



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:13 AM UTC

PDB ID : 9RIF / pdb_00009rif
Title : The histone fold domain heterodimer of oocyst rupture proteins 1 and 2 from Plasmodium berghei
Authors : Gourlay, L.J.; Nardini, M.
Deposited on : 2025-06-11
Resolution : 3.10 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

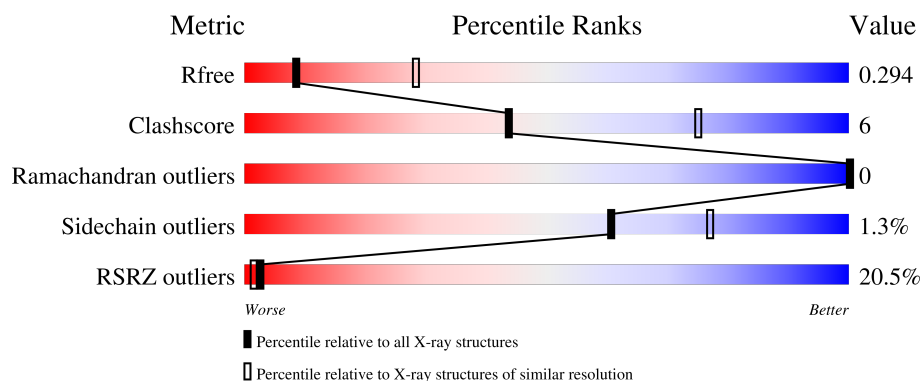
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	114	11% 67%8%25%
1	C	114	11% 61%15%24%
1	E	114	19% 66%11%24%
1	G	114	12% 61%15%25%
1	I	114	24% 68%6%25%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	114	15% 66% 6% 28%
2	B	111	16% 82% 9% 8%
2	D	111	26% 79% 15% 5%
2	F	111	23% 86% 6% 7%
2	H	111	18% 80% 10% 10%
2	J	111	17% 83% 10% 7%
2	L	111	10% 59% 9% 32%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9120 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 Oocyst rupture protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	85	Total	C	N	O	S	0	0	0
			697	448	116	130	3			
1	C	87	Total	C	N	O	S	0	0	0
			716	459	120	134	3			
1	E	87	Total	C	N	O	S	0	0	0
			716	459	120	134	3			
1	G	86	Total	C	N	O	S	0	0	0
			706	454	118	131	3			
1	I	85	Total	C	N	O	S	0	0	0
			697	448	116	130	3			
1	K	82	Total	C	N	O	S	0	0	0
			666	427	110	126	3			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	MET	-	initiating methionine	UNP A0A509AJ88
A	748	GLY	-	expression tag	UNP A0A509AJ88
A	749	SER	-	expression tag	UNP A0A509AJ88
A	750	SER	-	expression tag	UNP A0A509AJ88
A	751	HIS	-	expression tag	UNP A0A509AJ88
A	752	HIS	-	expression tag	UNP A0A509AJ88
A	753	HIS	-	expression tag	UNP A0A509AJ88
A	754	HIS	-	expression tag	UNP A0A509AJ88
A	755	HIS	-	expression tag	UNP A0A509AJ88
A	756	HIS	-	expression tag	UNP A0A509AJ88
A	757	SER	-	expression tag	UNP A0A509AJ88
A	758	SER	-	expression tag	UNP A0A509AJ88
A	759	GLY	-	expression tag	UNP A0A509AJ88
A	760	LEU	-	expression tag	UNP A0A509AJ88
A	761	VAL	-	expression tag	UNP A0A509AJ88
A	762	PRO	-	expression tag	UNP A0A509AJ88
A	763	ARG	-	expression tag	UNP A0A509AJ88

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	764	GLY	-	expression tag	UNP A0A509AJ88
A	765	SER	-	expression tag	UNP A0A509AJ88
A	766	HIS	-	expression tag	UNP A0A509AJ88
A	767	MET	-	expression tag	UNP A0A509AJ88
C	747	MET	-	initiating methionine	UNP A0A509AJ88
C	748	GLY	-	expression tag	UNP A0A509AJ88
C	749	SER	-	expression tag	UNP A0A509AJ88
C	750	SER	-	expression tag	UNP A0A509AJ88
C	751	HIS	-	expression tag	UNP A0A509AJ88
C	752	HIS	-	expression tag	UNP A0A509AJ88
C	753	HIS	-	expression tag	UNP A0A509AJ88
C	754	HIS	-	expression tag	UNP A0A509AJ88
C	755	HIS	-	expression tag	UNP A0A509AJ88
C	756	HIS	-	expression tag	UNP A0A509AJ88
C	757	SER	-	expression tag	UNP A0A509AJ88
C	758	SER	-	expression tag	UNP A0A509AJ88
C	759	GLY	-	expression tag	UNP A0A509AJ88
C	760	LEU	-	expression tag	UNP A0A509AJ88
C	761	VAL	-	expression tag	UNP A0A509AJ88
C	762	PRO	-	expression tag	UNP A0A509AJ88
C	763	ARG	-	expression tag	UNP A0A509AJ88
C	764	GLY	-	expression tag	UNP A0A509AJ88
C	765	SER	-	expression tag	UNP A0A509AJ88
C	766	HIS	-	expression tag	UNP A0A509AJ88
C	767	MET	-	expression tag	UNP A0A509AJ88
E	747	MET	-	initiating methionine	UNP A0A509AJ88
E	748	GLY	-	expression tag	UNP A0A509AJ88
E	749	SER	-	expression tag	UNP A0A509AJ88
E	750	SER	-	expression tag	UNP A0A509AJ88
E	751	HIS	-	expression tag	UNP A0A509AJ88
E	752	HIS	-	expression tag	UNP A0A509AJ88
E	753	HIS	-	expression tag	UNP A0A509AJ88
E	754	HIS	-	expression tag	UNP A0A509AJ88
E	755	HIS	-	expression tag	UNP A0A509AJ88
E	756	HIS	-	expression tag	UNP A0A509AJ88
E	757	SER	-	expression tag	UNP A0A509AJ88
E	758	SER	-	expression tag	UNP A0A509AJ88
E	759	GLY	-	expression tag	UNP A0A509AJ88
E	760	LEU	-	expression tag	UNP A0A509AJ88
E	761	VAL	-	expression tag	UNP A0A509AJ88
E	762	PRO	-	expression tag	UNP A0A509AJ88
E	763	ARG	-	expression tag	UNP A0A509AJ88

