Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 03:45 am BST

PDB ID	:	4XKT
Title	:	E coli BFR variant Y149F
Authors	:	Bradley, J.M.; Hemmings, A.M.; Le Brun, N.E.
Deposited on	:	2015-01-12
Resolution	:	1.82 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 following versions of software and data (see references ⓘ) were used in the production of this report:

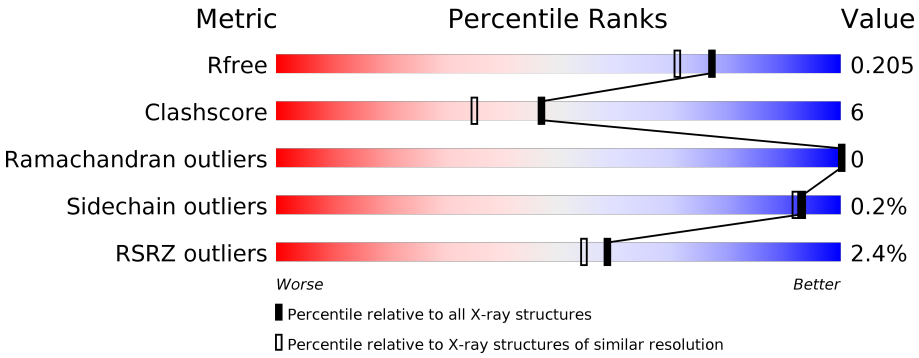
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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}	130704	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

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 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 <=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% 89% 11%
1	B	158	3% 87% 13%
1	C	158	3% 91% 9%
1	D	158	2% 87% 13%
1	E	158	3% 87% 13%
1	F	158	3% 86% 13%

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Mol	Chain	Length	Quality of chain
1	G	158	3% 85% 15%
1	H	158	2% 87% 13%
1	I	158	3% 88% 12%
1	J	158	2% 89% 11%
1	K	158	2% 89% 11%
1	L	158	3% 85% 15%

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	J	201	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19321 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	15	1
			1393	879	231	276	7			
1	B	158	Total	C	N	O	S	0	16	1
			1396	883	234	272	7			
1	C	158	Total	C	N	O	S	0	14	1
			1376	872	229	268	7			
1	D	158	Total	C	N	O	S	0	12	1
			1365	864	231	263	7			
1	E	158	Total	C	N	O	S	0	13	1
			1374	870	229	268	7			
1	F	158	Total	C	N	O	S	0	15	1
			1390	877	236	270	7			
1	G	158	Total	C	N	O	S	0	16	1
			1392	881	233	271	7			
1	H	158	Total	C	N	O	S	0	13	1
			1379	868	233	271	7			
1	I	158	Total	C	N	O	S	0	14	1
			1375	869	232	267	7			
1	J	158	Total	C	N	O	S	0	8	1
			1337	845	225	260	7			
1	K	158	Total	C	N	O	S	0	10	1
			1350	852	227	264	7			
1	L	158	Total	C	N	O	S	0	11	1
			1360	860	228	265	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	PHE	TYR	engineered mutation	UNP E2QFJ1
B	149	PHE	TYR	engineered mutation	UNP E2QFJ1
C	149	PHE	TYR	engineered mutation	UNP E2QFJ1
D	149	PHE	TYR	engineered mutation	UNP E2QFJ1
E	149	PHE	TYR	engineered mutation	UNP E2QFJ1

