



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:35 AM UTC

PDB ID : 7LRH / pdb_00007lrh
Title : C-terminal domain of RibD from Brucella abortus (5-amino-6-ribosylamino-2,4(1H,3H)-pyrimidinedione 5'-phosphate reductase)
Authors : Bonomi, H.R.; Cerutti, M.L.; Posadas, D.M.; Goldbaum, F.A.; Klinke, S.
Deposited on : 2021-02-16
Resolution : 1.92 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

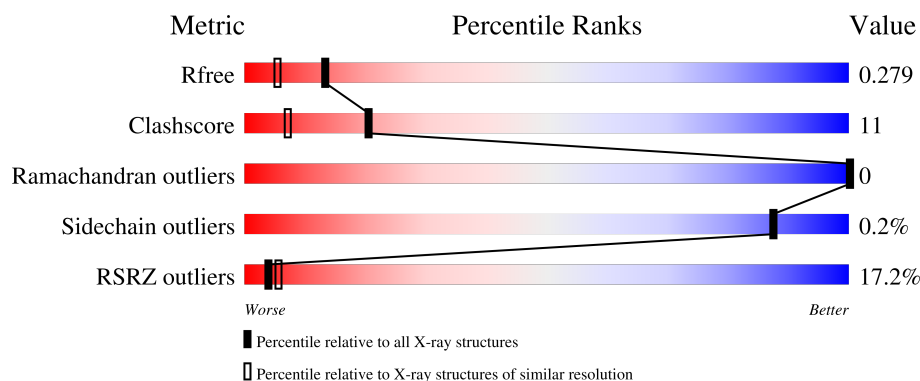
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.92 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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	225	12% 70% 23% 6%
1	B	225	21% 79% 15% 5%
1	C	225	17% 76% 17% 6%
1	D	225	14% 76% 18% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	301	-	-	X	-
2	SO4	B	301	-	-	X	-
2	SO4	B	303	-	-	X	-
2	SO4	D	303	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6426 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 Riboflavin biosynthesis protein RibD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	0	0
			1576	986	287	297	6			
1	B	213	Total	C	N	O	S	0	0	0
			1586	992	290	298	6			
1	C	212	Total	C	N	O	S	0	0	0
			1578	988	289	295	6			
1	D	213	Total	C	N	O	S	0	0	0
			1586	992	290	298	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A4V1RP59
A	2	HIS	-	expression tag	UNP A0A4V1RP59
A	3	HIS	-	expression tag	UNP A0A4V1RP59
A	4	HIS	-	expression tag	UNP A0A4V1RP59
A	5	HIS	-	expression tag	UNP A0A4V1RP59
A	6	HIS	-	expression tag	UNP A0A4V1RP59
A	7	HIS	-	expression tag	UNP A0A4V1RP59
B	1	MET	-	initiating methionine	UNP A0A4V1RP59
B	2	HIS	-	expression tag	UNP A0A4V1RP59
B	3	HIS	-	expression tag	UNP A0A4V1RP59
B	4	HIS	-	expression tag	UNP A0A4V1RP59
B	5	HIS	-	expression tag	UNP A0A4V1RP59
B	6	HIS	-	expression tag	UNP A0A4V1RP59
B	7	HIS	-	expression tag	UNP A0A4V1RP59
C	1	MET	-	initiating methionine	UNP A0A4V1RP59
C	2	HIS	-	expression tag	UNP A0A4V1RP59
C	3	HIS	-	expression tag	UNP A0A4V1RP59
C	4	HIS	-	expression tag	UNP A0A4V1RP59
C	5	HIS	-	expression tag	UNP A0A4V1RP59
C	6	HIS	-	expression tag	UNP A0A4V1RP59
C	7	HIS	-	expression tag	UNP A0A4V1RP59

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP A0A4V1RP59
D	2	HIS	-	expression tag	UNP A0A4V1RP59
D	3	HIS	-	expression tag	UNP A0A4V1RP59
D	4	HIS	-	expression tag	UNP A0A4V1RP59
D	5	HIS	-	expression tag	UNP A0A4V1RP59
D	6	HIS	-	expression tag	UNP A0A4V1RP59
D	7	HIS	-	expression tag	UNP A0A4V1RP59

- 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		
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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	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		

