



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:08 PM UTC

PDB ID : 2D69 / pdb_00002d69
Title : Crystal structure of the complex of sulfate ion and octameric ribulose-1,5-bisphosphate carboxylase/oxygenase (Rubisco) from *Pyrococcus horikoshii* OT3 (form-2 crystal)
Authors : Mizohata, E.; Mishima, C.; Akasaka, R.; Uda, H.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-11-10
Resolution : 1.90 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

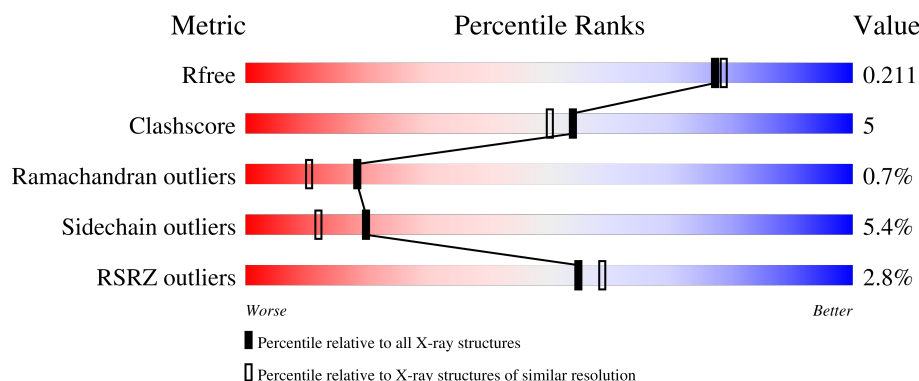
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	430	2% 84% 12% ..
1	B	430	3% 84% 12% ..
1	D	430	2% 83% 13% ..
1	E	430	4% 79% 13% 5%

2 Entry composition [i](#)

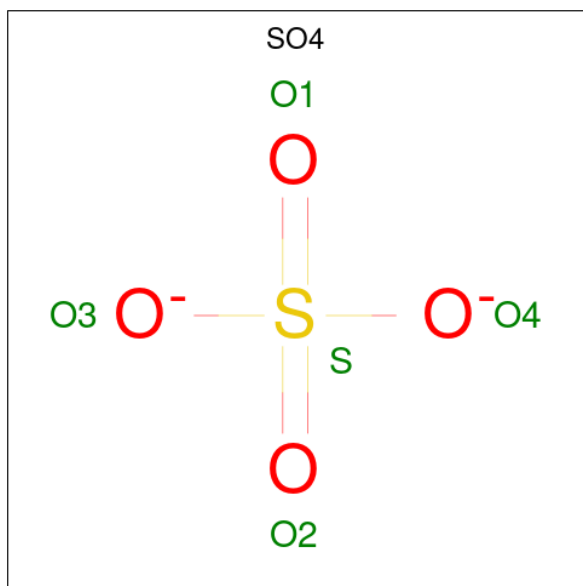
There are 3 unique types of molecules in this entry. The entry contains 14062 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3351	2150	577	606	18			
1	B	418	Total	C	N	O	S	0	0	0
			3301	2118	568	600	15			
1	D	419	Total	C	N	O	S	0	0	0
			3319	2130	571	600	18			
1	E	410	Total	C	N	O	S	0	0	0
			3246	2082	558	591	15			

- 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	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	225	Total	O	0	0
			225	225		
3	B	181	Total	O	0	0
			181	181		

