LYS:HB2	2.14	0.47
1:A:177:VAL:O	1:A:181:ARG:HG3	2.15	0.47
1:A:251:ASP:HA	1:B:260:ARG:HD3	1.96	0.47
1:B:68:ARG:NH2	3:B:787:HOH:O	2.48	0.47
1:A:290:ASN:HD22	1:A:290:ASN:N	2.12	0.47
1:B:327:MET:CE	1:B:336:ILE:HD12	2.45	0.47
1:A:237:ASN:ND2	1:A:241:ASN:H	2.08	0.46
1:A:373:ARG:O	1:B:374:ALA:HA	2.15	0.46
1:B:1:MET:HA	3:B:700:HOH:O	2.15	0.46
1:B:237:ASN:HD21	1:B:241:ASN:HB3	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLU:HG2	3:B:431:HOH:O	2.15	0.46
1:A:229:GLN:OE1	1:A:268:LYS:HE2	2.16	0.46
1:A:128:ILE:HD11	1:A:155:ILE:HG22	1.97	0.46
1:A:236:TYR:HA	1:A:262:TRP:O	2.16	0.45
1:A:173:LEU:HD13	1:A:176:ARG:HH11	1.82	0.45
1:B:83:PRO:HB2	1:B:129:THR:HG22	1.97	0.45
1:B:216:TRP:CZ3	1:B:347:PRO:HD3	2.52	0.45
1:A:1:MET:HB2	1:A:2:THR:H	1.58	0.45
1:B:321:GLU:CB	1:B:322:PRO:HD3	2.31	0.45
1:B:191:THR:HG22	1:B:368:VAL:HG23	1.98	0.45
1:A:260:ARG:NH2	1:B:260:ARG:NH1	2.65	0.44
1:B:42:ILE:HG12	2:B:400:SO4:O1	2.18	0.44
1:B:279:VAL:HG12	1:B:279:VAL:O	2.17	0.44
1:A:375:GLN:HA	1:A:375:GLN:NE2	2.31	0.44
1:A:204:PRO:HB2	1:A:208:ALA:HB3	1.99	0.44
1:B:240:GLY:HA2	1:B:262:TRP:CD1	2.53	0.43
1:B:249:LYS:O	1:B:252:PHE:HB2	2.18	0.43
1:B:249:LYS:HD2	1:B:282:PRO:HG2	2.00	0.43
1:A:225:ILE:HG22	1:A:227:MET:CE	2.47	0.43
1:B:184:ARG:HG2	1:B:375:GLN:CG	2.49	0.43
1:B:205:HIS:CG	1:B:206:PRO:HD2	2.53	0.43
1:B:225:ILE:HD12	1:B:342:GLN:HG3	2.00	0.43
1:B:232:PRO:O	1:B:233:SER:C	2.61	0.43
1:A:258:THR:HA	1:A:259:PRO:HD3	1.72	0.43
1:A:233:SER:O	1:A:234:SER:OG	2.27	0.42
1:B:74:GLY:O	1:B:116:PRO:HB3	2.20	0.42
1:B:227:MET:HE1	1:B:279:VAL:HG11	2.01	0.42
1:A:227:MET:HE1	1:A:300:ALA:HB1	2.02	0.42
1:A:252:PHE:HZ	1:A:299:LEU:HD22	1.84	0.42
1:A:260:ARG:NH1	1:B:250:ALA:O	2.53	0.42
1:A:137:MET:H	1:A:137:MET:HG3	1.61	0.42
1:A:181:ARG:NE	1:A:381:GLU:OE2	2.43	0.42
1:A:189:LYS:HB3	1:A:189:LYS:NZ	2.34	0.42
1:A:341:LEU:HD12	1:A:341:LEU:HA	1.93	0.42
1:B:31:LYS:C	1:B:33:PRO:HD3	2.45	0.41
1:B:1:MET:SD	1:B:2:THR:N	2.83	0.41
1:A:234:SER:HA	1:B:234:SER:HA	2.01	0.41
1:A:82:ARG:O	1:A:84:TYR:N	2.54	0.41
1:A:280:ARG:NH2	1:A:297:ARG:CD	2.75	0.41
1:B:258:THR:HA	1:B:259:PRO:HD3	1.86	0.41
1:A:74:GLY:O	1:A:116:PRO:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:LEU:HB2	1:A:256:HIS:CD2	2.56	0.41
1:A:1:MET:CE	1:A:2:THR:H	2.34	0.41
1:A:218:ARG:O	1:A:219:LEU:C	2.63	0.41
1:A:239:GLU:HB2	1:A:241:ASN:HD21	1.86	0.41
1:A:280:ARG:HD2	1:A:280:ARG:HA	1.55	0.41
1:A:372:LYS:HD3	3:A:668:HOH:O	2.21	0.41
1:B:111:ARG:CD	1:B:116:PRO:HD3	2.51	0.41
1:A:225:ILE:CG2	1:A:227:MET:HE3	2.45	0.41
1:B:283:VAL:CG2	1:B:283:VAL:O	2.55	0.41
1:A:223:CYS:SG	1:A:302:LEU:HB3	2.61	0.40
1:B:247:GLN:HE21	1:B:297:ARG:HG2	1.85	0.40
1:A:1:MET:HG2	3:A:691:HOH:O	2.20	0.40
1:B:206:PRO:HA	1:B:216:TRP:CH2	2.56	0.40
1:B:320:LEU:O	1:B:321:GLU:C	2.63	0.40
1:A:176:ARG:CD	1:B:176:ARG:HD3	2.50	0.40
1:A:273:GLY:O	1:A:310:ARG:CD	2.68	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	386/412 (94%)	372 (96%)	13 (3%)	1 (0%)	36	28
1	B	387/412 (94%)	365 (94%)	21 (5%)	1 (0%)	36	28
All	All	773/824 (94%)	737 (95%)	34 (4%)	2 (0%)	36	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	297	ARG
1	B	4	GLY