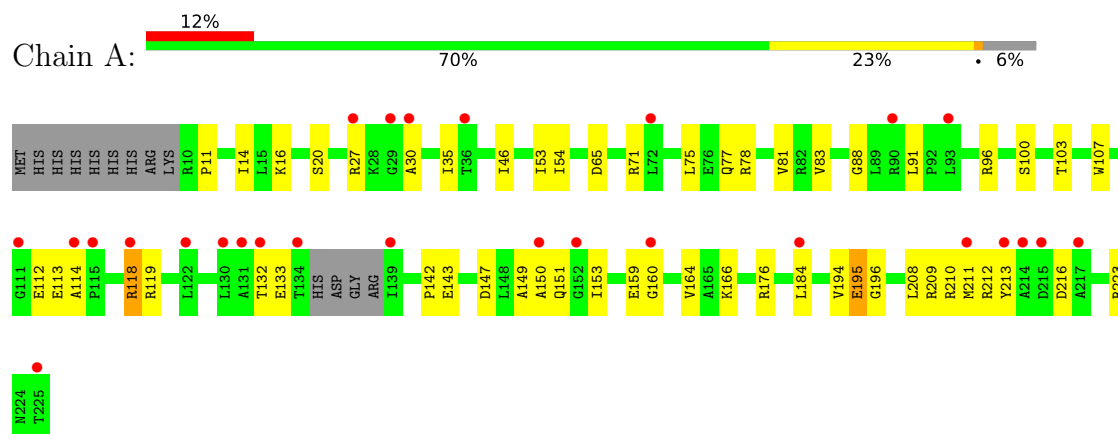
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	7	Total	O	0	0
			7	7		
3	C	7	Total	O	0	0
			7	7		
3	D	18	Total	O	0	0
			18	18		

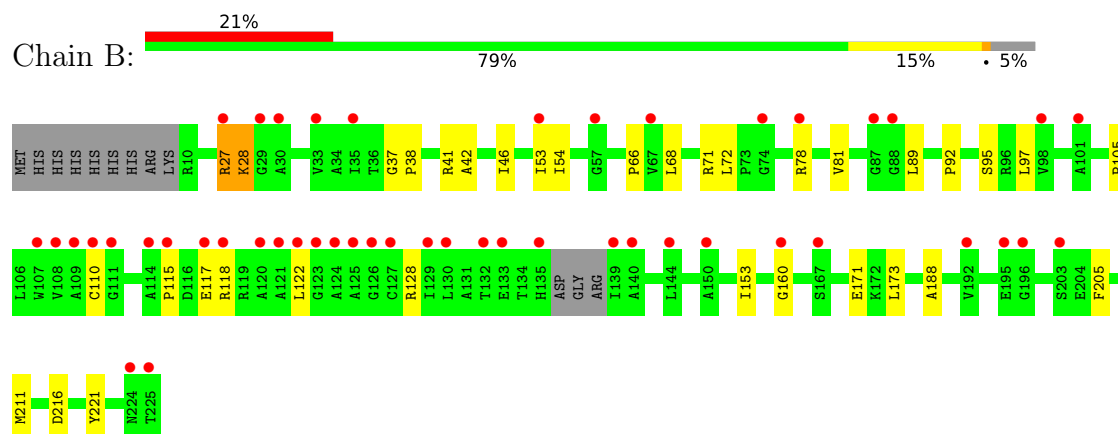
3 Residue-property plots [i](#)

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.

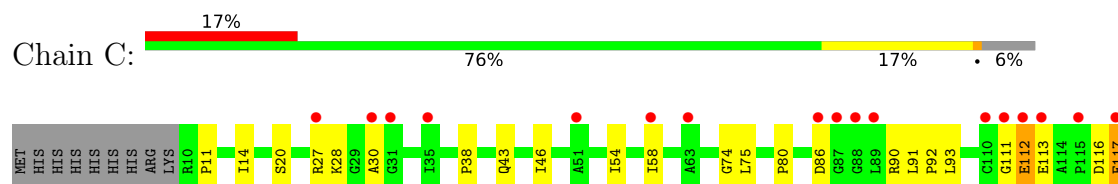
• Molecule 1: Riboflavin biosynthesis protein RibD