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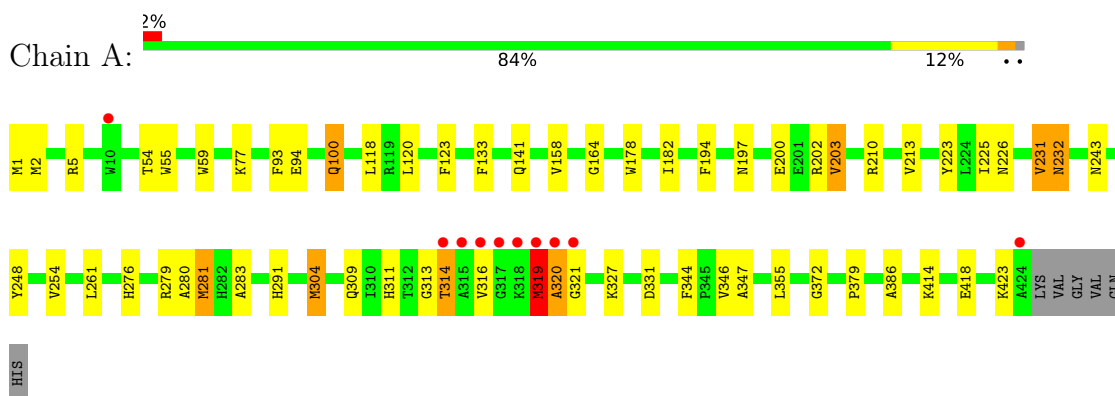
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	173	Total 173	O 173	0	0
3	E	171	Total 171	O 171	0	0

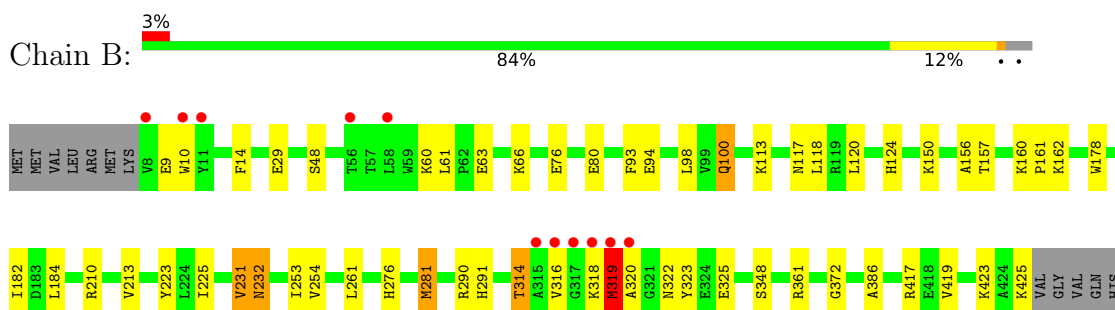
3 Residue-property plots

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.

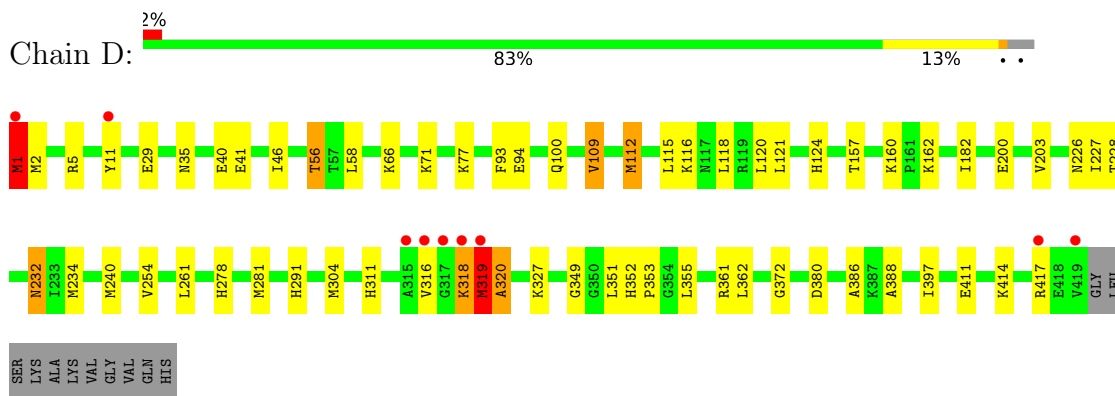
• Molecule 1: Ribulose biphosphate carboxylase



