



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:00 PM GMT

PDB ID : 2D69
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

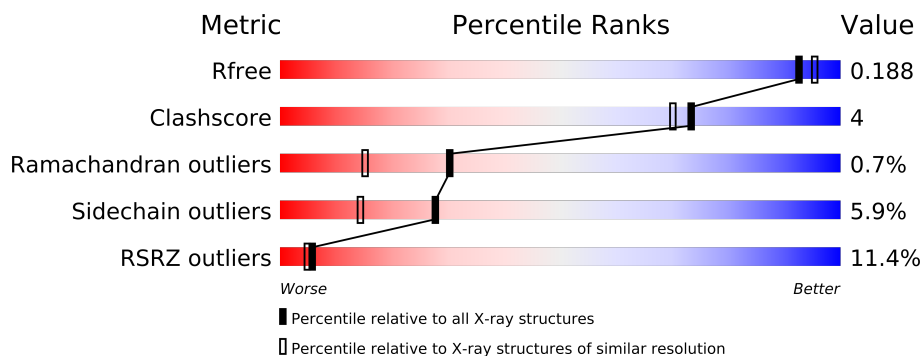
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3684 (1.90-1.90)
Clashscore	79885	4465 (1.90-1.90)
Ramachandran outliers	78287	4413 (1.90-1.90)
Sidechain outliers	78261	4414 (1.90-1.90)
RSRZ outliers	66119	3686 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	430	
1	B	430	
1	D	430	
1	E	430	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	A	1003	-	X
2	SO4	A	1004	-	X
2	SO4	A	1005	-	X
2	SO4	B	2003	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	SO4	B	2004	-	X
2	SO4	B	2005	-	X
2	SO4	E	4003	-	X
2	SO4	E	4005	-	X

2 Entry composition i

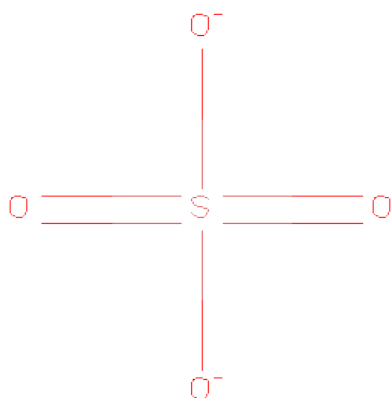
There are 3 unique types of molecules in this entry. The entry contains 14062 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: 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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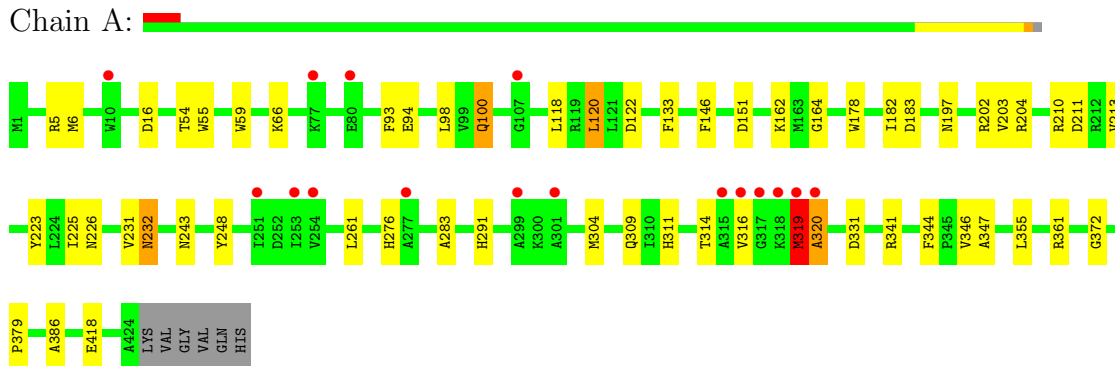
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	173	Total 173	O 173	0	0
3	E	171	Total 171	O 171	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