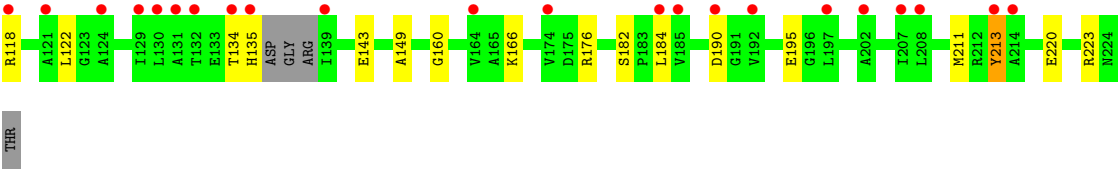


• Molecule 1: Riboflavin biosynthesis protein RibD

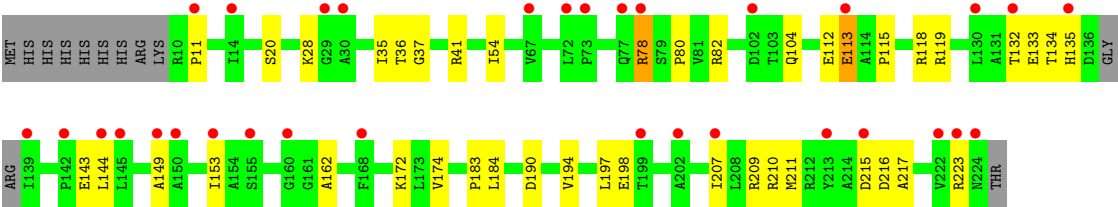
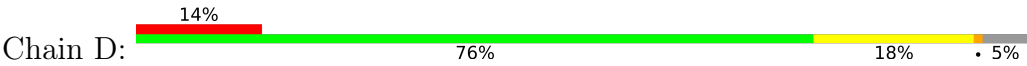


• Molecule 1: Riboflavin biosynthesis protein RibD





● Molecule 1: Riboflavin biosynthesis protein RibD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.91Å 56.70Å 79.60Å 95.99° 91.25° 113.16°	Depositor
Resolution (Å)	50.36 – 1.92 50.36 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.36-1.92) 98.0 (50.36-1.92)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 1.92Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, REFMAC (from ARP/wARP)	Depositor
R, R_{free}	0.234 , 0.274 0.239 , 0.279	Depositor DCC
R_{free} test set	3276 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	46.3	Xtriage
Anisotropy	0.159	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6426	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% 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	0.68	0/1593	0.97	8/2157 (0.4%)
1	B	0.65	0/1604	0.92	5/2172 (0.2%)
1	C	0.65	0/1596	1.00	12/2162 (0.6%)
1	D	0.67	0/1604	0.92	6/2173 (0.3%)
All	All	0.66	0/6397	0.95	31/8664 (0.4%)

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	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	112	GLU	CB-CG-CD	-9.73	96.05	112.60
1	C	112	GLU	N-CA-CB	-9.38	95.23	110.42
1	C	112	GLU	CA-CB-CG	8.64	131.38	114.10
1	A	142	PRO	CA-C-N	-7.79	109.69	122.54
1	A	142	PRO	C-N-CA	-7.79	109.69	122.54
1	A	143	GLU	CB-CA-C	7.46	122.55	110.09
1	D	113	GLU	CB-CG-CD	-7.45	99.94	112.60
1	C	117	GLU	CG-CD-OE1	-7.34	101.52	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	117	GLU	CB-CG-CD	7.33	125.06	112.60
1	C	117	GLU	CA-CB-CG	-7.26	99.59	114.10
1	D	78	ARG	CG-CD-NE	7.16	127.75	112.00
1	B	28	LYS	CA-C-N	-7.09	110.06	122.83
1	B	28	LYS	C-N-CA	-7.09	110.06	122.83
1	C	223	ARG	CG-CD-NE	-7.07	96.45	112.00
1	C	111	GLY	CA-C-N	6.46	134.86	121.94
1	C	111	GLY	C-N-CA	6.46	134.86	121.94
1	A	194	VAL	CA-C-N	-6.44	112.56	122.09
1	A	194	VAL	C-N-CA	-6.44	112.56	122.09
1	A	195	GLU	CA-CB-CG	-6.34	101.43	114.10
1	C	116	ASP	CA-C-N	-6.20	110.13	120.68
1	C	116	ASP	C-N-CA	-6.20	110.13	120.68
1	B	27	ARG	NE-CZ-NH1	-5.83	115.67	121.50
1	D	172	LYS	CG-CD-CE	5.81	124.66	111.30
1	B	117	GLU	CB-CG-CD	-5.77	102.79	112.60
1	D	215	ASP	N-CA-C	5.68	119.36	110.32
1	D	78	ARG	CA-CB-CG	-5.64	102.82	114.10
1	B	27	ARG	NE-CZ-NH2	5.55	124.19	119.20
1	C	112	GLU	CB-CA-C	5.51	120.57	110.11
1	A	118	ARG	CB-CG-CD	5.19	123.24	111.30
1	A	195	GLU	CB-CG-CD	-5.19	103.77	112.60
1	D	78	ARG	CB-CA-C	-5.07	102.03	110.81