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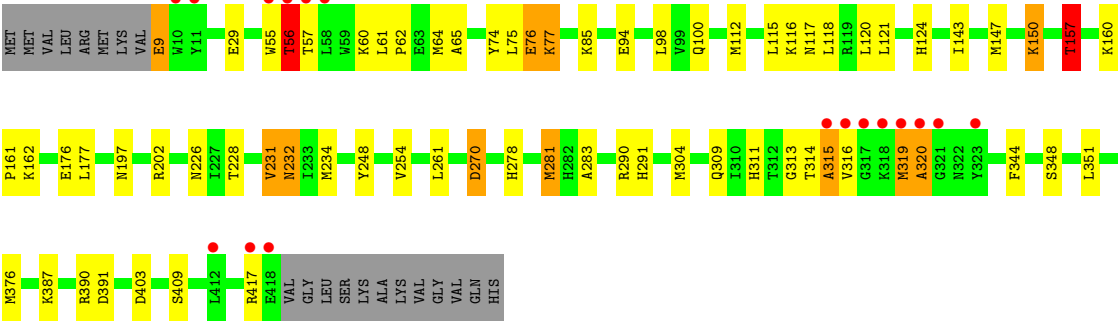
Chain E:

4%

79%

13%

5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	172.59Å 148.77Å 108.45Å 90.00° 126.49° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.90) 94.3 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.180 , 0.209 (Not available) , 0.211	Depositor DCC
R_{free} test set	7994 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.008 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14062	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	1.09	7/3430 (0.2%)	1.04	7/4631 (0.2%)
1	B	1.07	1/3380 (0.0%)	1.02	3/4566 (0.1%)
1	D	1.09	5/3398 (0.1%)	1.07	1/4589 (0.0%)
1	E	1.12	6/3325 (0.2%)	1.07	6/4493 (0.1%)
All	All	1.09	19/13533 (0.1%)	1.05	17/18279 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	304	MET	SD-CE	-11.27	1.51	1.79
1	E	304	MET	SD-CE	-10.19	1.54	1.79
1	D	112	MET	SD-CE	-10.15	1.54	1.79
1	A	281	MET	SD-CE	-9.05	1.56	1.79
1	A	304	MET	SD-CE	-8.18	1.59	1.79
1	B	281	MET	SD-CE	-8.04	1.59	1.79
1	E	147	MET	SD-CE	7.79	1.99	1.79
1	A	194	PHE	C-O	7.26	1.29	1.24
1	E	234	MET	C-O	-5.99	1.17	1.24
1	E	281	MET	SD-CE	-5.88	1.64	1.79
1	E	390	ARG	CA-C	5.69	1.60	1.52
1	E	403	ASP	CA-C	5.69	1.60	1.52
1	D	2	MET	SD-CE	5.59	1.93	1.79
1	D	240	MET	SD-CE	5.58	1.93	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1	MET	SD-CE	5.49	1.93	1.79
1	A	200	GLU	C-O	5.43	1.30	1.24
1	A	141	GLN	C-O	-5.20	1.17	1.24
1	A	319	MET	SD-CE	5.14	1.92	1.79
1	A	2	MET	SD-CE	5.08	1.92	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	231	VAL	CB-CA-C	-8.16	101.13	112.14
1	B	314	THR	N-CA-C	6.64	120.00	109.65
1	E	231	VAL	N-CA-CB	6.40	119.25	110.54
1	E	387	LYS	N-CA-C	-6.33	104.46	111.36
1	E	157	THR	N-CA-CB	-6.27	101.22	110.37
1	B	231	VAL	CB-CA-C	-6.02	104.02	112.14
1	A	313	GLY	CA-C-O	-5.98	118.15	122.45
1	A	321	GLY	N-CA-C	-5.85	103.64	112.60
1	B	253	ILE	N-CA-C	5.63	118.13	111.09
1	A	158	VAL	CB-CA-C	-5.55	104.77	110.71
1	A	203	VAL	N-CA-CB	5.54	117.03	110.55
1	A	314	THR	N-CA-C	5.53	117.38	109.14
1	A	248	TYR	CA-CB-CG	5.36	123.55	113.90
1	A	231	VAL	CB-CA-C	-5.32	104.95	112.14
1	E	270	ASP	N-CA-C	5.23	117.88	111.82
1	D	93	PHE	N-CA-C	5.20	118.21	109.95
1	E	344	PHE	CB-CA-C	-5.11	101.24	109.67

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	315	ALA	Peptide
1	E	56	THR	Peptide

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	3351	0	3356	33	0
1	B	3301	0	3293	25	0
1	D	3319	0	3319	36	0
1	E	3246	0	3225	39	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
2	D	20	0	0	0	0
2	E	25	0	0	1	0
3	A	225	0	0	1	0
3	B	181	0	0	2	0
3	D	173	0	0	1	0
3	E	171	0	0	2	0
All	All	14062	0	13193	129	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 5.

