



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 10:59 PM UTC

PDB ID : 4XKU / pdb_00004xku
Title : E coli BFR variant Y114F
Authors : Hemmings, A.M.; Le Brun, N.E.; Bradley, J.M.
Deposited on : 2015-01-12
Resolution : 1.78 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

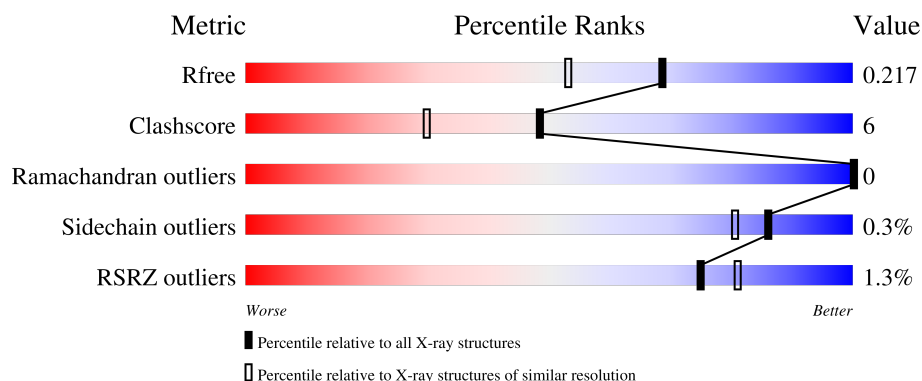
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	158	2% 88% 12%
1	B	158	% 85% 15%
1	C	158	% 93% 7%
1	D	158	% 84% 16%
1	E	158	% 90% 9%

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Mol	Chain	Length	Quality of chain
1	F	158	91% 9%
1	G	158	89% 10%
1	H	158	93% 6%
1	I	158	92% 8%
1	J	158	91% 9%
1	K	158	85% 15%
1	L	158	87% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19042 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 Bacterioferritin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	8	1
			1333	842	226	256	9			
1	B	158	Total	C	N	O	S	0	10	1
			1345	853	226	257	9			
1	C	158	Total	C	N	O	S	0	7	1
			1330	842	225	256	7			
1	D	158	Total	C	N	O	S	0	8	1
			1328	840	223	256	9			
1	E	158	Total	C	N	O	S	0	7	1
			1331	842	225	255	9			
1	F	158	Total	C	N	O	S	0	8	1
			1337	844	231	254	8			
1	G	158	Total	C	N	O	S	0	7	1
			1325	838	224	254	9			
1	H	158	Total	C	N	O	S	0	7	1
			1321	833	225	256	7			
1	I	158	Total	C	N	O	S	0	9	1
			1337	843	226	260	8			
1	J	158	Total	C	N	O	S	0	7	1
			1329	841	228	252	8			
1	K	158	Total	C	N	O	S	0	7	1
			1322	836	222	255	9			
1	L	158	Total	C	N	O	S	0	10	1
			1342	850	228	255	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	114	PHE	TYR	engineered mutation	UNP P0ABD3
B	114	PHE	TYR	engineered mutation	UNP P0ABD3
C	114	PHE	TYR	engineered mutation	UNP P0ABD3
D	114	PHE	TYR	engineered mutation	UNP P0ABD3
E	114	PHE	TYR	engineered mutation	UNP P0ABD3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	114	PHE	TYR	engineered mutation	UNP P0ABD3
G	114	PHE	TYR	engineered mutation	UNP P0ABD3
H	114	PHE	TYR	engineered mutation	UNP P0ABD3
I	114	PHE	TYR	engineered mutation	UNP P0ABD3
J	114	PHE	TYR	engineered mutation	UNP P0ABD3
K	114	PHE	TYR	engineered mutation	UNP P0ABD3
L	114	PHE	TYR	engineered mutation	UNP P0ABD3