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	GLY	Peptide
1	B	160	GLY	Peptide
1	B	27	ARG	Sidechain
1	C	160	GLY	Peptide
1	C	213	TYR	Sidechain
1	D	113	GLU	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	1576	0	1635	57	1
1	B	1586	0	1642	33	2
1	C	1578	0	1635	32	0
1	D	1586	0	1639	33	1
2	A	15	0	0	5	0
2	B	15	0	0	7	0
2	C	15	0	0	0	0
2	D	15	0	0	3	0
3	A	8	0	0	0	0
3	B	7	0	0	1	0
3	C	7	0	0	0	0
3	D	18	0	0	1	0
All	All	6426	0	6551	145	2

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 11.

All (145) 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:A:27:ARG:HG3	1:A:30:ALA:HB3	1.39	1.04
1:D:41:ARG:NH2	2:D:303:SO4:O2	1.99	0.96
1:D:41:ARG:NH2	2:D:303:SO4:S	2.44	0.89
1:C:38:PRO:HD2	1:D:78:ARG:HH21	1.39	0.88
1:A:210:ARG:NH1	1:A:212:ARG:NH1	2.22	0.88
1:C:134:THR:O	1:C:135:HIS:ND1	2.12	0.83
1:D:41:ARG:NH2	2:D:303:SO4:O1	2.12	0.83
1:D:194:VAL:HG23	1:D:197:LEU:HB2	1.62	0.81
1:A:112:GLU:O	1:A:113:GLU:HG3	1.82	0.80
1:A:210:ARG:HH11	1:A:212:ARG:NH1	1.80	0.80
1:C:27:ARG:HG3	1:C:30:ALA:HB3	1.63	0.80
1:A:71:ARG:NH2	2:A:301:SO4:O2	2.16	0.79
1:D:198:GLU:OE1	3:D:401:HOH:O	2.01	0.77
1:A:88:GLY:O	1:A:118:ARG:NH1	2.18	0.77
2:B:302:SO4:O2	3:B:401:HOH:O	2.04	0.75
1:A:112:GLU:C	1:A:113:GLU:HG3	2.11	0.74
1:A:114:ALA:O	1:A:119:ARG:NH2	2.20	0.74
1:B:211:MET:HE2	1:B:216:ASP:HB3	1.70	0.73
1:A:16:LYS:NZ	1:A:159:GLU:OE2	2.21	0.72
1:B:71:ARG:NH2	2:B:301:SO4:O4	2.19	0.72
1:D:35:ILE:O	1:D:41:ARG:HD2	1.89	0.72
1:A:210:ARG:HH11	1:A:212:ARG:CZ	2.03	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:NH2	2:B:301:SO4:S	2.63	0.71
1:B:41:ARG:NH1	2:B:303:SO4:S	2.64	0.70
1:A:71:ARG:NH2	2:A:301:SO4:S	2.65	0.69
1:C:38:PRO:HD2	1:D:78:ARG:NH2	2.08	0.69
1:A:46:ILE:HG13	1:B:46:ILE:CD1	2.24	0.68
1:B:71:ARG:NH2	2:B:301:SO4:O2	2.28	0.66
1:D:115:PRO:HG2	1:D:118:ARG:HD2	1.78	0.65
1:A:27:ARG:CG	1:A:30:ALA:HB3	2.22	0.65
1:A:71:ARG:NH2	2:A:301:SO4:O3	2.30	0.65
1:C:28:LYS:HD2	1:C:190:ASP:HA	1.78	0.65
1:D:174:VAL:O	1:D:223:ARG:HD3	1.99	0.63
1:C:118:ARG:O	1:C:122:LEU:HD13	1.99	0.62
1:D:28:LYS:HG2	1:D:190:ASP:O	2.00	0.62
1:A:210:ARG:NH1	1:A:212:ARG:HH12	1.97	0.62
1:B:66:PRO:HD2	1:B:97:LEU:HD11	1.82	0.61
1:A:46:ILE:HG13	1:B:46:ILE:HD12	1.82	0.60
1:C:143:GLU:OE2	1:C:143:GLU:N	2.32	0.60
1:C:112:GLU:OE1	1:C:134:THR:CG2	2.49	0.60
1:B:115:PRO:HD2	1:B:118:ARG:HH21	1.65	0.60