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	764	GLY	-	expression tag	UNP A0A509AJ88
E	765	SER	-	expression tag	UNP A0A509AJ88
E	766	HIS	-	expression tag	UNP A0A509AJ88
E	767	MET	-	expression tag	UNP A0A509AJ88
G	747	MET	-	initiating methionine	UNP A0A509AJ88
G	748	GLY	-	expression tag	UNP A0A509AJ88
G	749	SER	-	expression tag	UNP A0A509AJ88
G	750	SER	-	expression tag	UNP A0A509AJ88
G	751	HIS	-	expression tag	UNP A0A509AJ88
G	752	HIS	-	expression tag	UNP A0A509AJ88
G	753	HIS	-	expression tag	UNP A0A509AJ88
G	754	HIS	-	expression tag	UNP A0A509AJ88
G	755	HIS	-	expression tag	UNP A0A509AJ88
G	756	HIS	-	expression tag	UNP A0A509AJ88
G	757	SER	-	expression tag	UNP A0A509AJ88
G	758	SER	-	expression tag	UNP A0A509AJ88
G	759	GLY	-	expression tag	UNP A0A509AJ88
G	760	LEU	-	expression tag	UNP A0A509AJ88
G	761	VAL	-	expression tag	UNP A0A509AJ88
G	762	PRO	-	expression tag	UNP A0A509AJ88
G	763	ARG	-	expression tag	UNP A0A509AJ88
G	764	GLY	-	expression tag	UNP A0A509AJ88
G	765	SER	-	expression tag	UNP A0A509AJ88
G	766	HIS	-	expression tag	UNP A0A509AJ88
G	767	MET	-	expression tag	UNP A0A509AJ88
I	747	MET	-	initiating methionine	UNP A0A509AJ88
I	748	GLY	-	expression tag	UNP A0A509AJ88
I	749	SER	-	expression tag	UNP A0A509AJ88
I	750	SER	-	expression tag	UNP A0A509AJ88
I	751	HIS	-	expression tag	UNP A0A509AJ88
I	752	HIS	-	expression tag	UNP A0A509AJ88
I	753	HIS	-	expression tag	UNP A0A509AJ88
I	754	HIS	-	expression tag	UNP A0A509AJ88
I	755	HIS	-	expression tag	UNP A0A509AJ88
I	756	HIS	-	expression tag	UNP A0A509AJ88
I	757	SER	-	expression tag	UNP A0A509AJ88
I	758	SER	-	expression tag	UNP A0A509AJ88
I	759	GLY	-	expression tag	UNP A0A509AJ88
I	760	LEU	-	expression tag	UNP A0A509AJ88
I	761	VAL	-	expression tag	UNP A0A509AJ88
I	762	PRO	-	expression tag	UNP A0A509AJ88
I	763	ARG	-	expression tag	UNP A0A509AJ88

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
I	764	GLY	-	expression tag	UNP A0A509AJ88
I	765	SER	-	expression tag	UNP A0A509AJ88
I	766	HIS	-	expression tag	UNP A0A509AJ88
I	767	MET	-	expression tag	UNP A0A509AJ88
K	747	MET	-	initiating methionine	UNP A0A509AJ88
K	748	GLY	-	expression tag	UNP A0A509AJ88
K	749	SER	-	expression tag	UNP A0A509AJ88
K	750	SER	-	expression tag	UNP A0A509AJ88
K	751	HIS	-	expression tag	UNP A0A509AJ88
K	752	HIS	-	expression tag	UNP A0A509AJ88
K	753	HIS	-	expression tag	UNP A0A509AJ88
K	754	HIS	-	expression tag	UNP A0A509AJ88
K	755	HIS	-	expression tag	UNP A0A509AJ88
K	756	HIS	-	expression tag	UNP A0A509AJ88
K	757	SER	-	expression tag	UNP A0A509AJ88
K	758	SER	-	expression tag	UNP A0A509AJ88
K	759	GLY	-	expression tag	UNP A0A509AJ88
K	760	LEU	-	expression tag	UNP A0A509AJ88
K	761	VAL	-	expression tag	UNP A0A509AJ88
K	762	PRO	-	expression tag	UNP A0A509AJ88
K	763	ARG	-	expression tag	UNP A0A509AJ88
K	764	GLY	-	expression tag	UNP A0A509AJ88
K	765	SER	-	expression tag	UNP A0A509AJ88
K	766	HIS	-	expression tag	UNP A0A509AJ88
K	767	MET	-	expression tag	UNP A0A509AJ88