All (129) 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:323:TYR:OH	3:B:2101:HOH:O	2.00	0.80
1:E:248:TYR:OH	1:E:309:GLN:NE2	2.14	0.80
1:E:118:LEU:H	1:E:291:HIS:HD2	1.29	0.79
1:A:316:VAL:O	1:A:320:ALA:HB2	1.83	0.79
1:E:391:ASP:OD2	1:E:409:SER:OG	2.02	0.77
1:E:270:ASP:OD1	3:E:4105:HOH:O	2.05	0.73
1:B:232:ASN:HD22	1:B:232:ASN:H	1.36	0.72
1:D:227:ILE:O	1:D:234:MET:HG2	1.89	0.72
1:A:118:LEU:H	1:A:291:HIS:HD2	1.35	0.72
1:E:313:GLY:O	3:E:4128:HOH:O	2.07	0.72
1:B:29:GLU:OE1	1:B:124:HIS:HE1	1.73	0.71
1:D:1:MET:H1	1:D:1:MET:CE	2.07	0.68
1:D:316:VAL:HG13	1:D:355:LEU:CD1	2.24	0.68
1:B:157:THR:HG23	1:B:372:GLY:HA2	1.75	0.67
1:E:143:ILE:HD13	1:E:309:GLN:HE21	1.57	0.67
1:D:29:GLU:OE1	1:D:124:HIS:HE1	1.77	0.66
1:D:109:VAL:HG13	1:D:118:LEU:HD21	1.77	0.66
1:D:232:ASN:H	1:D:232:ASN:HD22	1.44	0.66
1:D:56:THR:HG22	3:D:3113:HOH:O	1.97	0.65
1:E:74:TYR:CZ	1:E:76:GLU:HG3	2.33	0.64
1:D:1:MET:H1	1:D:1:MET:HE2	1.63	0.63
1:E:9:GLU:N	1:E:56:THR:HG1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:VAL:HG13	1:D:118:LEU:CD2	2.28	0.63
1:A:316:VAL:HG13	1:A:355:LEU:CD1	2.28	0.62
1:A:118:LEU:H	1:A:291:HIS:CD2	2.17	0.61
1:D:316:VAL:HG13	1:D:355:LEU:HD13	1.84	0.60
1:D:361:ARG:NH1	1:D:362:LEU:HD21	2.17	0.60
1:E:29:GLU:OE1	1:E:124:HIS:HE1	1.85	0.60
1:B:118:LEU:H	1:B:291:HIS:HD2	1.51	0.59
1:D:1:MET:HE2	1:D:1:MET:N	2.18	0.58
1:A:232:ASN:HD22	1:A:232:ASN:H	1.50	0.58
1:A:223:TYR:CE2	1:A:225:ILE:HD12	2.39	0.57
1:A:254:VAL:HG12	1:A:281:MET:HE2	1.87	0.57
1:E:118:LEU:H	1:E:291:HIS:CD2	2.16	0.57
1:E:157:THR:CG2	1:E:177:LEU:HD13	2.35	0.57
1:D:380:ASP:OD1	1:D:414:LYS:HE3	2.05	0.57
1:E:55:TRP:O	1:E:56:THR:HB	2.03	0.56
1:D:112:MET:HE3	1:D:115:LEU:HD11	1.87	0.56
1:E:232:ASN:HD22	1:E:232:ASN:H	1.54	0.56
1:E:150:LYS:NZ	2:E:4004:SO4:O3	2.24	0.56
1:A:283:ALA:O	1:E:291:HIS:HE1	1.89	0.56
1:D:316:VAL:HG13	1:D:355:LEU:HD11	1.88	0.56
1:D:109:VAL:HA	1:D:112:MET:HE2	1.88	0.55
1:B:232:ASN:HD22	1:B:232:ASN:N	2.01	0.55
1:E:315:ALA:C	1:E:316:VAL:HG23	2.32	0.55
1:A:379:PRO:CG	1:A:418:GLU:HG3	2.37	0.54
1:B:210:ARG:HD2	1:B:210:ARG:C	2.33	0.54
1:D:157:THR:HG23	1:D:372:GLY:HA2	1.90	0.53
1:B:63:GLU:O	3:B:2084:HOH:O	2.18	0.53
1:E:112:MET:HE3	1:E:115:LEU:HD11	1.89	0.53
1:D:118:LEU:H	1:D:291:HIS:HD2	1.57	0.53
1:D:232:ASN:HD22	1:D:232:ASN:N	2.07	0.53
1:B:94:GLU:H	1:B:100:GLN:NE2	2.07	0.53
1:A:118:LEU:N	1:A:291:HIS:HD2	2.07	0.52
1:B:118:LEU:H	1:B:291:HIS:CD2	2.29	0.51
1:E:157:THR:O	1:E:157:THR:HG22	2.10	0.51
1:B:182:ILE:HG12	1:B:386:ALA:HB1	1.93	0.50
1:B:223:TYR:CE2	1:B:225:ILE:HD12	2.46	0.50
1:A:316:VAL:HG13	1:A:355:LEU:HD13	1.92	0.50
1:E:157:THR:CG2	1:E:157:THR:O	2.60	0.49
1:E:112:MET:HE3	1:E:115:LEU:CD1	2.43	0.49
1:E:160:LYS:HA	1:E:161:PRO:C	2.37	0.49
1:A:94:GLU:H	1:A:100:GLN:NE2	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:ASN:ND2	1:E:228:THR:H	2.12	0.48
1:E:29:GLU:HG2	1:E:85:LYS:HG2	1.95	0.48
1:D:388:ALA:HB2	1:D:411:GLU:C	2.39	0.48
1:A:314:THR:HG22	1:A:347:ALA:HB1	1.94	0.47