1:B:53:ILE:HG12	1:B:81:VAL:HG13	1.84	0.60
1:A:71:ARG:NH1	2:A:302:SO4:O4	2.34	0.60
1:A:210:ARG:NH1	1:A:212:ARG:CZ	2.65	0.59
1:A:27:ARG:NE	1:A:30:ALA:CB	2.66	0.59
1:A:150:ALA:HB3	1:A:151:GLN:OE1	2.02	0.59
1:C:91:LEU:HD12	1:C:92:PRO:HD2	1.87	0.57
1:D:132:THR:HG21	1:D:144:LEU:HD12	1.87	0.56
1:A:75:LEU:HD21	1:B:38:PRO:HB2	1.87	0.56
1:A:211:MET:HE3	1:A:213:TYR:HD2	1.69	0.56
1:C:182:SER:HB3	1:C:184:LEU:H	1.71	0.56
1:C:58:ILE:HG12	1:C:90:ARG:HG3	1.87	0.56
1:A:164:VAL:HG23	2:A:303:SO4:O3	2.05	0.55
1:B:53:ILE:HG12	1:B:81:VAL:CG1	2.36	0.55
1:D:211:MET:HE3	1:D:217:ALA:HB3	1.88	0.55
1:A:210:ARG:HH12	1:A:212:ARG:HH12	1.53	0.55
1:D:54:ILE:HG13	1:D:80:PRO:HG2	1.88	0.54
1:C:112:GLU:OE1	1:C:134:THR:HG21	2.08	0.54
1:A:27:ARG:HG3	1:A:30:ALA:CB	2.25	0.54
1:A:213:TYR:CE2	1:B:78:ARG:NH2	2.76	0.53
1:B:53:ILE:HG13	1:B:153:ILE:HD12	1.88	0.53
1:D:37:GLY:O	1:D:41:ARG:HG2	2.08	0.53
1:A:14:ILE:HD13	1:A:176:ARG:HH21	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:11:PRO:HD3	1:C:149:ALA:HB2	1.91	0.52
1:A:75:LEU:CD2	1:B:38:PRO:HB2	2.40	0.52
1:A:100:SER:O	1:A:103:THR:HG22	2.09	0.52
1:D:36:THR:HG21	1:D:183:PRO:HD2	1.91	0.52
1:D:20:SER:HB2	1:D:184:LEU:O	2.10	0.51
1:D:143:GLU:OE1	1:D:143:GLU:N	2.44	0.51
1:A:11:PRO:HD3	1:A:149:ALA:HB2	1.91	0.51
1:A:65:ASP:O	1:A:96:ARG:HD3	2.10	0.50
1:C:43:GLN:O	1:C:46:ILE:HG22	2.12	0.50
1:C:20:SER:HA	1:C:182:SER:HB2	1.94	0.50
1:C:166:LYS:NZ	1:C:195:GLU:O	2.37	0.50
1:B:46:ILE:HG13	1:B:72:LEU:HD11	1.94	0.49
1:B:89:LEU:HD22	1:B:122:LEU:CD1	2.42	0.49
1:A:209:ARG:HH21	1:A:211:MET:HG3	1.78	0.49
1:B:115:PRO:CD	1:B:118:ARG:HH21	2.25	0.49
1:C:86:ASP:OD1	1:C:90:ARG:HG2	2.12	0.49
1:B:41:ARG:NH1	2:B:303:SO4:O4	2.46	0.49
1:B:54:ILE:HD13	1:B:68:LEU:HB3	1.95	0.49
1:D:207:ILE:HG21	1:D:210:ARG:NH2	2.27	0.49
1:C:54:ILE:HG13	1:C:80:PRO:CG	2.43	0.49
1:C:117:GLU:O	1:C:117:GLU:CG	2.51	0.49
1:D:115:PRO:CG	1:D:118:ARG:HD2	2.43	0.49
1:D:132:THR:HG22	1:D:133:GLU:H	1.78	0.49
1:D:194:VAL:CG2	1:D:197:LEU:HB2	2.36	0.49
1:A:27:ARG:CZ	1:A:30:ALA:HB1	2.43	0.48
1:C:74:GLY:C	1:C:75:LEU:HD23	2.38	0.48
1:A:77:GLN:HG2	1:A:78:ARG:HD3	1.95	0.48
1:A:223:ARG:HG3	1:A:223:ARG:NH1	2.28	0.48
1:A:132:THR:HG22	1:A:133:GLU:H	1.78	0.48
1:A:147:ASP:O	1:A:151:GLN:OE1	2.32	0.48
1:B:81:VAL:HG23	1:B:105:PRO:HB2	1.96	0.47