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

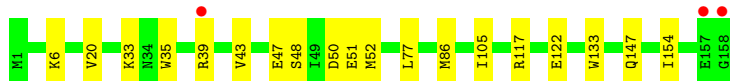
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	243	Total	O	0	0
			243	243		
3	C	234	Total	O	0	0
			234	234		
3	D	231	Total	O	0	0
			231	231		
3	E	271	Total	O	0	0
			271	271		
3	F	273	Total	O	0	0
			273	273		
3	G	255	Total	O	0	0
			255	255		
3	H	259	Total	O	0	0
			259	259		
3	I	241	Total	O	0	0
			241	241		
3	J	260	Total	O	0	0
			260	260		
3	K	243	Total	O	0	0
			243	243		
3	L	243	Total	O	0	0
			243	243		

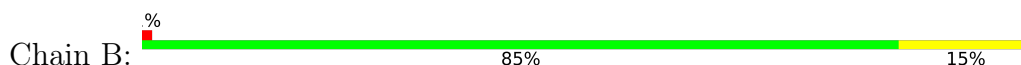
3 Residue-property plots [i](#)

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: Bacterioferritin



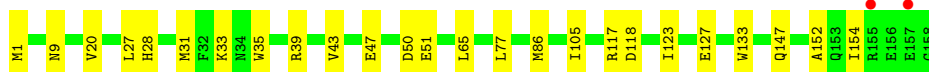
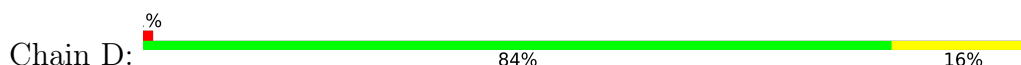
- Molecule 1: Bacterioferritin



- Molecule 1: Bacterioferritin



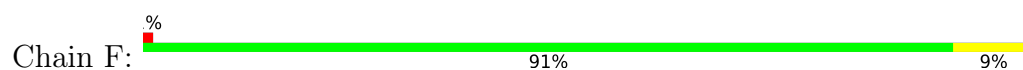
- Molecule 1: Bacterioferritin



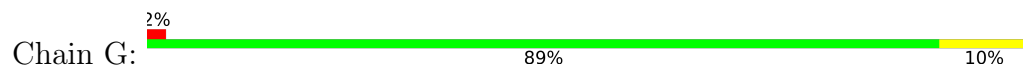
- Molecule 1: Bacterioferritin



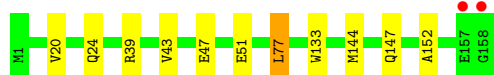
- Molecule 1: Bacterioferritin



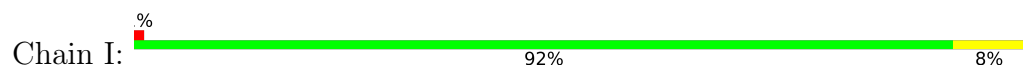
• Molecule 1: Bacterioferritin



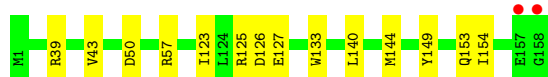
• Molecule 1: Bacterioferritin



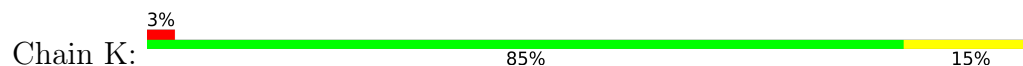
• Molecule 1: Bacterioferritin



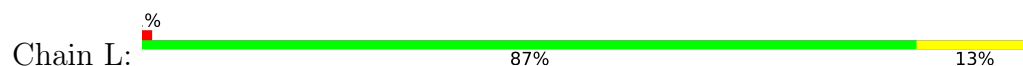
• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