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	335/354 (95%)	321 (96%)	14 (4%)	26	16
1	B	336/354 (95%)	326 (97%)	10 (3%)	36	27
All	All	671/708 (95%)	647 (96%)	24 (4%)	31	21

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	THR
1	A	94	ASP
1	A	173	LEU
1	A	189	LYS
1	A	193	LEU
1	A	233	SER
1	A	280	ARG
1	A	286	THR
1	A	290	ASN
1	A	291	LEU
1	A	341	LEU
1	A	352	GLU
1	A	375	GLN
1	B	1	MET
1	B	13	ARG
1	B	25	GLU
1	B	129	THR
1	B	173	LEU
1	B	255	LEU
1	B	287	ASN
1	B	336	ILE
1	B	377	GLU
1	B	398	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	98	GLN
1	A	188	GLN
1	A	237	ASN
1	A	241	ASN
1	A	256	HIS
1	A	287	ASN
1	A	290	ASN
1	A	375	GLN
1	B	98	GLN
1	B	148	ASN
1	B	205	HIS
1	B	241	ASN
1	B	343	ASN
1	B	366	GLN
1	B	375	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](#)

15 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	400	-	4,4,4	0.28	0	6,6,6	0.27	0
2	SO4	B	405	-	4,4,4	0.30	0	6,6,6	0.15	0
2	SO4	A	403	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	405	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	B	400	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	A	402	-	4,4,4	0.27	0	6,6,6	0.25	0
2	SO4	B	403	-	4,4,4	0.27	0	6,6,6	0.06	0
2	SO4	A	404	-	4,4,4	0.23	0	6,6,6	0.09	0
2	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.37	0
2	SO4	B	402	-	4,4,4	0.21	0	6,6,6	0.21	0
2	SO4	B	404	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	B	406	-	4,4,4	0.22	0	6,6,6	0.27	0
2	SO4	A	399	-	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	B	399	-	4,4,4	0.25	0	6,6,6	0.11	0
2	SO4	A	401	-	4,4,4	0.24	0	6,6,6	0.23	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	SO4	1	0
2	B	400	SO4	1	0
2	A	399	SO4	1	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	390/412 (94%)	0.16	14 (3%) 46 53	16, 31, 62, 90	1 (0%)
1	B	391/412 (94%)	0.22	22 (5%) 30 35	17, 33, 69, 96	1 (0%)
All	All	781/824 (94%)	0.19	36 (4%) 37 43	16, 32, 65, 96	2 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	VAL	8.5
1	B	284	GLY	5.4
1	A	252	PHE	5.1
1	A	233	SER	4.8
1	B	240	GLY	4.1
1	A	335	ALA	4.0
1	B	398	LEU	3.6
1	B	377	GLU	3.5
1	B	237	ASN	3.5
1	A	253	GLY	3.5
1	A	281	ALA	3.3
1	B	3	GLU	3.2
1	B	239	GLU	3.2
1	A	251	ASP	3.1
1	A	263	CYS	3.1
1	B	282	PRO	3.0
1	B	281	ALA	3.0
1	B	374	ALA	3.0
1	B	262	TRP	2.9
1	B	325	SER	2.8
1	B	233	SER	2.7
1	B	263	CYS	2.7
1	B	376	ALA	2.6
1	B	230	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	291	LEU	2.6
1	B	1	MET	2.3
1	B	378	THR	2.3
1	B	242	GLY	2.3
1	A	325	SER	2.3
1	A	237	ASN	2.3
1	B	279	VAL	2.2
1	B	391	ASP	2.1
1	A	209	ASP	2.1
1	A	258	THR	2.1
1	A	256	HIS	2.1
1	A	31	LYS	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	A	401	5/5	0.79	0.10	59,60,93,94	0
2	SO4	A	403	5/5	0.79	0.08	73,79,80,109	0
2	SO4	B	402	5/5	0.80	0.11	63,67,97,103	0
2	SO4	A	404	5/5	0.88	0.08	46,57,83,93	0
2	SO4	A	402	5/5	0.88	0.15	43,44,69,90	0
2	SO4	B	405	5/5	0.88	0.14	53,73,93,94	0
2	SO4	B	404	5/5	0.90	0.07	67,68,85,102	0
2	SO4	A	405	5/5	0.91	0.12	41,49,64,68	0
2	SO4	B	403	5/5	0.91	0.12	46,54,78,83	0
2	SO4	B	399	5/5	0.93	0.11	47,48,62,64	0
2	SO4	B	406	5/5	0.93	0.14	49,53,63,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	401	5/5	0.95	0.10	37,41,51,57	0
2	SO4	B	400	5/5	0.96	0.08	37,37,45,56	0
2	SO4	A	399	5/5	0.97	0.10	36,37,42,62	0
2	SO4	A	400	5/5	0.98	0.06	35,37,39,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.