1:B:93:PHE:HA	1:B:100:GLN:HE22	1.79	0.47
1:A:210:ARG:HD2	1:A:210:ARG:C	2.40	0.47
1:A:291:HIS:HE1	1:E:283:ALA:O	1.96	0.47
1:A:311:HIS:CD2	3:A:1217:HOH:O	2.67	0.47
1:B:314:THR:HG23	1:B:348:SER:O	2.15	0.47
1:D:112:MET:HE3	1:D:115:LEU:CD1	2.45	0.47
1:A:182:ILE:HG12	1:A:386:ALA:HB1	1.96	0.46
1:D:35:ASN:HD22	1:D:116:LYS:NZ	2.14	0.46
1:A:54:THR:C	1:A:55:TRP:CD1	2.94	0.45
1:E:319:MET:O	1:E:320:ALA:HB3	2.16	0.45
1:A:319:MET:O	1:A:320:ALA:C	2.60	0.45
1:B:182:ILE:HG12	1:B:386:ALA:CB	2.47	0.45
1:D:94:GLU:H	1:D:100:GLN:NE2	2.14	0.45
1:D:316:VAL:HG12	1:D:318:LYS:H	1.80	0.45
1:E:254:VAL:HG12	1:E:281:MET:HE2	1.99	0.45
1:B:178:TRP:HB3	1:B:213:VAL:HG11	1.99	0.45
1:A:164:GLY:O	1:E:64:MET:HB2	2.17	0.45
1:A:197:ASN:OD1	1:A:202:ARG:HD3	2.17	0.44
1:B:322:ASN:HD22	1:B:325:GLU:HB2	1.82	0.44
1:D:319:MET:O	1:D:320:ALA:HB3	2.17	0.44
1:E:197:ASN:OD1	1:E:202:ARG:HD3	2.17	0.44
1:E:278:HIS:HA	1:E:311:HIS:HD2	1.82	0.44
1:E:160:LYS:O	1:E:376:MET:HE2	2.17	0.44
1:E:232:ASN:HD22	1:E:232:ASN:N	2.15	0.44
1:B:254:VAL:HG12	1:B:281:MET:HE2	1.98	0.43
1:D:254:VAL:HG12	1:D:281:MET:HE2	2.00	0.43
1:E:94:GLU:H	1:E:100:GLN:NE2	2.15	0.43
1:B:276:HIS:CD2	1:B:276:HIS:C	2.96	0.43
1:A:311:HIS:HA	1:A:346:VAL:HB	1.99	0.43
1:E:77:LYS:HA	1:E:77:LYS:HD2	1.68	0.43
1:E:157:THR:HG21	1:E:177:LEU:HD22	2.01	0.43
1:A:276:HIS:CE1	1:A:346:VAL:HG21	2.53	0.43
1:E:75:LEU:C	1:E:76:GLU:HG2	2.42	0.43
1:E:117:ASN:HB3	1:E:290:ARG:O	2.19	0.43
1:B:319:MET:SD	1:B:320:ALA:N	2.92	0.43
1:D:46:ILE:HG12	1:D:112:MET:HE1	2.01	0.42
1:E:62:PRO:HG2	1:E:65:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:118:LEU:H	1:D:291:HIS:CD2	2.36	0.42
1:D:352:HIS:HB2	1:D:353:PRO:CD	2.48	0.42
1:A:93:PHE:HA	1:A:100:GLN:HE22	1.83	0.42
1:A:123:PHE:CE1	1:A:304:MET:HE1	2.54	0.42
1:A:178:TRP:HB3	1:A:213:VAL:HG11	2.00	0.42
1:D:11:TYR:CD1	1:D:41:GLU:HA	2.55	0.42
1:A:279:ARG:O	1:A:280:ALA:C	2.61	0.41
1:D:352:HIS:HB2	1:D:353:PRO:HD2	2.01	0.41
1:D:316:VAL:HG22	1:D:351:LEU:HD23	2.02	0.41
1:A:327:LYS:NZ	1:A:331:ASP:OD2	2.48	0.41
1:B:14:PHE:CE2	1:B:48:SER:HB3	2.56	0.41
1:A:59:TRP:CH2	1:E:176:GLU:HG3	2.56	0.41
1:A:133:PHE:CG	1:A:304:MET:HG2	2.56	0.41
1:A:182:ILE:HG12	1:A:386:ALA:CB	2.51	0.41
1:A:309:GLN:HB3	1:A:344:PHE:HB2	2.02	0.41
1:B:156:ALA:HA	1:B:184:LEU:O	2.21	0.41
1:B:316:VAL:H	1:B:320:ALA:HB2	1.86	0.41
1:D:226:ASN:ND2	1:D:228:THR:H	2.19	0.41
1:D:278:HIS:HA	1:D:311:HIS:HD2	1.86	0.41
1:D:182:ILE:HG12	1:D:386:ALA:CB	2.51	0.41
1:D:200:GLU:O	1:D:203:VAL:HG22	2.22	0.40
1:E:314:THR:HG23	1:E:348:SER:O	2.21	0.40
1:A:226:ASN:C	1:A:226:ASN:HD22	2.28	0.40
1:B:117:ASN:HB3	1:B:290:ARG:O	2.21	0.40
1:B:160:LYS:HA	1:B:161:PRO:C	2.46	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	422/430 (98%)	407 (96%)	12 (3%)	3 (1%)	18 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	416/430 (97%)	401 (96%)	14 (3%)	1 (0%)	43	36
1	D	417/430 (97%)	401 (96%)	13 (3%)	3 (1%)	18	10
1	E	408/430 (95%)	389 (95%)	15 (4%)	4 (1%)	12	5
All	All	1663/1720 (97%)	1598 (96%)	54 (3%)	11 (1%)	18	10