• Molecule 1: Bacterioferritin



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.56Å 207.56Å 142.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	102.27 – 1.78 102.27 – 1.78	Depositor EDS
% Data completeness (in resolution range)	95.9 (102.27-1.78) 96.2 (102.27-1.78)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.188 , 0.217 0.188 , 0.217	Depositor DCC
R_{free} test set	14159 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	14.9	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19042	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1847e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.36	0/1375	0.64	0/1850
1	B	0.36	0/1396	0.62	0/1878
1	C	0.38	0/1369	0.63	0/1843
1	D	0.38	0/1372	0.62	0/1846
1	E	0.37	0/1372	0.63	0/1844
1	F	0.37	0/1378	0.62	0/1854
1	G	0.37	0/1363	0.62	0/1834
1	H	0.37	0/1363	0.63	0/1837
1	I	0.36	0/1381	0.61	0/1859
1	J	0.38	0/1371	0.66	0/1842
1	K	0.38	0/1362	0.65	0/1833
1	L	0.36	0/1393	0.62	0/1872
All	All	0.37	0/16495	0.63	0/22192

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	1333	0	1310	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1345	0	1332	21	0
1	C	1330	0	1303	10	0
1	D	1328	0	1306	21	0
1	E	1331	0	1319	13	0
1	F	1337	0	1320	15	0
1	G	1325	0	1304	15	0
1	H	1321	0	1287	9	0
1	I	1337	0	1311	15	0
1	J	1329	0	1317	12	0
1	K	1322	0	1306	19	0
1	L	1342	0	1339	18	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	D	5	0	0	0	0
2	E	15	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	15	0	0	0	0
2	K	5	0	0	1	0
2	L	10	0	0	0	0
3	A	234	0	0	7	1
3	B	243	0	0	6	0
3	C	234	0	0	2	1
3	D	231	0	0	5	0
3	E	271	0	0	1	2
3	F	273	0	0	8	0
3	G	255	0	0	5	2
3	H	259	0	0	4	0
3	I	241	0	0	2	1
3	J	260	0	0	6	0
3	K	243	0	0	3	1
3	L	243	0	0	3	0
All	All	19042	0	15754	176	4