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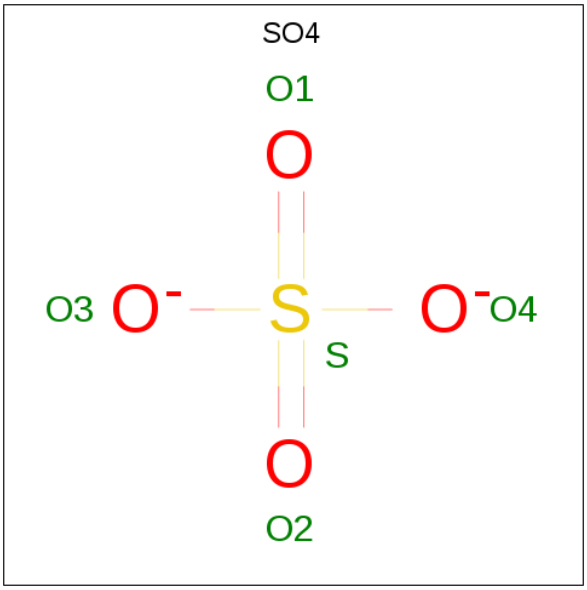
Chain	Residue	Modelled	Actual	Comment	Reference
F	149	PHE	TYR	engineered mutation	UNP E2QFJ1
G	149	PHE	TYR	engineered mutation	UNP E2QFJ1
H	149	PHE	TYR	engineered mutation	UNP E2QFJ1
I	149	PHE	TYR	engineered mutation	UNP E2QFJ1
J	149	PHE	TYR	engineered mutation	UNP E2QFJ1
K	149	PHE	TYR	engineered mutation	UNP E2QFJ1
L	149	PHE	TYR	engineered mutation	UNP E2QFJ1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

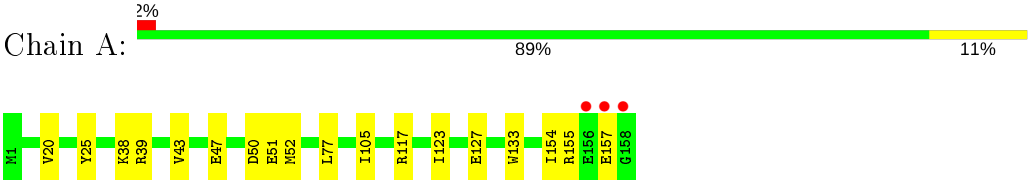
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	233	Total O 233 233	0	0
3	B	234	Total O 234 234	0	0
3	C	246	Total O 246 246	0	0
3	D	231	Total O 231 231	0	0
3	E	228	Total O 228 228	0	0
3	F	232	Total O 232 232	0	0
3	G	236	Total O 236 236	0	0
3	H	220	Total O 220 220	0	0
3	I	219	Total O 219 219	0	0
3	J	229	Total O 229 229	0	0
3	K	230	Total O 230 230	0	0
3	L	231	Total O 231 231	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 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.

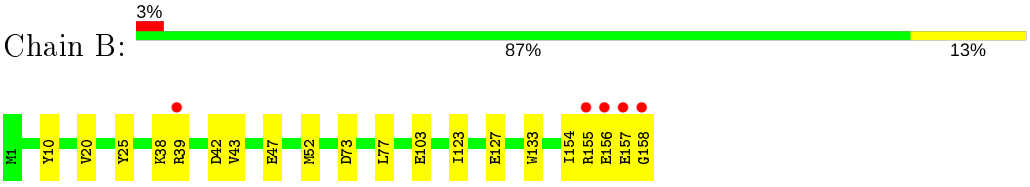
- Molecule 1: Bacterioferritin

Chain A:



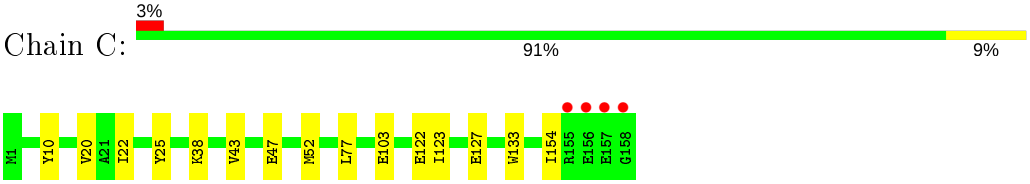
- Molecule 1: Bacterioferritin

Chain B:



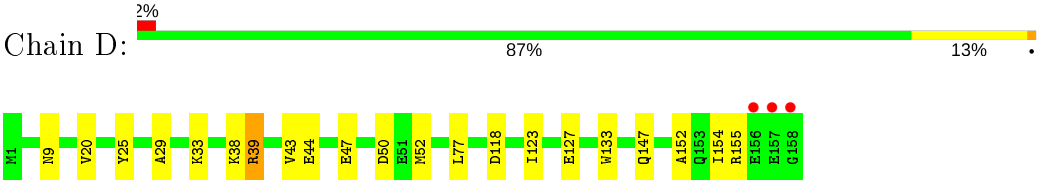
- Molecule 1: Bacterioferritin

Chain C:



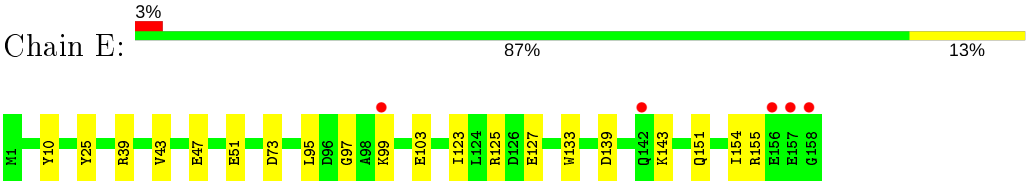
- Molecule 1: Bacterioferritin

Chain D:



- Molecule 1: Bacterioferritin

Chain E:

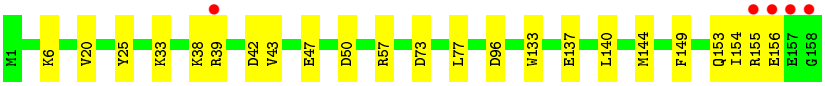


- Molecule 1: Bacterioferritin

Chain F:

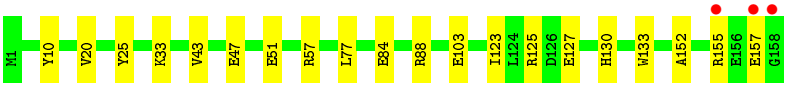
• Molecule 1: Bacterioferritin

Chain G:



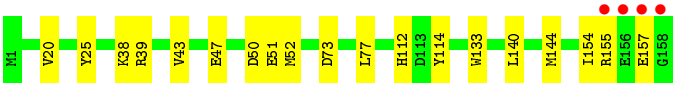
• Molecule 1: Bacterioferritin

Chain H:



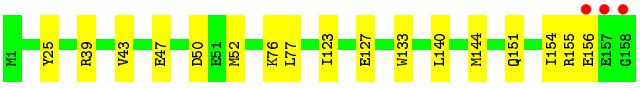
• Molecule 1: Bacterioferritin

Chain I:



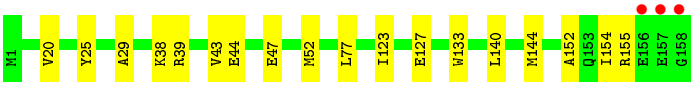
• Molecule 1: Bacterioferritin

Chain J:



• Molecule 1: Bacterioferritin

Chain K:



• Molecule 1: Bacterioferritin

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α, β, γ	208.47Å 208.47Å 142.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.75 – 1.82 31.74 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.5 (31.75-1.82) 99.8 (31.74-1.82)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.64 (at 1.82Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.167 , 0.206 0.170 , 0.205	Depositor DCC
R_{free} test set	13933 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	14.8	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	19321	wwPDB-VP
Average B, all atoms (Å^2)	14.0	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 49.41 % 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 7.4915e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/1447	0.41	0/1947
1	B	0.34	0/1454	0.43	0/1956
1	C	0.34	0/1434	0.44	0/1930
1	D	0.33	0/1417	0.42	0/1907
1	E	0.33	0/1431	0.43	0/1924
1	F	0.34	0/1440	0.43	0/1936
1	G	0.33	0/1447	0.43	0/1947
1	H	0.38	0/1421	0.43	0/1913
1	I	0.33	0/1430	0.46	0/1926
1	J	0.33	0/1379	0.43	0/1856
1	K	0.34	0/1397	0.43	0/1881
1	L	0.33	0/1408	0.42	0/1894
All	All	0.34	0/17105	0.43	0/23017

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

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	1393	0	1357	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1396	0	1368	24	0
1	C	1376	0	1347	12	0
1	D	1365	0	1338	19	0
1	E	1374	0	1357	24	0
1	F	1390	0	1365	17	0
1	G	1392	0	1363	27	0
1	H	1379	0	1334	20	0
1	I	1375	0	1347	18	0
1	J	1337	0	1310	13	0
1	K	1350	0	1322	12	0
1	L	1360	0	1338	22	0
2	B	5	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	10	0	0	0	0
2	J	5	0	0	1	0
2	K	5	0	0	1	0
2	L	5	0	0	0	0
3	A	233	0	0	5	0
3	B	234	0	0	6	1
3	C	246	0	0	1	0
3	D	231	0	0	8	0
3	E	228	0	0	4	0
3	F	232	0	0	4	0
3	G	236	0	0	12	0
3	H	220	0	0	4	1
3	I	219	0	0	6	0
3	J	229	0	0	2	0
3	K	230	0	0	1	0
3	L	231	0	0	4	0
All	All	19321	0	16146	203	1