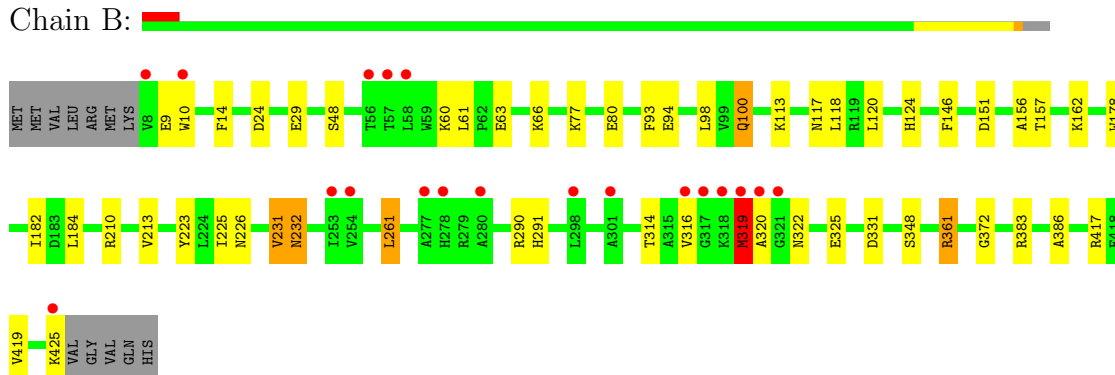
- Molecule 1: Ribulose biphosphate carboxylase

Chain A:



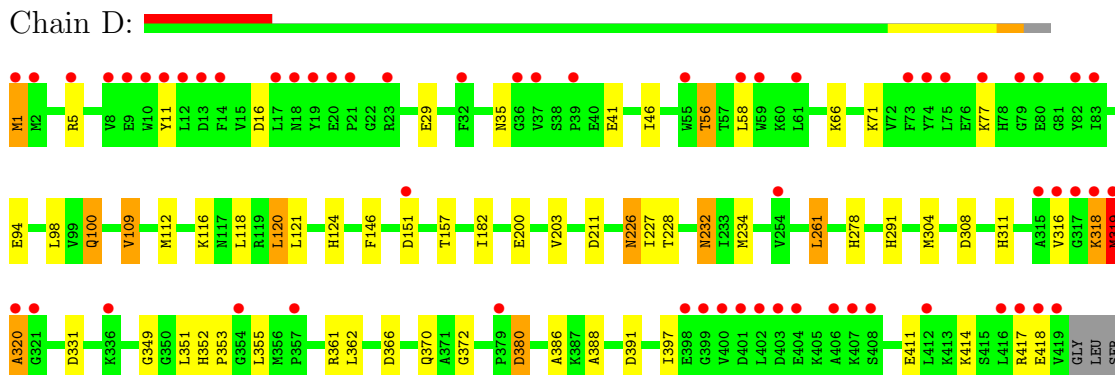
- Molecule 1: Ribulose biphosphate carboxylase

Chain B:



- Molecule 1: Ribulose biphosphate carboxylase

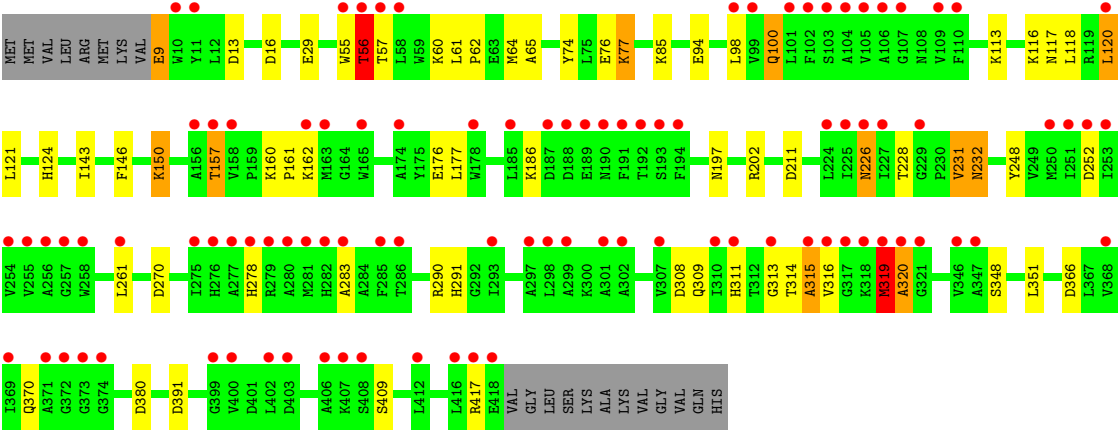
Chain D:



LYS
ALA
LYS
VAL
LEU
ARG
MET
LYS
VAL
GLN
HIS

• Molecule 1: Ribulose biphosphate carboxylase

Chain E:



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 46.70 – 1.90	Depositor EDS
% Data completeness (in resolution range)	94.3 (50.00-1.90) 94.2 (46.70-1.90)	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 0.188 , 0.188	Depositor DCC
R_{free} test set	7994 reflections (5.17%)	DCC
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 , 32.9	EDS
Estimated twinning fraction	0.008 for -h-2*1,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 162742 reflections	Xtriage
F_o, F_c correlation	0.95	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.