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 (176) 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:I:73:ASP:O	3:I:201:HOH:O	1.97	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:50[B]:ASP:OD1	3:L:301:HOH:O	2.03	0.76
3:A:530:HOH:O	1:B:31[B]:MET:SD	2.41	0.76
1:K:27:LEU:HG	1:K:31[B]:MET:HE2	1.68	0.75
1:A:35:TRP:HH2	1:A:86[B]:MET:HE1	1.54	0.73
1:G:158:GLY:N	3:G:302:HOH:O	2.22	0.71
1:F:39[B]:ARG:NH2	3:F:301:HOH:O	2.23	0.70
1:H:39:ARG:NH2	3:H:401:HOH:O	2.24	0.69
1:I:27:LEU:HG	1:I:31[B]:MET:HE2	1.74	0.69
1:H:20:VAL:HG13	1:H:77:LEU:HD22	1.74	0.69
1:I:31[B]:MET:SD	3:J:457:HOH:O	2.48	0.69
1:E:27:LEU:HG	1:E:31[B]:MET:HE2	1.76	0.67
1:L:35:TRP:HH2	1:L:86[B]:MET:HE1	1.59	0.66
1:D:39:ARG:NH2	3:D:304:HOH:O	2.28	0.66
1:K:38:LYS:NZ	1:K:154:ILE:O	2.26	0.66
1:B:27:LEU:HG	1:B:31[B]:MET:HE2	1.78	0.65
1:A:35:TRP:CH2	1:A:86[B]:MET:HE1	2.31	0.65
1:G:20:VAL:HG13	1:G:77:LEU:HD22	1.78	0.65
1:B:50[A]:ASP:OD1	3:B:301:HOH:O	2.14	0.65
1:G:27:LEU:HG	1:G:31[B]:MET:HE2	1.78	0.65
1:F:6:LYS:NZ	3:F:302:HOH:O	2.30	0.64
1:D:147:GLN:NE2	3:D:302:HOH:O	2.17	0.64
2:K:201:SO4:O2	3:K:301:HOH:O	2.14	0.64
1:E:31[B]:MET:SD	3:F:567:HOH:O	2.45	0.64
1:D:33:LYS:NZ	3:D:305:HOH:O	2.30	0.64
1:L:35:TRP:CH2	1:L:86[B]:MET:HE1	2.34	0.62
1:L:27:LEU:HG	1:L:31[B]:MET:HE2	1.82	0.62
1:G:31[B]:MET:HE3	1:G:86:MET:HE3	1.82	0.61
1:J:57:ARG:NH2	3:J:203:HOH:O	2.34	0.60
1:L:20:VAL:HG13	1:L:77:LEU:HD23	1.84	0.60
1:D:35:TRP:CH2	1:D:86[B]:MET:HE1	2.36	0.60
1:C:43:VAL:O	1:C:47[A]:GLU:HG2	2.02	0.59
1:F:57:ARG:NH2	3:F:304:HOH:O	2.35	0.59
1:D:27:LEU:HG	1:D:31[B]:MET:HE2	1.84	0.59
1:D:35:TRP:HH2	1:D:86[B]:MET:HE1	1.66	0.59
1:I:28:HIS:HA	1:I:31[B]:MET:HE3	1.83	0.59
1:I:20:VAL:HG13	1:I:77:LEU:HD23	1.84	0.59
1:B:20:VAL:HG13	1:B:77[A]:LEU:HD23	1.83	0.59
1:G:57:ARG:NH2	3:G:305:HOH:O	2.37	0.58
1:G:43:VAL:O	1:G:47:GLU:HG2	2.02	0.58
1:E:31[B]:MET:HE3	1:E:86:MET:HE3	1.86	0.58
1:D:50[A]:ASP:OD1	3:D:301:HOH:O	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2:LYS:NZ	3:F:305:HOH:O	2.37	0.58
1:A:6:LYS:NZ	3:A:306:HOH:O	2.36	0.58
1:A:147:GLN:NE2	3:A:303:HOH:O	2.22	0.58
1:B:9[B]:ASN:ND2	3:B:305:HOH:O	2.31	0.57
1:H:43:VAL:O	1:H:47[A]:GLU:HG2	2.04	0.57
1:F:43:VAL:O	1:F:47:GLU:HG2	2.05	0.57
1:B:31[B]:MET:HE3	1:B:86:MET:HE3	1.86	0.57
1:J:39[A]:ARG:NH2	3:J:207:HOH:O	2.37	0.56
1:A:33:LYS:NZ	3:A:307:HOH:O	2.38	0.56
1:A:50[A]:ASP:OD2	3:A:301:HOH:O	2.18	0.56
3:K:538:HOH:O	1:L:31[B]:MET:SD	2.51	0.56
1:E:43:VAL:O	1:E:47[A]:GLU:HG2	2.07	0.54
1:A:39:ARG:NH2	3:A:309:HOH:O	2.40	0.54