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	319	MET
1	E	57	THR
1	B	319	MET
1	E	56	THR
1	E	319	MET
1	A	319	MET
1	A	320	ALA
1	A	372	GLY
1	E	320	ALA
1	D	320	ALA
1	D	349	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	346/351 (99%)	333 (96%)	13 (4%)	29	21
1	B	340/351 (97%)	317 (93%)	23 (7%)	14	7
1	D	343/351 (98%)	323 (94%)	20 (6%)	18	10
1	E	334/351 (95%)	316 (95%)	18 (5%)	20	12
All	All	1363/1404 (97%)	1289 (95%)	74 (5%)	20	12

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	5	ARG
1	A	77	LYS
1	A	100	GLN
1	A	120	LEU
1	A	203	VAL
1	A	231	VAL
1	A	232	ASN
1	A	243	ASN
1	A	261	LEU
1	A	319	MET
1	A	414	LYS
1	A	423	LYS
1	B	9	GLU
1	B	10	TRP
1	B	60	LYS
1	B	61	LEU
1	B	66	LYS
1	B	76	GLU
1	B	80	GLU
1	B	98	LEU
1	B	100	GLN
1	B	113	LYS
1	B	120	LEU
1	B	150	LYS
1	B	162	LYS
1	B	231	VAL
1	B	232	ASN
1	B	261	LEU
1	B	318	LYS
1	B	319	MET
1	B	361	ARG
1	B	417	ARG
1	B	419	VAL
1	B	423	LYS
1	B	425	LYS
1	D	1	MET
1	D	5	ARG
1	D	40	GLU
1	D	56	THR
1	D	58	LEU
1	D	66	LYS
1	D	71	LYS