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	0.89	0/3430	0.90	11/4631 (0.2%)
1	B	0.88	1/3380 (0.0%)	0.90	8/4566 (0.2%)
1	D	0.85	0/3398	0.93	12/4589 (0.3%)
1	E	0.90	1/3325 (0.0%)	0.93	9/4493 (0.2%)
All	All	0.88	2/13533 (0.0%)	0.91	40/18279 (0.2%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	231	VAL	CB-CG2	-6.44	1.39	1.52
1	B	231	VAL	CB-CG2	-5.36	1.41	1.52

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ASP	CB-CG-OD2	7.60	125.14	118.30
1	D	380	ASP	CB-CG-OD2	7.54	125.08	118.30
1	E	380	ASP	CB-CG-OD2	7.42	124.97	118.30
1	B	261	LEU	CB-CG-CD2	7.29	123.39	111.00
1	D	151	ASP	CB-CG-OD2	6.91	124.52	118.30
1	D	211	ASP	CB-CG-OD2	6.73	124.36	118.30
1	D	331	ASP	CB-CG-OD2	6.49	124.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CB-CG-OD2	6.47	124.12	118.30
1	E	211	ASP	CB-CG-OD2	6.33	124.00	118.30
1	D	261	LEU	CB-CG-CD2	6.31	121.73	111.00
1	D	391	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	16	ASP	CB-CG-OD2	6.24	123.92	118.30
1	D	308	ASP	CB-CG-OD2	6.22	123.90	118.30
1	D	366	ASP	CB-CG-OD2	6.17	123.85	118.30
1	E	16	ASP	CB-CG-OD2	6.14	123.83	118.30
1	E	308	ASP	CB-CG-OD2	6.09	123.78	118.30
1	E	13	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	211	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	361	ARG	NE-CZ-NH2	5.95	123.27	120.30
1	B	383	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	120	LEU	CA-CB-CG	5.87	128.79	115.30
1	E	120	LEU	CA-CB-CG	5.72	128.45	115.30
1	B	361	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	151	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	16	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	151	ASP	CB-CG-OD2	5.66	123.39	118.30
1	D	1	MET	CG-SD-CE	5.66	109.25	100.20
1	A	361	ARG	NE-CZ-NH2	5.61	123.11	120.30
1	A	341	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	24	ASP	CB-CG-OD2	5.52	123.27	118.30
1	E	366	ASP	CB-CG-OD2	5.45	123.21	118.30
1	E	231	VAL	CB-CA-C	-5.41	101.13	111.40
1	D	120	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	248	TYR	CA-CB-CG	5.34	123.55	113.40
1	A	204	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	D	304	MET	CG-SD-CE	-5.26	91.79	100.20
1	A	122	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	183	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	252	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	383	ARG	NE-CZ-NH1	5.01	122.81	120.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3351	0	3356	28	0
1	B	3301	0	3293	21	0
1	D	3319	0	3319	31	0
1	E	3246	0	3225	34	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	1	0
3	D	173	0	0	1	0
3	E	171	0	0	2	0
All	All	14062	0	13193	110	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (110) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:270:ASP:OD1	3:E:4105:HOH:O	2.05	0.73
1:B:232:ASN:H	1:B:232:ASN:HD22	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:391:ASP:OD2	1:E:409:SER:OG	2.02	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:232:ASN:HD22	1:D:232:ASN:H	1.44	0.66
1:E:9:GLU:N	1:E:56:THR:HG1	1.94	0.66
1:E:150:LYS:NZ	2:E:4004:SO4:O3	2.24	0.65
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: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:109:VAL:HG22	1:D:112:MET:HE2	1.84	0.60