- Molecule 2 is a protein called Oocyst rupture protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	102	Total	C	N	O	S	0	0	0
			841	536	143	156	6			
2	D	106	Total	C	N	O	S	0	0	0
			877	559	149	163	6			
2	F	103	Total	C	N	O	S	0	0	0
			852	542	144	160	6			
2	H	100	Total	C	N	O	S	0	0	0
			827	529	140	152	6			
2	J	103	Total	C	N	O	S	0	0	0
			854	544	145	159	6			
2	L	75	Total	C	N	O	S	0	0	0
			620	400	104	111	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	L	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	C	O	0	0
			4	2	2		

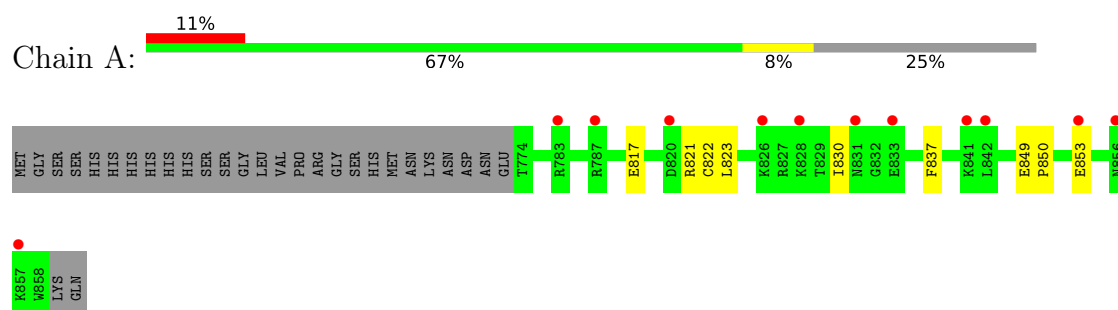
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	2	Total	O	0	0
			2	2		
5	D	2	Total	O	0	0
			2	2		
5	F	6	Total	O	0	0
			6	6		
5	H	2	Total	O	0	0
			2	2		
5	J	4	Total	O	0	0
			4	4		

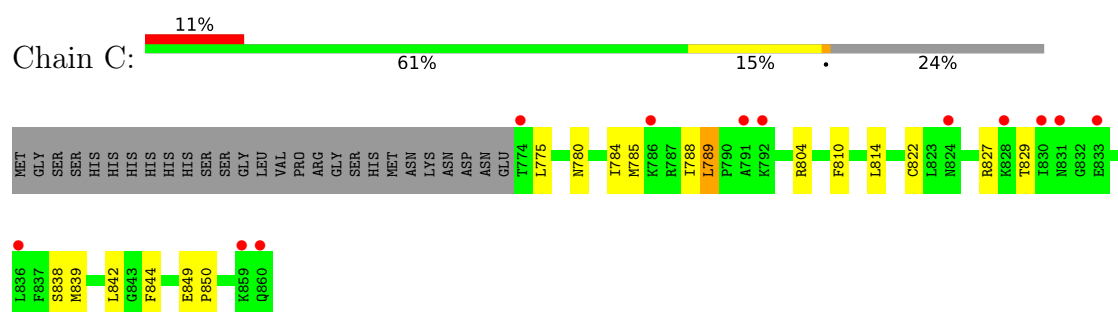
3 Residue-property plots [i](#)

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.