1:B:43:VAL:O	1:B:47[A]:GLU:HG2	2.08	0.54
1:B:28:HIS:HA	1:B:31[B]:MET:HE3	1.89	0.53
1:L:6:LYS:HD3	1:L:107:TYR:CZ	2.44	0.53
1:L:28:HIS:HA	1:L:31[B]:MET:HE3	1.91	0.53
1:G:96:ASP:OD1	3:G:301:HOH:O	2.18	0.53
1:H:152:ALA:HB1	1:I:154:ILE:HD11	1.91	0.53
1:B:152:ALA:HB1	1:E:154:ILE:HD11	1.91	0.52
1:F:9[B]:ASN:ND2	3:F:308:HOH:O	2.41	0.52
1:E:96:ASP:O	1:E:99:LYS:HG3	2.09	0.52
1:B:39:ARG:NH2	3:B:308:HOH:O	2.42	0.52
1:G:39:ARG:NH1	3:G:310:HOH:O	2.43	0.52
1:A:43:VAL:HG11	1:A:133:TRP:CZ2	2.43	0.52
1:D:28:HIS:HA	1:D:31[B]:MET:HE3	1.92	0.52
1:I:43:VAL:O	1:I:47[B]:GLU:HG2	2.10	0.52
1:K:28:HIS:HA	1:K:31[B]:MET:HE3	1.91	0.52
1:K:31[B]:MET:HE3	1:K:86:MET:HE3	1.91	0.52
1:I:9[B]:ASN:OD1	3:I:202:HOH:O	2.19	0.51
1:C:20:VAL:HG13	1:C:77[A]:LEU:HD23	1.91	0.51
1:C:157:GLU:OE2	3:C:201:HOH:O	2.19	0.51
1:L:57:ARG:NH2	3:L:309:HOH:O	2.41	0.51
1:F:9[B]:ASN:ND2	3:F:303:HOH:O	2.33	0.51
1:A:43:VAL:HG11	1:A:133:TRP:CE2	2.47	0.50
1:B:43:VAL:HG11	1:B:133:TRP:CE2	2.47	0.50
1:K:139:ASP:O	1:K:142[B]:GLN:HG2	2.12	0.50
1:E:28:HIS:HA	1:E:31[B]:MET:HE3	1.93	0.50
1:B:125:ARG:NH2	3:B:310:HOH:O	2.44	0.50
1:A:105:ILE:HG23	1:A:117:ARG:HG3	1.95	0.49
1:K:39:ARG:NH2	3:K:306:HOH:O	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:HIS:HD2	1:L:31[B]:MET:CE	2.26	0.49
1:B:57:ARG:NH2	3:B:307:HOH:O	2.42	0.49
1:I:31[A]:MET:SD	3:J:457:HOH:O	2.60	0.49
3:H:403:HOH:O	1:L:125:ARG:NH2	2.46	0.48
1:B:157:GLU:OE2	3:B:302:HOH:O	2.20	0.48
1:J:43:VAL:HG11	1:J:133:TRP:CE2	2.48	0.48
1:D:43:VAL:HG11	1:D:133:TRP:CE2	2.49	0.48
1:F:43:VAL:HG11	1:F:133:TRP:CE2	2.48	0.48
1:J:43:VAL:HG11	1:J:133:TRP:CZ2	2.48	0.48
1:E:48:SER:O	1:E:52[B]:MET:HG3	2.14	0.48
1:B:27:LEU:HD23	1:B:79:ILE:HD12	1.95	0.48
1:A:122:GLU:OE1	3:A:302:HOH:O	2.20	0.47
1:G:43:VAL:HG11	1:G:133:TRP:CE2	2.49	0.47
1:K:43:VAL:HG11	1:K:133:TRP:CE2	2.49	0.47
1:J:125:ARG:NH1	3:J:213:HOH:O	2.46	0.47
1:B:148:ASN:O	1:E:151:GLN:NE2	2.47	0.47
1:H:24:GLN:HB2	1:H:77:LEU:HD13	1.96	0.47
1:H:147:GLN:NE2	3:H:402:HOH:O	2.29	0.47
1:I:28:HIS:HD2	1:I:31[B]:MET:CE	2.28	0.47
1:C:43:VAL:HG11	1:C:133:TRP:CZ2	2.49	0.47
1:F:43:VAL:HG11	1:F:133:TRP:CZ2	2.51	0.46
1:B:49:ILE:HA	1:B:52[B]:MET:HE2	1.96	0.46
1:I:43:VAL:HG11	1:I:133:TRP:CE2	2.50	0.46
1:D:105:ILE:HG23	1:D:117:ARG:HG3	1.98	0.46
1:J:126:ASP:HB3	3:J:216:HOH:O	2.16	0.46
1:E:9[A]:ASN:ND2	3:E:308:HOH:O	2.42	0.46
1:G:9[B]:ASN:ND2	3:G:314:HOH:O	2.49	0.45
1:D:47:GLU:O	1:D:51[B]:GLU:HG2	2.16	0.45
1:J:144:MET:HE1	1:K:154:ILE:HD13	1.98	0.45
1:A:47:GLU:O	1:A:51[B]:GLU:HG2	2.16	0.45