1:E:29:GLU:OE1	1:E:124:HIS:HE1	1.85	0.60
1:D:361:ARG:NH1	1:D:362:LEU:HD21	2.17	0.60
1:B:118:LEU:H	1:B:291:HIS:HD2	1.51	0.59
1:E:55:TRP:O	1:E:56:THR:HB	2.03	0.59
1:A:232:ASN:H	1:A:232:ASN:HD22	1.50	0.58
1:A:223:TYR:CE2	1:A:225:ILE:HD12	2.39	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:232:ASN:HD22	1:E:232:ASN:H	1.54	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:B:232:ASN:N	1:B:232:ASN:HD22	2.01	0.55
1:A:379:PRO:CG	1:A:418:GLU:HG3	2.37	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:D:118:LEU:H	1:D:291:HIS:HD2	1.57	0.53
1:D:232:ASN:N	1:D:232:ASN:HD22	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:HG22	1:E:157:THR:O	2.10	0.51
1:B:223:TYR:CE2	1:B:225:ILE:HD12	2.46	0.50
1:B:182:ILE:HG12	1:B:386:ALA:HB1	1.93	0.50
1:A:316:VAL:HG13	1:A:355:LEU:HD13	1.92	0.50
1:E:315:ALA:C	1:E:316:VAL:HG23	2.32	0.50
1:E:157:THR:O	1:E:157:THR:CG2	2.60	0.49
1:B:210:ARG:HD2	1:B:210:ARG:C	2.33	0.49
1:A:94:GLU:H	1:A:100:GLN:NE2	2.10	0.49
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:A:314:THR:HG22	1:A:347:ALA:HB1	1.94	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:PHE:HA	1:B:100:GLN:HE22	1.79	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:35:ASN:HD22	1:D:116:LYS:NZ	2.14	0.46
1:A:182:ILE:HG12	1:A:386:ALA:HB1	1.96	0.46
1:E:319:MET:O	1:E:320:ALA:HB3	2.16	0.45
1:D:316:VAL:HG12	1:D:318:LYS:H	1.80	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: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:E:160:LYS:HA	1:E:161:PRO:C	2.37	0.45
1:D:46:ILE:HG12	1:D:112:MET:HE1	1.99	0.44
1:E:278:HIS:HA	1:E:311:HIS:HD2	1.82	0.44
1:E:197:ASN:OD1	1:E: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:A:197:ASN:OD1	1:A:202:ARG:HD3	2.17	0.44
1:E:232:ASN:HD22	1:E:232:ASN:N	2.15	0.44
1:E:94:GLU:H	1:E:100:GLN:NE2	2.15	0.43
1:A:311:HIS:HA	1:A:346:VAL:HB	1.99	0.43
1:E:157:THR:HG21	1:E:177:LEU:HD22	2.01	0.43
1:E:77:LYS:HA	1:E:77:LYS:HD2	1.68	0.43
1:A:276:HIS:CE1	1:A:346:VAL:HG21	2.53	0.43
1:D:388:ALA:HB2	1:D:411:GLU:C	2.39	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:E:62:PRO:HG2	1:E:65:ALA:HB2	2.01	0.42
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:210:ARG:C	1:A:210:ARG:HD2	2.40	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:D:1:MET:N	1:D:1:MET:CE	2.84	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: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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:316:VAL:H	1:B:320:ALA:HB2	1.86	0.41
1:D:278:HIS:HA	1:D:311:HIS:HD2	1.86	0.41
1:D:226:ASN:ND2	1:D:228:THR:H	2.19	0.41
1:A:309:GLN:HB3	1:A:344:PHE:HB2	2.02	0.41
1:A:54:THR:C	1:A:55:TRP:CD1	2.94	0.41
1:B:156:ALA:HA	1:B:184:LEU:O	2.21	0.41
1:D:182:ILE:HG12	1:D:386:ALA:CB	2.51	0.41
1:A:319:MET:O	1:A:320:ALA:C	2.60	0.40
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:B:117:ASN:HB3	1:B:290:ARG:O	2.21	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%)	30	15
1	B	416/430 (97%)	401 (96%)	14 (3%)	1 (0%)	56	44
1	D	417/430 (97%)	401 (96%)	13 (3%)	3 (1%)	30	15
1	E	408/430 (95%)	389 (95%)	15 (4%)	4 (1%)	22	8
All	All	1663/1720 (97%)	1598 (96%)	54 (3%)	11 (1%)	30	15