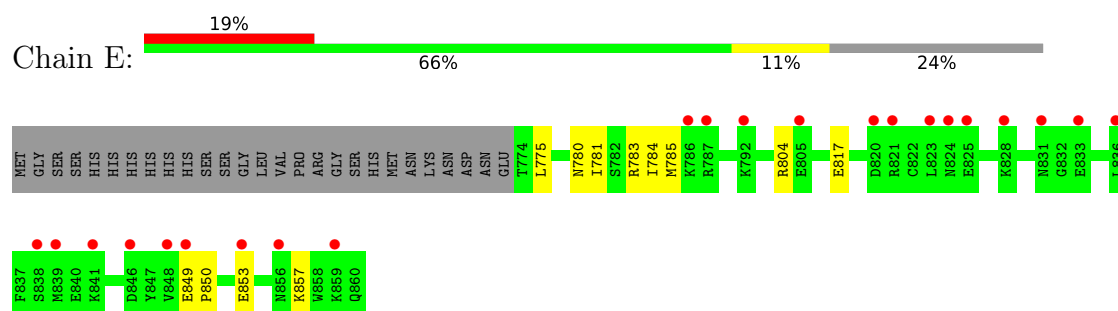
• Molecule 1: Oocyst rupture protein 1



• Molecule 1: Oocyst rupture protein 1

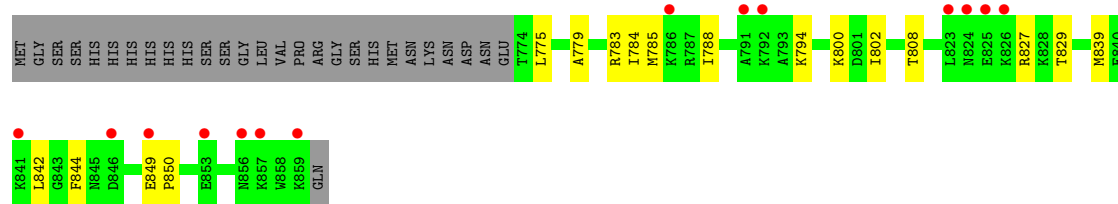


• Molecule 1: Oocyst rupture protein 1

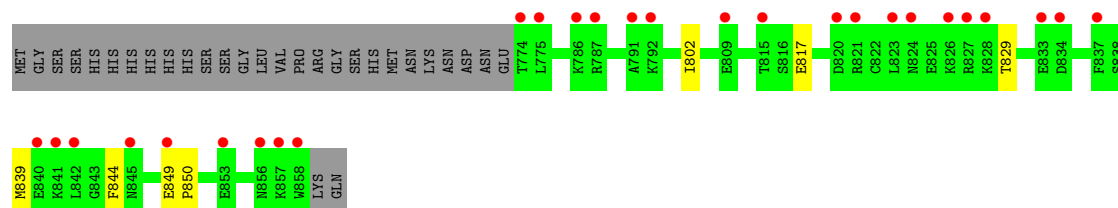


• Molecule 1: Oocyst rupture protein 1

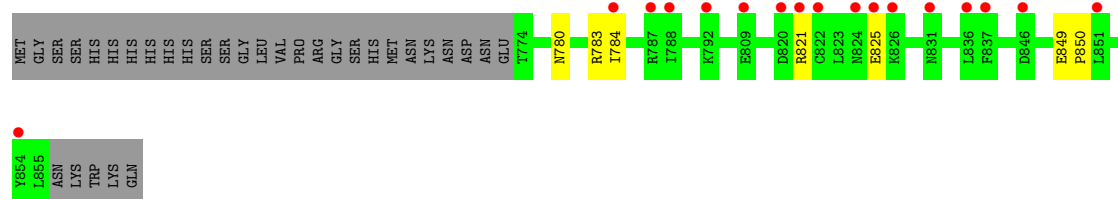




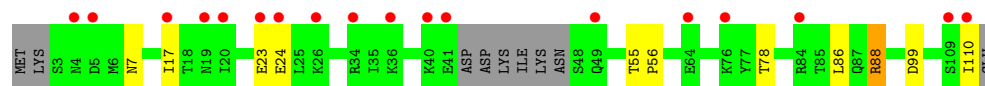
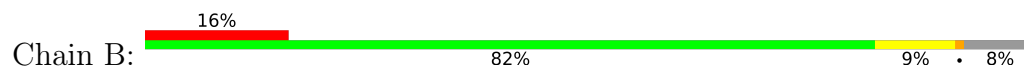
• Molecule 1: Oocyst rupture protein 1



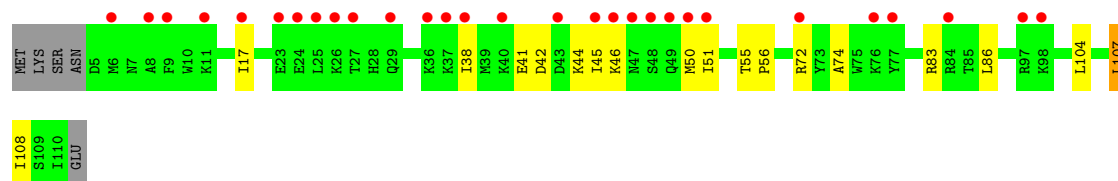
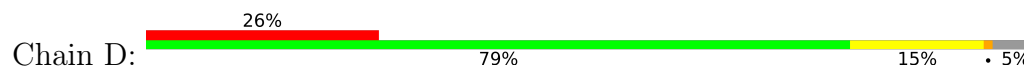
• Molecule 1: Oocyst rupture protein 1



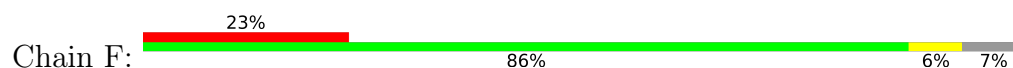
• Molecule 2: Oocyst rupture protein 2

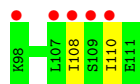


• Molecule 2: Oocyst rupture protein 2



• Molecule 2: Oocyst rupture protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.67Å 112.92Å 145.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.70 – 3.10 66.70 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (66.70-3.10) 99.7 (66.70-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 3.13Å)	Xtriage
Refinement program	PHENIX (1.21.2_5419)	Depositor
R, R_{free}	0.274 , 0.295 0.276 , 0.294	Depositor DCC
R_{free} test set	1196 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å ²)	92.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 151.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9120	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, 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	0.25	0/708	0.52	0/951
1	C	0.34	0/727	0.60	0/974
1	E	0.25	0/727	0.49	0/974
1	G	0.30	0/717	0.54	0/962
1	I	0.33	0/708	0.55	0/951
1	K	0.24	0/675	0.54	0/906
2	B	0.32	0/854	0.51	0/1148
2	D	0.45	0/891	0.61	0/1198
2	F	0.24	0/865	0.46	0/1163
2	H	0.26	0/840	0.48	0/1129
2	J	0.23	0/867	0.48	0/1165
2	L	0.28	0/628	0.47	0/841
All	All	0.30	0/9207	0.52	0/12362

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	697	0	720	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	716	0	741	13	0
1	E	716	0	741	14	0
1	G	706	0	733	13	0
1	I	697	0	720	6	0
1	K	666	0	691	3	0
2	B	841	0	855	8	0
2	D	877	0	896	14	0
2	F	852	0	860	32	0
2	H	827	0	844	10	0
2	J	854	0	866	9	0
2	L	620	0	647	5	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	I	5	0	0	0	0
3	L	5	0	0	1	0
4	L	4	0	6	1	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	D	2	0	0	0	0
5	F	6	0	0	0	0
5	H	2	0	0	0	0
5	J	4	0	0	1	0
All	All	9120	0	9320	103	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 6.