1:D:123:ILE:O	1:D:127:GLU:HG2	2.17	0.45
1:I:31[B]:MET:HE3	1:I:86:MET:HE3	1.98	0.45
1:C:43:VAL:HG11	1:C:133:TRP:CE2	2.52	0.45
1:A:154:ILE:HD11	1:D:152:ALA:HB1	1.99	0.45
1:J:39[B]:ARG:HD2	1:K:155:ARG:NH2	2.32	0.45
1:K:20:VAL:HG13	1:K:77:LEU:HD23	1.99	0.45
1:C:20:VAL:HG13	1:C:77[B]:LEU:HD12	1.98	0.45
1:J:140:LEU:O	1:J:144:MET:HG2	2.17	0.44
1:L:147:GLN:NE2	3:L:305:HOH:O	2.35	0.44
1:G:28:HIS:HA	1:G:31[B]:MET:HE3	1.99	0.44
1:D:28:HIS:HD2	1:D:31[B]:MET:CE	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52[B]:MET:HE3	1:F:52[B]:MET:HB2	1.73	0.44
1:G:39:ARG:NH2	1:G:157:GLU:OE1	2.44	0.44
1:D:20:VAL:HG13	1:D:77:LEU:HD23	1.99	0.44
1:B:45:TYR:O	1:B:49:ILE:HG12	2.18	0.44
1:L:47:GLU:O	1:L:51:GLU:HG2	2.18	0.44
1:L:28:HIS:HD2	1:L:31[B]:MET:HE1	1.82	0.44
1:H:43:VAL:HG11	1:H:133:TRP:CZ2	2.52	0.43
1:K:49:ILE:HD13	1:K:52[B]:MET:HE2	2.01	0.43
1:A:20:VAL:HG13	1:A:77:LEU:HD23	2.00	0.43
1:L:43:VAL:HG11	1:L:133:TRP:CZ2	2.53	0.43
1:C:154:ILE:HD11	1:F:152:ALA:HB1	1.99	0.43
1:I:43:VAL:HG11	1:I:133:TRP:CZ2	2.54	0.43
1:A:48:SER:O	1:A:52[B]:MET:HG3	2.19	0.43
1:C:110:SER:HB3	3:C:268:HOH:O	2.18	0.43
1:K:123:ILE:O	1:K:127:GLU:HG2	2.19	0.43
1:D:118:ASP:OD2	1:F:125:ARG:NH2	2.47	0.42
1:H:144:MET:HE2	1:H:144:MET:HB3	1.85	0.42
1:D:154:ILE:HD11	1:K:152:ALA:HB1	2.02	0.42
1:E:43:VAL:HG11	1:E:133:TRP:CZ2	2.53	0.42
1:K:49:ILE:HA	1:K:52[B]:MET:HE2	2.01	0.42
1:L:43:VAL:HG11	1:L:133:TRP:CE2	2.54	0.42
1:J:39[B]:ARG:HD3	1:J:153:GLN:OE1	2.20	0.42
1:E:95:LEU:O	1:E:99:LYS:HG2	2.20	0.42
1:I:28:HIS:HD2	1:I:31[B]:MET:HE1	1.83	0.42
1:D:1:MET:O	1:D:65:LEU:HA	2.20	0.42
1:J:149:TYR:O	1:J:153:GLN:HG2	2.20	0.41
1:F:125:ARG:NH2	3:F:322:HOH:O	2.54	0.41
1:K:27:LEU:HD23	1:K:79:ILE:HD12	2.02	0.41
1:D:9[B]:ASN:ND2	3:D:318:HOH:O	2.52	0.41
1:D:28:HIS:HD2	1:D:31[B]:MET:HE1	1.84	0.41
1:F:39[B]:ARG:HD2	1:F:157:GLU:HB2	2.02	0.41
1:K:47:GLU:O	1:K:51:GLU:HG2	2.20	0.41
1:L:140:LEU:O	1:L:144:MET:HG2	2.21	0.41
1:C:123:ILE:O	1:C:127:GLU:HG2	2.20	0.41
1:G:31[B]:MET:SD	3:H:648:HOH:O	2.61	0.41
1:K:43:VAL:HG11	1:K:133:TRP:CZ2	2.56	0.41
1:F:149:TYR:O	1:F:153:GLN:HG2	2.21	0.41
1:B:123:ILE:O	1:B:127:GLU:HG2	2.21	0.41
1:D:47:GLU:O	1:D:51[A]:GLU:HG2	2.20	0.41
1:A:47:GLU:O	1:A:51[A]:GLU:HG2	2.20	0.40
1:B:77[B]:LEU:HD23	1:B:79:ILE:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:VAL:HG11	1:G:133:TRP:CZ2	2.56	0.40
1:G:105:ILE:HG23	1:G:117:ARG:HG3	2.03	0.40
1:K:28:HIS:HD2	1:K:31[B]:MET:CE	2.35	0.40
1:J:123:ILE:O	1:J:127:GLU:HG2	2.21	0.40
1:K:144:MET:HE2	1:K:144:MET:HB3	1.88	0.40