1:C:117:GLU:O	1:C:117:GLU:HG3	2.14	0.47
1:A:53:ILE:HG13	1:A:153:ILE:HD12	1.96	0.47
1:B:188:ALA:HB2	1:D:210:ARG:HD2	1.97	0.47
1:D:54:ILE:HG13	1:D:80:PRO:CG	2.44	0.47
1:D:198:GLU:H	1:D:198:GLU:CD	2.22	0.46
1:B:89:LEU:HG	1:B:110:CYS:SG	2.54	0.46
1:C:14:ILE:HD12	1:C:176:ARG:HB3	1.97	0.46
1:C:176:ARG:HD3	1:D:209:ARG:NH2	2.29	0.46
1:C:213:TYR:CD1	1:C:213:TYR:N	2.78	0.46
1:B:171:GLU:C	1:B:173:LEU:HD22	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:GLU:C	1:A:113:GLU:CG	2.86	0.45
1:A:27:ARG:NE	1:A:30:ALA:HB1	2.30	0.45
1:D:115:PRO:O	1:D:119:ARG:HG3	2.17	0.45
1:A:195:GLU:HG3	1:A:196:GLY:N	2.31	0.45
1:B:78:ARG:HA	1:B:78:ARG:HD2	1.58	0.45
1:A:77:GLN:HE21	1:A:78:ARG:HH21	1.63	0.45
1:A:77:GLN:HE21	1:A:78:ARG:NH2	2.15	0.45
1:C:93:LEU:HD11	1:C:122:LEU:CD1	2.47	0.44
1:D:11:PRO:HD3	1:D:149:ALA:HB2	2.00	0.44
1:A:223:ARG:HG3	1:A:223:ARG:HH11	1.81	0.44
1:A:46:ILE:HD11	1:B:42:ALA:CB	2.48	0.43
1:B:95:SER:HG	1:B:97:LEU:HB2	1.82	0.43
1:A:35:ILE:HD13	1:A:35:ILE:HA	1.84	0.43
1:C:43:GLN:HA	1:C:46:ILE:HG22	2.00	0.43
1:A:14:ILE:HD13	1:A:176:ARG:NH2	2.34	0.43
1:A:166:LYS:HE3	1:A:166:LYS:HB2	1.80	0.43
1:A:213:TYR:CZ	1:B:78:ARG:NH2	2.84	0.43
1:B:37:GLY:O	1:B:41:ARG:HG3	2.19	0.43
1:C:46:ILE:HD12	1:C:46:ILE:HA	1.68	0.43
1:B:205:PHE:HB3	1:B:221:TYR:HB3	2.01	0.43
1:C:176:ARG:NH1	1:C:220:GLU:OE1	2.52	0.42
1:C:211:MET:HG3	1:C:213:TYR:CD2	2.54	0.42
1:B:41:ARG:HD2	2:B:303:SO4:O1	2.19	0.42
1:A:91:LEU:HD12	1:A:91:LEU:HA	1.81	0.42
1:A:208:LEU:HA	1:A:208:LEU:HD23	1.72	0.42
1:C:54:ILE:HG13	1:C:80:PRO:HG3	2.01	0.42
1:A:83:VAL:HA	1:A:107:TRP:O	2.19	0.42
1:B:92:PRO:O	1:B:95:SER:HB3	2.19	0.42
1:B:89:LEU:HD22	1:B:122:LEU:HD12	2.02	0.42
1:A:54:ILE:HD11	1:A:159:GLU:CD	2.45	0.41
1:D:11:PRO:HB3	1:D:153:ILE:O	2.20	0.41
1:C:93:LEU:HD11	1:C:122:LEU:HD12	2.02	0.41
1:D:162:ALA:HA	1:D:194:VAL:HG12	2.01	0.41
1:A:20:SER:HB2	1:A:184:LEU:O	2.20	0.41
1:D:37:GLY:HA3	1:D:216:ASP:OD1	2.21	0.41
1:D:82:ARG:HD3	1:D:104:GLN:CD	2.44	0.41
1:A:53:ILE:HG12	1:A:81:VAL:HB	2.03	0.41
1:C:112:GLU:OE1	1:C:134:THR:HG23	2.20	0.40
1:A:211:MET:HE2	1:A:216:ASP:O	2.21	0.40
1:A:166:LYS:NZ	1:A:195:GLU:H	2.20	0.40
1:D:134:THR:O	1:D:135:HIS:ND1	2.54	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LYS:NZ	1:D:112:GLU:OE1[1_445]	2.06	0.14
1:A:147:ASP:OD1	1:B:128:ARG:NH2[1_665]	2.19	0.01