All (103) 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:823:LEU:HD11	2:F:24:GLU:CG	1.84	1.06
2:F:110:ILE:HD12	1:G:802:ILE:HD13	1.33	1.04
1:A:823:LEU:HD11	2:F:24:GLU:HG2	1.40	1.03
1:E:850:PRO:HA	2:F:17:ILE:HD11	1.51	0.93
1:C:788:ILE:HG13	2:D:72:ARG:HD3	1.55	0.89
2:F:110:ILE:HD11	2:H:92:ILE:HG12	1.54	0.88
1:A:823:LEU:HD11	2:F:24:GLU:HG3	1.58	0.85
1:A:823:LEU:HD21	2:F:24:GLU:HG2	1.57	0.82
1:C:822:CYS:SG	1:C:827:ARG:HB2	2.20	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:823:LEU:CD1	2:F:24:GLU:HG2	2.11	0.79
1:C:827:ARG:HB3	3:C:901:SO4:O4	1.86	0.76
2:F:110:ILE:HD11	2:H:92:ILE:CG1	2.23	0.68
1:A:823:LEU:CD2	2:F:24:GLU:HG2	2.24	0.67
1:E:850:PRO:HA	2:F:17:ILE:CD1	2.26	0.65
1:C:788:ILE:CG1	2:D:72:ARG:HD3	2.27	0.65
2:D:55:THR:OG1	2:D:56:PRO:HD3	1.96	0.64
1:C:829:THR:HA	2:D:50:MET:O	1.98	0.64
1:E:850:PRO:O	2:F:17:ILE:HD12	2.00	0.61
2:D:42:ASP:C	2:D:44:LYS:H	2.08	0.61
1:E:850:PRO:CA	2:F:17:ILE:HD11	2.26	0.61
2:F:110:ILE:HG22	2:F:110:ILE:O	1.99	0.61
2:F:110:ILE:HG23	2:H:107:LEU:CD1	2.32	0.59
1:A:822:CYS:SG	1:A:830:ILE:HA	2.42	0.58
1:E:850:PRO:CA	2:F:17:ILE:CD1	2.84	0.56
1:I:802:ILE:HD11	2:J:88:ARG:HG2	1.87	0.55
1:C:810:PHE:CZ	1:C:814:LEU:HD11	2.43	0.54
2:F:110:ILE:HG23	2:H:107:LEU:HD11	1.90	0.54
1:E:850:PRO:O	2:F:17:ILE:CD1	2.55	0.54
1:A:817:GLU:OE1	1:E:783:ARG:NH2	2.41	0.53
2:F:17:ILE:HA	2:F:20:ILE:HD11	1.90	0.53
1:C:780:ASN:O	1:C:784:ILE:HG12	2.08	0.53
2:L:84:ARG:N	3:L:201:SO4:O2	2.39	0.52
1:C:849:GLU:HB3	1:C:850:PRO:HD3	1.93	0.51
2:F:110:ILE:HG12	2:H:108:ILE:HG12	1.92	0.51
1:G:775:LEU:HD23	1:G:808:THR:HG21	1.90	0.51
1:E:849:GLU:HB3	1:E:850:PRO:HD3	1.93	0.51
1:A:823:LEU:CG	2:F:24:GLU:HG2	2.39	0.51
2:B:99:ASP:OD2	2:D:83:ARG:NH1	2.45	0.50
1:C:838:SER:O	1:C:842:LEU:HD23	2.11	0.50
2:B:55:THR:HB	2:B:56:PRO:HD3	1.95	0.49
2:F:17:ILE:O	2:F:20:ILE:HD12	2.12	0.48
1:I:850:PRO:HA	2:J:17:ILE:HD11	1.96	0.47
2:J:64:GLU:OE2	5:J:201:HOH:O	2.20	0.47
1:E:853:GLU:O	1:E:857:LYS:HD3	2.15	0.47
2:B:88:ARG:NH2	2:D:108:ILE:O	2.43	0.47
2:J:92:ILE:HG12	2:L:110:ILE:HD11	1.96	0.47
1:E:775:LEU:HD12	1:E:804:ARG:HG2	1.97	0.46
2:F:17:ILE:HA	2:F:20:ILE:CG1	2.46	0.46
2:F:110:ILE:CD1	1:G:802:ILE:HG21	2.46	0.46
1:A:822:CYS:SG	1:A:830:ILE:HG13	2.56	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:780:ASN:O	1:E:784:ILE:HG12	2.16	0.45
2:F:20:ILE:CG2	2:F:25:LEU:HG	2.45	0.45
2:J:55:THR:HB	2:J:56:PRO:HD3	1.98	0.45
1:C:814:LEU:HD13	1:C:839:MET:HE1	1.97	0.45
2:F:17:ILE:O	2:F:20:ILE:CD1	2.65	0.45
2:H:83:ARG:NH2	2:H:90:ASP:OD2	2.49	0.45
2:D:42:ASP:C	2:D:44:LYS:N	2.74	0.45
1:C:839:MET:HG3	1:C:844:PHE:HB2	1.98	0.45
1:G:779:ALA:O	1:G:783:ARG:HG2	2.17	0.45
1:C:785:MET:O	1:C:789:LEU:HD22	2.16	0.45
1:G:849:GLU:HB3	1:G:850:PRO:HD3	1.99	0.45
2:H:17:ILE:C	2:H:17:ILE:HD12	2.42	0.44
2:D:45:ILE:O	2:D:46:LYS:C	2.61	0.43
2:H:64:GLU:HG2	2:H:68:MET:HE2	2.01	0.43
2:F:20:ILE:HG22	2:F:25:LEU:HG	2.00	0.43
2:D:38:ILE:O	2:D:41:GLU:HG2	2.19	0.43
2:F:17:ILE:HA	2:F:20:ILE:HG13	2.01	0.43
1:K:849:GLU:HB2	1:K:850:PRO:HD3	1.99	0.43
1:A:821:ARG:HD2	1:A:837:PHE:CD2	2.54	0.43