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 (203) 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:G:155:ARG:HH21	1:L:39:ARG:HD2	1.27	1.00
1:D:52:MET:SD	3:D:531:HOH:O	2.27	0.93
1:I:52:MET:SD	3:I:418:HOH:O	2.28	0.92
1:A:52:MET:SD	3:B:531:HOH:O	2.27	0.91
3:I:418:HOH:O	1:J:52:MET:SD	2.26	0.91
1:K:52:MET:SD	3:L:529:HOH:O	2.29	0.91
1:L:52:MET:SD	3:L:529:HOH:O	2.28	0.91
1:C:52:MET:SD	3:D:531:HOH:O	2.30	0.89
1:J:155:ARG:O	1:K:155:ARG:NH2	2.07	0.87
1:B:39:ARG:HD2	1:E:155:ARG:HH21	1.39	0.86
1:B:52:MET:SD	3:B:531:HOH:O	2.35	0.84
1:A:155:ARG:O	1:J:155:ARG:NH2	2.13	0.81
1:A:39:ARG:NH2	3:A:202:HOH:O	2.13	0.80
1:C:20:VAL:HG13	1:C:77:LEU:HD23	1.65	0.79
1:K:38:LYS:NZ	1:K:154:ILE:O	2.18	0.75
1:K:43:VAL:O	1:K:47[A]:GLU:HG2	1.87	0.75
1:D:147:GLN:NE2	3:D:304:HOH:O	2.21	0.73
1:G:155:ARG:NH2	1:L:39:ARG:HD2	2.01	0.73
1:L:125:ARG:NH2	3:L:301:HOH:O	2.22	0.72
1:B:39:ARG:HD2	1:E:155:ARG:NH2	2.05	0.72
1:D:155:ARG:NH2	1:K:155:ARG:O	2.19	0.71
1:I:39[B]:ARG:NH2	1:I:157:GLU:OE1	2.23	0.71
1:J:43:VAL:O	1:J:47[A]:GLU:HG2	1.89	0.71
1:H:47[B]:GLU:OE2	3:H:301:HOH:O	2.09	0.70
1:F:43:VAL:O	1:F:47[A]:GLU:HG2	1.92	0.69
1:G:43:VAL:O	1:G:47[A]:GLU:HG2	1.93	0.69
1:F:50[A]:ASP:OD1	3:F:301:HOH:O	2.10	0.68
1:L:38:LYS:NZ	1:L:154:ILE:O	2.26	0.68
1:A:43:VAL:O	1:A:47[A]:GLU:HG2	1.92	0.68
1:L:43:VAL:O	1:L:47[A]:GLU:HG2	1.94	0.67
1:G:57:ARG:NH2	3:G:307:HOH:O	2.28	0.67
1:A:50[A]:ASP:OD1	3:A:201:HOH:O	2.13	0.67
1:B:73[A]:ASP:O	3:B:301:HOH:O	2.13	0.67
1:B:73[B]:ASP:O	3:B:301:HOH:O	2.13	0.67
2:G:201:SO4:O4	3:G:301:HOH:O	2.11	0.66
1:K:20:VAL:HG13	1:K:77:LEU:HD23	1.77	0.66
1:G:73[A]:ASP:O	3:G:302:HOH:O	2.13	0.66
1:G:73[B]:ASP:O	3:G:302:HOH:O	2.13	0.66
1:I:50[A]:ASP:OD1	3:I:202:HOH:O	2.14	0.66
1:E:73[A]:ASP:O	3:E:301:HOH:O	2.14	0.65
1:E:73[B]:ASP:O	3:E:301:HOH:O	2.14	0.65
1:D:50[A]:ASP:OD1	3:D:301:HOH:O	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:ASP:OD2	1:G:156:GLU:HG2	1.96	0.65
1:L:20:VAL:HG13	1:L:77:LEU:HD23	1.78	0.65
1:C:43:VAL:O	1:C:47[A]:GLU:HG2	1.97	0.65