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	208/225 (92%)	203 (98%)	5 (2%)	0	100	100
1	B	209/225 (93%)	205 (98%)	4 (2%)	0	100	100
1	C	208/225 (92%)	204 (98%)	4 (2%)	0	100	100
1	D	209/225 (93%)	204 (98%)	5 (2%)	0	100	100
All	All	834/900 (93%)	816 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	163/175 (93%)	163 (100%)	0	100	100
1	B	164/175 (94%)	164 (100%)	0	100	100
1	C	163/175 (93%)	162 (99%)	1 (1%)	78	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	164/175 (94%)	164 (100%)	0	100	100
All	All	654/700 (93%)	653 (100%)	1 (0%)	87	87

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	113	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	B	32	GLN
1	D	32	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](#)

12 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	D	302	-	4,4,4	0.36	0	6,6,6	0.54	0
2	SO4	C	303	-	4,4,4	0.41	0	6,6,6	0.72	0
2	SO4	B	301	-	4,4,4	0.29	0	6,6,6	0.26	0
2	SO4	A	302	-	4,4,4	0.25	0	6,6,6	0.45	0
2	SO4	A	301	-	4,4,4	0.23	0	6,6,6	0.50	0
2	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.42	0
2	SO4	D	303	-	4,4,4	0.18	0	6,6,6	0.54	0
2	SO4	B	303	-	4,4,4	0.35	0	6,6,6	0.33	0
2	SO4	C	301	-	4,4,4	0.40	0	6,6,6	0.73	0
2	SO4	A	303	-	4,4,4	0.25	0	6,6,6	0.47	0
2	SO4	C	302	-	4,4,4	0.31	0	6,6,6	0.49	0
2	SO4	D	301	-	4,4,4	0.30	0	6,6,6	0.75	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.