2:J:74:ALA:CB	2:J:86:LEU:HD11	2.49	0.43
2:B:78:THR:OG1	2:B:86:LEU:HD12	2.20	0.42
1:G:785:MET:HE1	1:G:800:LYS:HA	2.01	0.42
1:G:827:ARG:HG3	1:G:829:THR:H	1.84	0.42
1:I:849:GLU:HB3	1:I:850:PRO:HD3	1.99	0.42
2:F:17:ILE:HA	2:F:20:ILE:CD1	2.48	0.42
2:B:17:ILE:HD12	2:B:17:ILE:C	2.44	0.42
1:G:788:ILE:O	1:G:788:ILE:HG13	2.19	0.42
1:G:839:MET:HE2	1:G:844:PHE:HB2	2.01	0.42
1:A:849:GLU:HB3	1:A:850:PRO:HD3	2.02	0.42
1:C:775:LEU:HD13	1:C:804:ARG:HD3	2.00	0.42
1:E:817:GLU:HA	1:K:783:ARG:HH22	1.85	0.42
1:G:783:ARG:HH22	1:I:817:GLU:HA	1.85	0.42
1:I:839:MET:HE2	1:I:844:PHE:CB	2.50	0.42
1:K:780:ASN:O	1:K:784:ILE:HG12	2.20	0.41
2:L:55:THR:OG1	2:L:56:PRO:HD3	2.19	0.41
2:D:104:LEU:HA	2:D:107:LEU:HD21	2.01	0.41
2:F:17:ILE:CA	2:F:20:ILE:HD11	2.50	0.41
1:I:829:THR:HG22	2:J:50:MET:HB2	2.01	0.41
2:D:17:ILE:C	2:D:17:ILE:HD12	2.46	0.41
2:D:74:ALA:HB3	2:D:86:LEU:HD11	2.02	0.41
2:J:108:ILE:HG23	2:L:108:ILE:HG23	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:31:PRO:O	2:L:35:ILE:HG12	2.20	0.41
1:G:784:ILE:HD11	2:H:29:GLN:HB3	2.02	0.41
2:B:23:GLU:O	2:B:24:GLU:C	2.64	0.41
2:B:55:THR:HB	2:B:56:PRO:CD	2.51	0.41
1:A:853:GLU:HB2	2:B:17:ILE:HD13	2.03	0.41
2:D:104:LEU:HA	2:D:107:LEU:CD2	2.51	0.41
1:G:794:LYS:HB3	4:L:202:EDO:H22	2.03	0.41
1:E:781:ILE:CG2	1:E:785:MET:HE2	2.51	0.40
2:J:78:THR:OG1	2:J:86:LEU:HD12	2.21	0.40
1:E:850:PRO:HB3	2:F:17:ILE:HD13	2.02	0.40
2:F:78:THR:OG1	2:F:86:LEU:HD12	2.22	0.40
1:G:794:LYS:HB2	2:H:85:THR:HG22	2.03	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	83/114 (73%)	82 (99%)	1 (1%)	0	100	100
1	C	85/114 (75%)	83 (98%)	2 (2%)	0	100	100
1	E	85/114 (75%)	84 (99%)	1 (1%)	0	100	100
1	G	84/114 (74%)	84 (100%)	0	0	100	100
1	I	83/114 (73%)	81 (98%)	2 (2%)	0	100	100
1	K	80/114 (70%)	75 (94%)	5 (6%)	0	100	100
2	B	98/111 (88%)	93 (95%)	5 (5%)	0	100	100
2	D	104/111 (94%)	97 (93%)	7 (7%)	0	100	100
2	F	99/111 (89%)	94 (95%)	5 (5%)	0	100	100
2	H	96/111 (86%)	95 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	99/111 (89%)	95 (96%)	4 (4%)	0	100	100
2	L	71/111 (64%)	68 (96%)	3 (4%)	0	100	100
All	All	1067/1350 (79%)	1031 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	78/104 (75%)	78 (100%)	0	100	100
1	C	80/104 (77%)	79 (99%)	1 (1%)	61	77
1	E	80/104 (77%)	80 (100%)	0	100	100
1	G	79/104 (76%)	78 (99%)	1 (1%)	61	77
1	I	78/104 (75%)	78 (100%)	0	100	100
1	K	75/104 (72%)	73 (97%)	2 (3%)	39	67
2	B	94/103 (91%)	91 (97%)	3 (3%)	34	64
2	D	98/103 (95%)	96 (98%)	2 (2%)	48	72
2	F	95/103 (92%)	95 (100%)	0	100	100
2	H	92/103 (89%)	91 (99%)	1 (1%)	65	78
2	J	95/103 (92%)	95 (100%)	0	100	100
2	L	68/103 (66%)	65 (96%)	3 (4%)	25	56
All	All	1012/1242 (82%)	999 (99%)	13 (1%)	61	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	7	ASN
2	B	88	ARG
2	B	110	ILE
1	C	789	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	51	ILE
2	D	107	LEU
1	G	842	LEU
2	H	70	PHE
1	K	821	ARG
1	K	825	GLU
2	L	54	ASP
2	L	88	ARG
2	L	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	87	GLN
2	F	28	HIS
2	F	87	GLN
2	L	89	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](#)