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

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Mol	Chain	Res	Type
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%)	331 (96%)	15 (4%)	40	26
1	B	340/351 (97%)	318 (94%)	22 (6%)	24	11
1	D	343/351 (98%)	322 (94%)	21 (6%)	26	13
1	E	334/351 (95%)	311 (93%)	23 (7%)	22	10
All	All	1363/1404 (97%)	1282 (94%)	81 (6%)	28	14

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	MET
1	A	66	LYS
1	A	98	LEU
1	A	100	GLN
1	A	120	LEU
1	A	146	PHE
1	A	162	LYS
1	A	203	VAL
1	A	226	ASN
1	A	231	VAL
1	A	232	ASN
1	A	243	ASN
1	A	261	LEU
1	A	319	MET
1	B	9	GLU
1	B	10	TRP
1	B	60	LYS

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Mol	Chain	Res	Type
1	B	61	LEU
1	B	66	LYS
1	B	77	LYS
1	B	80	GLU
1	B	98	LEU
1	B	100	GLN
1	B	113	LYS
1	B	120	LEU
1	B	146	PHE
1	B	162	LYS
1	B	226	ASN
1	B	231	VAL
1	B	232	ASN
1	B	261	LEU
1	B	319	MET
1	B	361	ARG
1	B	417	ARG
1	B	419	VAL
1	B	425	LYS
1	D	5	ARG
1	D	56	THR
1	D	58	LEU
1	D	66	LYS
1	D	71	LYS
1	D	77	LYS
1	D	98	LEU
1	D	100	GLN
1	D	109	VAL
1	D	120	LEU
1	D	121	LEU
1	D	146	PHE
1	D	226	ASN
1	D	232	ASN
1	D	261	LEU
1	D	318	LYS
1	D	319	MET
1	D	370	GLN
1	D	397	ILE
1	D	417	ARG
1	D	418	GLU
1	E	9	GLU
1	E	60	LYS

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Mol	Chain	Res	Type
1	E	61	LEU
1	E	77	LYS
1	E	98	LEU
1	E	100	GLN
1	E	113	LYS
1	E	116	LYS
1	E	120	LEU
1	E	121	LEU
1	E	146	PHE
1	E	150	LYS
1	E	157	THR
1	E	162	LYS
1	E	186	LYS
1	E	226	ASN
1	E	231	VAL
1	E	232	ASN
1	E	261	LEU
1	E	319	MET
1	E	351	LEU
1	E	370	GLN
1	E	417	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

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

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Mol	Chain	Res	Type
1	D	124	HIS
1	D	226	ASN
1	D	232	ASN
1	D	291	HIS
1	D	309	GLN
1	D	330	ASN
1	E	35	ASN
1	E	100	GLN
1	E	124	HIS
1	E	137	GLN
1	E	226	ASN
1	E	232	ASN
1	E	291	HIS
1	E	309	GLN
1	E	322	ASN
1	E	330	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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	A	1001	-	4,4,4	0.54	0	6,6,6	0.23	0
2	SO4	A	1002	-	4,4,4	0.08	0	6,6,6	0.42	0
2	SO4	A	1003	-	4,4,4	0.19	0	6,6,6	0.34	0
2	SO4	A	1004	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	A	1005	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	B	2001	-	4,4,4	0.59	0	6,6,6	0.45	0
2	SO4	B	2002	-	4,4,4	0.10	0	6,6,6	0.31	0
2	SO4	B	2003	-	4,4,4	0.18	0	6,6,6	0.35	0
2	SO4	B	2004	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	B	2005	-	4,4,4	0.24	0	6,6,6	0.37	0
2	SO4	D	3001	-	4,4,4	0.61	0	6,6,6	0.42	0
2	SO4	D	3002	-	4,4,4	0.13	0	6,6,6	0.25	0
2	SO4	D	3003	-	4,4,4	0.15	0	6,6,6	0.16	0
2	SO4	D	3004	-	4,4,4	0.16	0	6,6,6	0.30	0
2	SO4	E	4001	-	4,4,4	0.53	0	6,6,6	0.48	0
2	SO4	E	4002	-	4,4,4	0.15	0	6,6,6	0.29	0
2	SO4	E	4003	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	E	4004	-	4,4,4	0.23	0	6,6,6	0.53	0
2	SO4	E	4005	-	4,4,4	0.24	0	6,6,6	0.21	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3001	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3002	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	3004	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4001	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4002	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4003	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	E	4004	-	-	0/0/0/0	0/0/0/0
2	SO4	E	4005	-	-	0/0/0/0	0/0/0/0

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.