7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	SO4	3	0
2	A	302	SO4	1	0
2	A	301	SO4	3	0
2	B	302	SO4	1	0
2	D	303	SO4	3	0
2	B	303	SO4	3	0
2	A	303	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	212/225 (94%)	1.21	27 (12%) 8 10	38, 54, 77, 96	0
1	B	213/225 (94%)	1.32	48 (22%) 2 2	39, 58, 80, 96	0
1	C	212/225 (94%)	1.29	39 (18%) 3 4	39, 55, 74, 87	0
1	D	213/225 (94%)	1.14	32 (15%) 5 7	37, 53, 77, 90	0
All	All	850/900 (94%)	1.24	146 (17%) 4 5	37, 55, 77, 96	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	TYR	5.5
1	B	129	ILE	5.0
1	A	213	TYR	4.8
1	B	160	GLY	4.4
1	B	110	CYS	4.2
1	A	214	ALA	4.0
1	A	150	ALA	4.0
1	C	184	LEU	3.9
1	C	130	LEU	3.7
1	C	139	ILE	3.7
1	A	115	PRO	3.7
1	A	215	ASP	3.6
1	B	109	ALA	3.5
1	B	139	ILE	3.4
1	A	225	THR	3.4
1	B	150	ALA	3.4
1	A	160	GLY	3.3
1	A	90	ARG	3.3
1	C	117	GLU	3.3
1	A	134	THR	3.3
1	B	107	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	88	GLY	3.3
1	D	78	ARG	3.2
1	D	11	PRO	3.2
1	B	133	GLU	3.2
1	A	29	GLY	3.2
1	A	152	GLY	3.1
1	B	135	HIS	3.1
1	B	225	THR	3.1
1	C	174	VAL	3.1
1	A	139	ILE	3.0
1	D	207	ILE	3.0
1	B	140	ALA	3.0
1	C	115	PRO	3.0
1	B	115	PRO	3.0
1	D	142	PRO	3.0
1	A	111	GLY	2.9
1	C	86	ASP	2.9
1	A	132	THR	2.9
1	A	30	ALA	2.9
1	A	114	ALA	2.9
1	C	214	ALA	2.9
1	D	30	ALA	2.9
1	C	131	ALA	2.8
1	D	149	ALA	2.8
1	D	224	ASN	2.8
1	C	129	ILE	2.8
1	D	135	HIS	2.8
1	B	127	CYS	2.8
1	C	207	ILE	2.8
1	D	102	ASP	2.8
1	D	153	ILE	2.7
1	A	118	ARG	2.7
1	A	130	LEU	2.7
1	A	131	ALA	2.6
1	B	124	ALA	2.6
1	C	110	CYS	2.6
1	D	139	ILE	2.6
1	C	111	GLY	2.6
1	D	113	GLU	2.6
1	C	135	HIS	2.6
1	B	111	GLY	2.6
1	D	215	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	113	GLU	2.6
1	C	132	THR	2.6
1	D	132	THR	2.6
1	B	144	LEU	2.6
1	C	118	ARG	2.6
1	A	27	ARG	2.5
1	D	160	GLY	2.5
1	B	132	THR	2.5
1	A	184	LEU	2.5
1	B	29	GLY	2.5
1	B	130	LEU	2.5
1	B	196	GLY	2.5
1	D	144	LEU	2.5
1	B	53	ILE	2.5
1	B	114	ALA	2.5
1	C	121	ALA	2.5
1	C	192	VAL	2.5
1	C	87	GLY	2.4
1	D	223	ARG	2.4
1	C	197	LEU	2.4
1	D	130	LEU	2.4
1	A	211	MET	2.4
1	A	217	ALA	2.4
1	D	29	GLY	2.4
1	D	145	LEU	2.4
1	B	30	ALA	2.4
1	B	35	ILE	2.4
1	D	150	ALA	2.4
1	C	164	VAL	2.3
1	C	134	THR	2.3
1	B	87	GLY	2.3
1	B	88	GLY	2.3
1	C	35	ILE	2.3
1	B	33	VAL	2.3
1	C	185	VAL	2.3
1	A	122	LEU	2.3
1	D	72	LEU	2.3
1	B	117	GLU	2.2
1	B	195	GLU	2.2
1	D	202	ALA	2.2
1	D	213	TYR	2.2
1	D	155	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	58	ILE	2.2
1	B	122	LEU	2.2
1	C	112	GLU	2.2
1	D	77	GLN	2.2
1	C	63	ALA	2.2
1	D	199	THR	2.2
1	A	72	LEU	2.2
1	D	73	PRO	2.2
1	B	121	ALA	2.2
1	B	125	ALA	2.2
1	D	67	VAL	2.2
1	B	123	GLY	2.2
1	B	120	ALA	2.2
1	D	14	ILE	2.1
1	B	108	VAL	2.1
1	C	31	GLY	2.1
1	B	78	ARG	2.1
1	C	89	LEU	2.1
1	C	124	ALA	2.1
1	B	27	ARG	2.1
1	B	57	GLY	2.1
1	B	192	VAL	2.1
1	D	222	VAL	2.1
1	A	93	LEU	2.1
1	C	190	ASP	2.1
1	B	74	GLY	2.1
1	B	126	GLY	2.1
1	B	224	ASN	2.1
1	C	208	LEU	2.1
1	C	30	ALA	2.1
1	C	51	ALA	2.1
1	C	202	ALA	2.1
1	B	118	ARG	2.1
1	B	167	SER	2.0
1	B	203	SER	2.0
1	B	67	VAL	2.0
1	B	98	VAL	2.0
1	B	101	ALA	2.0
1	C	27	ARG	2.0
1	D	168	PHE	2.0
1	A	36	THR	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	C	303	5/5	0.67	0.13	66,69,77,79	0
2	SO4	B	303	5/5	0.74	0.11	79,80,90,96	0
2	SO4	D	303	5/5	0.75	0.11	74,77,82,82	0
2	SO4	A	302	5/5	0.83	0.09	70,74,83,85	0
2	SO4	C	302	5/5	0.93	0.08	61,61,65,70	0
2	SO4	A	303	5/5	0.94	0.09	51,54,59,61	0
2	SO4	D	302	5/5	0.94	0.08	52,58,59,61	0
2	SO4	B	302	5/5	0.94	0.08	58,59,61,64	0
2	SO4	A	301	5/5	0.95	0.09	55,55,61,63	0
2	SO4	B	301	5/5	0.96	0.06	58,59,63,64	0
2	SO4	D	301	5/5	0.96	0.08	50,51,52,54	0
2	SO4	C	301	5/5	0.97	0.07	46,47,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.