7 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	$\# Z > 2$
3	SO4	D	201	-	4,4,4	0.25	0	6,6,6	0.10	0
3	SO4	A	901	-	4,4,4	0.30	0	6,6,6	0.09	0
3	SO4	B	201	-	4,4,4	0.24	0	6,6,6	0.05	0
4	EDO	L	202	-	3,3,3	0.44	0	2,2,2	0.54	0
3	SO4	I	901	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	C	901	-	4,4,4	0.30	0	6,6,6	0.08	0
3	SO4	L	201	-	4,4,4	0.23	0	6,6,6	0.12	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
4	EDO	L	202	-	-	0/1/1/1	-

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
4	L	202	EDO	1	0
3	C	901	SO4	1	0
3	L	201	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	85/114 (74%)	0.92	12 (14%) 6 3	41, 63, 92, 116	19 (22%)
1	C	87/114 (76%)	1.06	12 (13%) 6 4	37, 64, 95, 132	14 (16%)
1	E	87/114 (76%)	1.32	22 (25%) 1 1	37, 67, 103, 114	19 (21%)
1	G	86/114 (75%)	1.02	14 (16%) 4 2	36, 64, 89, 99	17 (19%)
1	I	85/114 (74%)	1.40	27 (31%) 1 0	36, 63, 88, 99	22 (25%)
1	K	82/114 (71%)	1.36	17 (20%) 2 1	41, 75, 103, 126	17 (20%)
2	B	102/111 (91%)	1.10	18 (17%) 4 2	32, 66, 109, 130	19 (18%)
2	D	106/111 (95%)	1.58	29 (27%) 1 1	32, 65, 108, 172	25 (23%)
2	F	103/111 (92%)	1.37	25 (24%) 2 1	29, 64, 95, 108	26 (25%)
2	H	100/111 (90%)	1.29	20 (20%) 3 1	35, 66, 103, 113	19 (19%)
2	J	103/111 (92%)	1.26	19 (18%) 3 1	32, 70, 117, 189	12 (11%)
2	L	75/111 (67%)	1.06	11 (14%) 6 3	34, 72, 117, 155	5 (6%)
All	All	1101/1350 (81%)	1.24	226 (20%) 2 1	29, 66, 106, 189	214 (19%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	48	SER	9.6
1	K	837	PHE	8.0
1	K	821	ARG	7.7
1	I	837	PHE	7.3
1	C	831	ASN	6.7
2	J	40	LYS	6.6
2	F	97	ARG	6.5
1	C	830	ILE	6.4
1	I	815	THR	6.2
1	I	827	ARG	6.2
1	A	853	GLU	6.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	H	79	GLU	5.9
2	H	82	LYS	5.8
2	D	23	GLU	5.7
2	F	111	GLU	5.7
2	F	5	ASP	5.7
2	F	23	GLU	5.6
2	B	19	ASN	5.6
2	D	40	LYS	5.4
1	K	825	GLU	5.3
1	I	786	LYS	5.3
1	E	853	GLU	5.2
2	D	36	LYS	5.1
2	J	26	LYS	5.1
2	J	44	LYS	5.0
1	I	856	ASN	5.0
2	D	29	GLN	5.0
1	E	841	LYS	5.0
2	F	109	SER	4.9
1	C	833	GLU	4.8
2	H	23	GLU	4.8
1	E	831	ASN	4.7
1	E	825	GLU	4.7
2	B	24	GLU	4.7
2	B	76	LYS	4.7
1	I	833	GLU	4.6
1	E	786	LYS	4.6
2	J	41	GLU	4.6
2	H	49	GLN	4.5
2	H	98	LYS	4.5
1	A	857	LYS	4.5
1	G	792	LYS	4.5
2	H	84	ARG	4.5
1	E	833	GLU	4.4
2	D	26	LYS	4.4
2	F	42	ASP	4.4
2	L	72	ARG	4.4
2	F	36	LYS	4.4
2	L	110	ILE	4.3
2	D	45	ILE	4.3
1	C	860	GLN	4.3
2	F	3	SER	4.3
1	G	786	LYS	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	77	TYR	4.2
1	I	845	ASN	4.1
1	I	824	ASN	4.1
2	D	47	ASN	4.1
1	K	826	LYS	4.0
1	G	853	GLU	4.0
1	E	792	LYS	4.0
1	C	824	ASN	4.0
1	G	849	GLU	4.0
2	D	24	GLU	4.0
2	B	23	GLU	4.0
2	F	50	MET	3.9
1	I	792	LYS	3.9
2	D	25	LEU	3.9
2	D	43	ASP	3.9
2	B	36	LYS	3.9
2	F	11	LYS	3.9
2	L	41	GLU	3.9
1	E	821	ARG	3.8
2	H	48	SER	3.8
2	L	76	LYS	3.8
2	F	19	ASN	3.8
2	D	98	LYS	3.7
2	D	50	MET	3.7
2	J	11	LYS	3.7
2	J	82	LYS	3.7
1	I	840	GLU	3.7
1	G	791	ALA	3.7
2	B	49	GLN	3.7