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	424/430 (98%)	0.26	16 (3%) 38 40	11, 17, 29, 68	0
1	B	418/430 (97%)	0.25	19 (4%) 32 32	10, 16, 36, 64	0
1	D	419/430 (97%)	0.55	60 (14%) 3 3	11, 19, 33, 63	0
1	E	410/430 (95%)	1.20	97 (23%) 1 1	11, 18, 38, 65	0
All	All	1671/1720 (97%)	0.56	192 (11%) 6 5	10, 18, 35, 68	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	317	GLY	12.6
1	D	317	GLY	12.4
1	B	317	GLY	10.7
1	A	316	VAL	8.7
1	E	55	TRP	7.4
1	D	318	LYS	6.9
1	E	254	VAL	6.8
1	E	58	LEU	6.7
1	E	316	VAL	6.6
1	B	316	VAL	6.3
1	E	255	VAL	6.3
1	E	318	LYS	6.2
1	D	1	MET	5.8
1	E	253	ILE	5.6
1	A	319	MET	5.4
1	E	256	ALA	5.1
1	B	56	THR	4.9
1	E	278	HIS	4.8
1	A	318	LYS	4.6
1	E	277	ALA	4.5
1	D	19	TYR	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	283	ALA	4.3
1	E	280	ALA	4.3
1	E	417	ARG	4.2
1	B	319	MET	4.2
1	D	316	VAL	4.2
1	B	58	LEU	4.2
1	D	58	LEU	4.1
1	E	315	ALA	4.1
1	E	158	VAL	4.1
1	E	346	VAL	4.1
1	E	257	GLY	4.1
1	D	2	MET	4.0
1	D	417	ARG	4.0
1	B	320	ALA	4.0
1	B	10	TRP	3.9
1	E	310	ILE	3.9
1	E	400	VAL	3.8
1	A	317	GLY	3.8
1	E	258	TRP	3.8
1	E	107	GLY	3.7
1	E	279	ARG	3.7
1	A	320	ALA	3.7
1	E	102	PHE	3.7
1	D	59	TRP	3.7
1	E	313	GLY	3.6
1	A	254	VAL	3.6
1	D	82	TYR	3.5
1	D	400	VAL	3.5
1	E	293	ILE	3.5
1	D	11	TYR	3.5
1	E	251	ILE	3.5
1	D	404	GLU	3.4
1	E	185	LEU	3.4
1	E	229	GLY	3.4
1	E	299	ALA	3.4
1	E	320	ALA	3.4
1	E	286	THR	3.3
1	E	301	ALA	3.3
1	D	36	GLY	3.3
1	D	399	GLY	3.3
1	E	412	LEU	3.3
1	E	192	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	E	307	VAL	3.2
1	E	416	LEU	3.2
1	E	191	PHE	3.2
1	E	11	TYR	3.2
1	E	371	ALA	3.2
1	E	163	MET	3.2
1	E	311	HIS	3.2
1	B	8	VAL	3.1
1	E	104	ALA	3.1
1	B	254	VAL	3.1
1	E	250	MET	3.1
1	D	12	LEU	3.1
1	D	17	LEU	3.1
1	D	80	GLU	3.1
1	E	418	GLU	3.1
1	E	57	THR	3.1
1	E	282	HIS	3.1
1	E	372	GLY	3.0
1	D	416	LEU	3.0
1	E	189	GLU	3.0
1	D	39	PRO	3.0
1	D	402	LEU	3.0
1	E	226	ASN	3.0
1	E	225	ILE	2.9
1	D	37	VAL	2.9
1	D	83	ILE	2.9
1	D	319	MET	2.9
1	E	319	MET	2.9
1	E	56	THR	2.9
1	D	20	GLU	2.9
1	D	321	GLY	2.8
1	D	403	ASP	2.8
1	D	61	LEU	2.8
1	D	73	PHE	2.8
1	E	402	LEU	2.8
1	B	321	GLY	2.7
1	E	99	VAL	2.7
1	D	336	LYS	2.7
1	A	253	ILE	2.7
1	D	357	PRO	2.7
1	D	401	ASP	2.7
1	D	13	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	297	ALA	2.7
1	D	418	GLU	2.7
1	E	109	VAL	2.7
1	D	32	PHE	2.7
1	D	55	TRP	2.6
1	E	224	LEU	2.6
1	E	261	LEU	2.6
1	E	275	ILE	2.6