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Mol	Chain	Res	Type
1	D	77	LYS
1	D	109	VAL
1	D	120	LEU
1	D	121	LEU
1	D	160	LYS
1	D	162	LYS
1	D	232	ASN
1	D	261	LEU
1	D	318	LYS
1	D	319	MET
1	D	327	LYS
1	D	397	ILE
1	D	417	ARG
1	E	9	GLU
1	E	56	THR
1	E	60	LYS
1	E	61	LEU
1	E	76	GLU
1	E	77	LYS
1	E	98	LEU
1	E	116	LYS
1	E	120	LEU
1	E	121	LEU
1	E	150	LYS
1	E	157	THR
1	E	162	LYS
1	E	231	VAL
1	E	232	ASN
1	E	261	LEU
1	E	351	LEU
1	E	417	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	100	GLN
1	A	226	ASN
1	A	232	ASN
1	A	291	HIS
1	A	309	GLN
1	A	322	ASN

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Mol	Chain	Res	Type
1	A	330	ASN
1	A	352	HIS
1	B	35	ASN
1	B	100	GLN
1	B	124	HIS
1	B	226	ASN
1	B	232	ASN
1	B	291	HIS
1	B	311	HIS
1	B	322	ASN
1	B	330	ASN
1	D	35	ASN
1	D	100	GLN
1	D	124	HIS
1	D	226	ASN
1	D	232	ASN
1	D	247	GLN
1	D	291	HIS
1	D	330	ASN
1	E	35	ASN
1	E	100	GLN
1	E	124	HIS
1	E	226	ASN
1	E	232	ASN
1	E	278	HIS
1	E	291	HIS
1	E	309	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