1	I	841	LYS	3.7
2	B	64	GLU	3.6
2	J	23	GLU	3.6
2	H	72	ARG	3.6
1	E	856	ASN	3.6
2	F	4	ASN	3.6
1	E	859	LYS	3.6
1	I	849	GLU	3.6
2	D	9	PHE	3.5
1	C	786	LYS	3.5
2	B	26	LYS	3.5
2	H	26	LYS	3.5
1	A	828	LYS	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	823	LEU	3.5
1	E	828	LYS	3.5
2	B	40	LYS	3.5
1	C	791	ALA	3.5
2	D	11	LYS	3.4
1	G	826	LYS	3.4
2	D	6	MET	3.4
2	B	17	ILE	3.4
2	L	109	SER	3.4
2	H	25	LEU	3.3
2	F	15	ASP	3.3
2	B	4	ASN	3.3
1	K	836	LEU	3.3
1	I	853	GLU	3.3
1	K	831	ASN	3.2
2	B	34	ARG	3.2
1	K	851	LEU	3.2
2	H	19	ASN	3.1
1	I	828	LYS	3.1
2	D	76	LYS	3.1
1	A	787	ARG	3.1
1	K	788	ILE	3.1
2	H	11	LYS	3.1
2	L	108	ILE	3.1
2	L	42	ASP	3.1
1	A	833	GLU	3.0
2	D	46	LYS	3.0
1	E	849	GLU	2.9
1	I	820	ASP	2.9
2	J	19	ASN	2.9
1	E	787	ARG	2.9
2	D	49	GLN	2.9
2	L	98	LYS	2.9
2	H	17	ILE	2.9
2	F	49	GLN	2.9
2	L	81	ASN	2.9
1	E	823	LEU	2.9
1	K	792	LYS	2.9
1	E	824	ASN	2.8
2	D	84	ARG	2.8
1	E	820	ASP	2.8
2	D	97	ARG	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	55	THR	2.8
1	G	859	LYS	2.8
2	B	109	SER	2.8
1	C	774	THR	2.8
2	H	41	GLU	2.8
1	K	846	ASP	2.8
1	A	831	ASN	2.8
1	I	809	GLU	2.8
2	F	110	ILE	2.8
2	J	20	ILE	2.8
1	I	821	ARG	2.7
1	G	857	LYS	2.7
1	C	859	LYS	2.7
1	K	824	ASN	2.7
2	H	37	LYS	2.7
1	I	826	LYS	2.7
2	B	5	ASP	2.7
2	B	110	ILE	2.7
2	J	50	MET	2.7
1	I	858	TRP	2.7
2	D	51	ILE	2.6
1	K	787	ARG	2.6
2	D	72	ARG	2.6
2	D	8	ALA	2.6
1	A	820	ASP	2.6
2	F	40	LYS	2.6
2	F	77	TYR	2.6
1	A	826	LYS	2.6
1	G	841	LYS	2.6
2	H	20	ILE	2.6
2	H	18	THR	2.6
2	J	108	ILE	2.6
2	H	50	MET	2.6
2	J	18	THR	2.6
2	H	51	ILE	2.6
2	F	21	SER	2.5
1	C	792	LYS	2.5
2	F	37	LYS	2.5
1	C	836	LEU	2.5
1	E	805	GLU	2.4
1	I	857	LYS	2.4
1	A	841	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	16	ASP	2.4
2	D	37	LYS	2.4
2	J	13	GLN	2.4
2	D	27	THR	2.4
1	I	774	THR	2.3
1	E	846	ASP	2.3
2	B	84	ARG	2.3
2	B	41	GLU	2.3
1	K	822	CYS	2.3
1	I	775	LEU	2.3
2	F	41	GLU	2.3
1	C	828	LYS	2.3
2	F	76	LYS	2.3
1	K	820	ASP	2.3
2	D	17	ILE	2.3
1	I	791	ALA	2.3
1	K	854	TYR	2.3
1	A	856	ASN	2.3
1	I	834	ASP	2.3
2	H	80	GLU	2.2
2	F	78	THR	2.2
1	G	856	ASN	2.2
2	L	107	LEU	2.2
1	G	825	GLU	2.2
2	J	32	ILE	2.2
1	E	848	VAL	2.2
2	J	25	LEU	2.2
2	J	43	ASP	2.2
1	K	784	ILE	2.1
2	B	20	ILE	2.1
2	D	38	ILE	2.1
1	I	842	LEU	2.1
2	L	50	MET	2.1
1	E	838	SER	2.1
1	A	783	ARG	2.1
1	E	839	MET	2.1
1	G	824	ASN	2.1
1	A	842	LEU	2.1
2	J	73	TYR	2.1
1	G	846	ASP	2.1
2	J	49	GLN	2.1
1	K	809	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	31	PRO	2.1
1	G	823	LEU	2.0
1	E	836	LEU	2.0
1	I	787	ARG	2.0
2	F	51	ILE	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
3	SO4	C	901	5/5	0.74	0.09	111,121,128,137	0
3	SO4	I	901	5/5	0.74	0.12	125,125,125,125	0
3	SO4	A	901	5/5	0.84	0.13	114,121,128,137	0
3	SO4	L	201	5/5	0.89	0.18	82,84,90,101	0
3	SO4	D	201	5/5	0.93	0.12	76,76,81,88	0
4	EDO	L	202	4/4	0.94	0.16	65,67,67,72	0
3	SO4	B	201	5/5	0.95	0.09	69,73,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.