1	E	252	ASP	2.6
1	E	157	THR	2.6
1	B	253	ILE	2.6
1	D	77	LYS	2.6
1	A	301	ALA	2.6
1	E	101	LEU	2.6
1	D	407	LYS	2.6
1	E	187	ASP	2.6
1	E	406	ALA	2.5
1	E	281	MET	2.5
1	E	174	ALA	2.5
1	E	285	PHE	2.5
1	A	10	TRP	2.5
1	E	110	PHE	2.5
1	E	98	LEU	2.5
1	D	8	VAL	2.5
1	D	18	ASN	2.5
1	D	9	GLU	2.5
1	E	403	ASP	2.5
1	B	280	ALA	2.5
1	B	318	LYS	2.5
1	E	368	VAL	2.4
1	A	315	ALA	2.4
1	E	302	ALA	2.4
1	D	151	ASP	2.4
1	E	188	ASP	2.4
1	E	276	HIS	2.4
1	D	419	VAL	2.4
1	D	5	ARG	2.4
1	D	14	PHE	2.4
1	E	106	ALA	2.4
1	E	194	PHE	2.4
1	A	251	ILE	2.4
1	B	425	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	354	GLY	2.4
1	D	23	ARG	2.3
1	E	162	LYS	2.3
1	E	407	LYS	2.3
1	A	80	GLU	2.3
1	D	21	PRO	2.3
1	E	408	SER	2.3
1	E	105	VAL	2.3
1	D	315	ALA	2.3
1	D	412	LEU	2.3
1	A	107	GLY	2.3
1	D	79	GLY	2.3
1	E	321	GLY	2.3
1	D	320	ALA	2.3
1	D	379	PRO	2.2
1	A	277	ALA	2.2
1	B	277	ALA	2.2
1	E	190	ASN	2.2
1	E	10	TRP	2.2
1	E	178	TRP	2.2
1	E	103	SER	2.2
1	B	298	LEU	2.2
1	E	369	ILE	2.2
1	D	254	VAL	2.2
1	E	120	LEU	2.2
1	A	77	LYS	2.2
1	E	347	ALA	2.2
1	E	227	ILE	2.2
1	E	165	TRP	2.2
1	D	398	GLU	2.1
1	D	10	TRP	2.1
1	D	408	SER	2.1
1	E	193	SER	2.1
1	E	298	LEU	2.1
1	E	373	GLY	2.1
1	E	374	GLY	2.1
1	D	75	LEU	2.1
1	A	299	ALA	2.1
1	B	301	ALA	2.1
1	B	57	THR	2.0
1	B	278	HIS	2.0
1	E	399	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	406	ALA	2.0
1	E	156	ALA	2.0
1	D	74	TYR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	1003	5/5	0.35	8.33	113,115,115,115	0
2	SO4	E	4003	5/5	0.35	6.08	111,111,112,112	0
2	SO4	B	2005	5/5	0.27	4.34	99,100,101,101	0
2	SO4	B	2004	5/5	0.27	3.92	110,112,112,113	0
2	SO4	B	2003	5/5	0.20	3.92	113,114,114,115	0
2	SO4	E	4005	5/5	0.32	3.84	124,125,125,125	0
2	SO4	A	1005	5/5	0.27	3.50	131,131,132,132	0
2	SO4	A	1004	5/5	0.28	3.09	115,116,117,118	0
2	SO4	E	4004	5/5	0.22	1.96	97,98,100,100	0
2	SO4	D	3004	5/5	0.27	1.39	103,103,104,105	0
2	SO4	D	3002	5/5	0.18	1.26	69,71,72,73	0
2	SO4	D	3003	5/5	0.19	0.66	122,123,123,123	0
2	SO4	A	1001	5/5	0.12	0.26	50,53,55,57	0
2	SO4	D	3001	5/5	0.13	0.23	52,55,56,58	0
2	SO4	B	2001	5/5	0.12	-0.26	46,48,49,50	0
2	SO4	A	1002	5/5	0.16	-0.42	77,79,80,80	0
2	SO4	B	2002	5/5	0.14	-0.54	60,65,66,66	0
2	SO4	E	4001	5/5	0.14	-1.65	53,56,56,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	E	4002	5/5	0.16	-1.84	68,71,72,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.