All (4) 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)
3:A:490:HOH:O	3:E:469:HOH:O[8_776]	2.14	0.06
3:E:460:HOH:O	3:I:222:HOH:O[8_776]	2.14	0.06
3:C:324:HOH:O	3:G:490:HOH:O[8_776]	2.16	0.04
3:G:476:HOH:O	3:K:493:HOH:O[8_776]	2.18	0.02

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	164/158 (104%)	163 (99%)	1 (1%)	0	100	100
1	B	166/158 (105%)	165 (99%)	1 (1%)	0	100	100
1	C	163/158 (103%)	162 (99%)	1 (1%)	0	100	100
1	D	164/158 (104%)	163 (99%)	1 (1%)	0	100	100
1	E	163/158 (103%)	162 (99%)	1 (1%)	0	100	100
1	F	164/158 (104%)	163 (99%)	1 (1%)	0	100	100
1	G	163/158 (103%)	163 (100%)	0	0	100	100
1	H	163/158 (103%)	162 (99%)	1 (1%)	0	100	100
1	I	165/158 (104%)	165 (100%)	0	0	100	100
1	J	163/158 (103%)	163 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	163/158 (103%)	163 (100%)	0	0	100	100
1	L	166/158 (105%)	165 (99%)	1 (1%)	0	100	100
All	All	1967/1896 (104%)	1959 (100%)	8 (0%)	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	145/139 (104%)	145 (100%)	0	100	100
1	B	147/139 (106%)	147 (100%)	0	100	100
1	C	143/139 (103%)	143 (100%)	0	100	100
1	D	144/139 (104%)	144 (100%)	0	100	100
1	E	145/139 (104%)	144 (99%)	1 (1%)	76	66
1	F	145/139 (104%)	145 (100%)	0	100	100
1	G	143/139 (103%)	142 (99%)	1 (1%)	76	66
1	H	143/139 (103%)	142 (99%)	1 (1%)	76	66
1	I	146/139 (105%)	146 (100%)	0	100	100
1	J	145/139 (104%)	143 (99%)	2 (1%)	59	44
1	K	144/139 (104%)	144 (100%)	0	100	100
1	L	148/139 (106%)	148 (100%)	0	100	100
All	All	1738/1668 (104%)	1733 (100%)	5 (0%)	86	80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	99	LYS
1	G	77	LEU
1	H	77	LEU
1	J	50	ASP