19 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	B	2001	-	4,4,4	0.28	0	6,6,6	0.71	0
2	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.38	0
2	SO4	A	1004	-	4,4,4	0.30	0	6,6,6	0.33	0
2	SO4	B	2002	-	4,4,4	0.30	0	6,6,6	0.37	0
2	SO4	D	3004	-	4,4,4	0.28	0	6,6,6	0.41	0
2	SO4	E	4001	-	4,4,4	0.23	0	6,6,6	0.55	0
2	SO4	A	1003	-	4,4,4	0.21	0	6,6,6	0.33	0
2	SO4	D	3002	-	4,4,4	0.23	0	6,6,6	0.24	0
2	SO4	A	1005	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.32	0
2	SO4	E	4003	-	4,4,4	0.20	0	6,6,6	0.13	0
2	SO4	E	4002	-	4,4,4	0.32	0	6,6,6	0.37	0
2	SO4	B	2003	-	4,4,4	0.22	0	6,6,6	0.30	0
2	SO4	E	4004	-	4,4,4	0.37	0	6,6,6	0.38	0
2	SO4	E	4005	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	D	3003	-	4,4,4	0.26	0	6,6,6	0.13	0
2	SO4	B	2005	-	4,4,4	0.30	0	6,6,6	0.32	0
2	SO4	B	2004	-	4,4,4	0.24	0	6,6,6	0.36	0
2	SO4	D	3001	-	4,4,4	0.40	0	6,6,6	0.36	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	4004	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	424/430 (98%)	-0.06	10 (2%) 59 63	11, 17, 29, 68	0
1	B	418/430 (97%)	-0.27	11 (2%) 57 61	10, 16, 36, 64	0
1	D	419/430 (97%)	-0.05	9 (2%) 63 67	11, 19, 33, 63	0
1	E	410/430 (95%)	0.07	17 (4%) 41 44	11, 18, 38, 65	0
All	All	1671/1720 (97%)	-0.08	47 (2%) 55 59	10, 18, 35, 68	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	317	GLY	7.7
1	D	419	VAL	7.3
1	B	317	GLY	6.5
1	E	316	VAL	5.7
1	A	316	VAL	5.6
1	D	317	GLY	5.3
1	D	315	ALA	5.2
1	E	315	ALA	5.1
1	E	55	TRP	5.0
1	B	316	VAL	4.8
1	E	10	TRP	4.8
1	B	315	ALA	4.7
1	A	319	MET	4.3
1	D	318	LYS	4.3
1	A	315	ALA	4.2
1	A	320	ALA	4.0
1	B	319	MET	3.7
1	D	319	MET	3.7
1	B	10	TRP	3.7
1	E	319	MET	3.5
1	E	58	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	56	THR	3.3
1	A	321	GLY	3.2
1	E	56	THR	3.2
1	A	318	LYS	3.1
1	E	318	LYS	3.1
1	B	58	LEU	3.1
1	E	321	GLY	3.1
1	E	418	GLU	3.1
1	B	8	VAL	3.1
1	E	320	ALA	3.0
1	B	320	ALA	3.0
1	D	316	VAL	2.9
1	A	10	TRP	2.9
1	D	417	ARG	2.9
1	A	317	GLY	2.8
1	E	11	TYR	2.8
1	A	424	ALA	2.7
1	E	412	LEU	2.6
1	E	57	THR	2.6
1	E	323	TYR	2.4
1	A	314	THR	2.2
1	D	1	MET	2.1
1	B	318	LYS	2.1
1	B	11	TYR	2.1
1	D	11	TYR	2.0
1	E	417	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
2	SO4	E	4004	5/5	0.46	0.17	97,98,100,100	0
2	SO4	A	1004	5/5	0.47	0.20	115,116,117,118	0
2	SO4	D	3004	5/5	0.52	0.16	103,103,104,105	0
2	SO4	B	2004	5/5	0.65	0.15	110,112,112,113	0
2	SO4	A	1002	5/5	0.70	0.14	77,79,80,80	0
2	SO4	A	1003	5/5	0.72	0.14	113,115,115,115	0
2	SO4	D	3002	5/5	0.73	0.12	69,71,72,73	0
2	SO4	E	4002	5/5	0.74	0.12	68,71,72,72	0
2	SO4	D	3003	5/5	0.77	0.14	122,123,123,123	0
2	SO4	E	4005	5/5	0.78	0.16	124,125,125,125	0
2	SO4	A	1005	5/5	0.81	0.17	131,131,132,132	0
2	SO4	B	2005	5/5	0.81	0.12	99,100,101,101	0
2	SO4	E	4003	5/5	0.83	0.12	111,111,112,112	0
2	SO4	B	2003	5/5	0.84	0.14	113,114,114,115	0
2	SO4	B	2002	5/5	0.85	0.09	60,65,66,66	0
2	SO4	D	3001	5/5	0.95	0.06	52,55,56,58	0
2	SO4	E	4001	5/5	0.95	0.07	53,56,56,58	0
2	SO4	B	2001	5/5	0.96	0.06	46,48,49,50	0
2	SO4	A	1001	5/5	0.96	0.06	50,53,55,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.