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Mol	Chain	Res	Type
1	J	154	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	34	ASN
1	A	100	ASN
1	B	17	ASN
1	B	100	ASN
1	C	17	ASN
1	C	34	ASN
1	C	100	ASN
1	C	142	GLN
1	D	17	ASN
1	D	34	ASN
1	D	100	ASN
1	D	112	HIS
1	E	34	ASN
1	F	34	ASN
1	G	34	ASN
1	G	130	HIS
1	H	34	ASN
1	I	34	ASN
1	J	17	ASN
1	J	100	ASN
1	K	34	ASN
1	L	34	ASN
1	L	130	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

15 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	201	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	H	201	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	L	201	-	4,4,4	0.30	0	6,6,6	0.13	0
2	SO4	H	202	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	E	203	-	4,4,4	0.20	0	6,6,6	0.22	0
2	SO4	E	201	-	4,4,4	0.22	0	6,6,6	0.22	0
2	SO4	D	201	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	202	-	4,4,4	0.19	0	6,6,6	0.23	0
2	SO4	F	202	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	G	201	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	F	201	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	H	203	-	4,4,4	0.30	0	6,6,6	0.17	0
2	SO4	L	202	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	K	201	-	4,4,4	0.30	0	6,6,6	0.17	0
2	SO4	A	201	-	4,4,4	0.69	0	6,6,6	0.79	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	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	158/158 (100%)	-0.42	3 (1%) 66 74	2, 7, 20, 43	8 (5%)
1	B	158/158 (100%)	-0.48	1 (0%) 85 89	2, 7, 18, 39	10 (6%)
1	C	158/158 (100%)	-0.42	1 (0%) 85 89	2, 6, 18, 44	7 (4%)
1	D	158/158 (100%)	-0.42	2 (1%) 75 81	2, 7, 19, 46	8 (5%)
1	E	158/158 (100%)	-0.43	1 (0%) 85 89	2, 7, 21, 47	7 (4%)
1	F	158/158 (100%)	-0.42	2 (1%) 75 81	3, 6, 19, 60	8 (5%)
1	G	158/158 (100%)	-0.44	3 (1%) 66 74	2, 6, 21, 53	7 (4%)
1	H	158/158 (100%)	-0.43	2 (1%) 75 81	2, 7, 19, 44	7 (4%)
1	I	158/158 (100%)	-0.49	1 (0%) 85 89	2, 6, 18, 41	9 (5%)
1	J	158/158 (100%)	-0.44	2 (1%) 75 81	2, 7, 19, 49	7 (4%)
1	K	158/158 (100%)	-0.41	4 (2%) 58 66	2, 7, 19, 50	7 (4%)
1	L	158/158 (100%)	-0.45	2 (1%) 75 81	2, 7, 20, 38	10 (6%)
All	All	1896/1896 (100%)	-0.44	24 (1%) 75 81	2, 7, 19, 60	95 (5%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	158	GLY	7.4
1	C	158	GLY	6.1
1	H	158	GLY	5.9
1	E	158	GLY	4.1
1	G	157	GLU	3.4
1	L	158	GLY	3.4
1	G	158	GLY	3.3
1	J	158	GLY	3.3
1	A	157	GLU	3.3
1	D	157	GLU	2.7
1	K	158	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	157	GLU	2.5
1	A	158	GLY	2.3
1	J	157	GLU	2.2
1	F	157	GLU	2.2
1	I	158	GLY	2.2
1	D	155	ARG	2.2
1	K	46	HIS	2.1
1	L	156	GLU	2.1
1	K	155	ARG	2.1
1	B	158	GLY	2.1
1	G	156	GLU	2.0
1	H	157	GLU	2.0
1	A	39	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	201	5/5	0.87	0.13	33,34,45,53	0
2	SO4	E	202	5/5	0.92	0.14	26,30,42,47	0
2	SO4	E	203	5/5	0.92	0.17	30,32,36,47	0
2	SO4	F	201	5/5	0.92	0.12	26,31,45,48	0
2	SO4	F	202	5/5	0.93	0.11	19,28,51,55	0
2	SO4	H	203	5/5	0.93	0.17	30,30,36,48	0
2	SO4	K	201	5/5	0.93	0.16	26,29,37,50	0
2	SO4	L	202	5/5	0.93	0.15	30,31,37,44	0
2	SO4	L	201	5/5	0.94	0.13	23,26,41,42	0
2	SO4	D	201	5/5	0.95	0.12	23,32,40,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	H	202	5/5	0.95	0.13	27,28,38,41	0
2	SO4	H	201	5/5	0.99	0.03	6,7,7,8	0
2	SO4	E	201	5/5	0.99	0.03	6,7,8,8	0
2	SO4	G	201	5/5	0.99	0.03	5,6,7,9	0
2	SO4	B	201	5/5	1.00	0.03	5,5,7,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.