1:F:147:GLN:NE2	3:F:305:HOH:O	2.29	0.65
1:L:42:ASP:OD2	1:L:156:GLU:HB3	1.97	0.64
1:L:46[B]:HIS:NE2	3:L:306:HOH:O	2.30	0.64
1:I:73[A]:ASP:O	3:I:201:HOH:O	2.14	0.64
1:I:73[B]:ASP:O	3:I:201:HOH:O	2.14	0.64
1:B:157:GLU:HB2	1:E:155:ARG:CZ	2.27	0.63
1:B:20:VAL:HG13	1:B:77:LEU:HD23	1.80	0.63
1:D:39[A]:ARG:HH22	1:D:133:TRP:HE1	1.47	0.63
1:E:125:ARG:HG3	1:E:125:ARG:HH11	1.64	0.63
1:G:155:ARG:HH21	1:L:39:ARG:CD	2.09	0.62
1:E:43:VAL:O	1:E:47[A]:GLU:HG2	2.00	0.61
1:I:43:VAL:O	1:I:47[A]:GLU:HG2	2.00	0.61
1:G:50[B]:ASP:OD1	3:G:303:HOH:O	2.16	0.61
1:D:39[A]:ARG:NH2	1:D:133:TRP:HE1	1.97	0.61
1:J:76:LYS:HE2	1:J:77:LEU:O	2.01	0.60
3:D:302:HOH:O	1:F:125:ARG:NH2	2.32	0.60
1:H:43:VAL:O	1:H:47[A]:GLU:HG2	2.02	0.60
1:F:42:ASP:OD2	1:F:156:GLU:HG2	2.01	0.60
1:D:20:VAL:HG13	1:D:77:LEU:HD23	1.83	0.59
1:G:33[B]:LYS:HG3	3:G:466:HOH:O	2.03	0.58
1:A:20:VAL:HG13	1:A:77:LEU:HD23	1.83	0.58
1:D:33[B]:LYS:NZ	3:D:309:HOH:O	2.36	0.58
1:H:20:VAL:HG13	1:H:77:LEU:HD23	1.86	0.57
1:B:43:VAL:O	1:B:47[A]:GLU:HG2	2.04	0.56
1:G:6[B]:LYS:NZ	3:G:311:HOH:O	2.37	0.56
1:G:38:LYS:NZ	1:G:154:ILE:O	2.29	0.56
1:B:155:ARG:O	1:E:155:ARG:NH2	2.38	0.56
1:B:39:ARG:HB2	1:E:155:ARG:NH2	2.21	0.56
1:G:39:ARG:HD3	3:G:313:HOH:O	2.05	0.56
1:I:38:LYS:NZ	1:I:154:ILE:O	2.36	0.56
1:D:118:ASP:OD2	3:D:302:HOH:O	2.18	0.55
1:E:125:ARG:NH1	1:E:125:ARG:HG3	2.20	0.55
1:H:57:ARG:NH2	3:H:304:HOH:O	2.29	0.55
1:H:125:ARG:NH2	3:J:303:HOH:O	2.39	0.55
1:G:39:ARG:NH1	3:G:313:HOH:O	2.40	0.55
1:E:95:LEU:O	1:E:99:LYS:HG3	2.08	0.54
1:J:39:ARG:HH22	1:J:133:TRP:HE1	1.55	0.54
1:B:38:LYS:NZ	1:B:154:ILE:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:157:GLU:HB2	1:I:155:ARG:NH1	2.24	0.53
1:A:154:ILE:HD11	1:D:152:ALA:HB1	1.91	0.52
1:A:39:ARG:HD3	3:A:232:HOH:O	2.08	0.52
1:H:155:ARG:O	1:I:155:ARG:NH2	2.43	0.52
1:I:20:VAL:HG13	1:I:77:LEU:HD23	1.92	0.52
1:L:6:LYS:HD3	1:L:107:TYR:CZ	2.44	0.51
1:E:97:GLY:HA3	3:E:451:HOH:O	2.09	0.51
2:J:201:SO4:O1	3:J:301:HOH:O	2.18	0.51
1:C:122:GLU:OE1	3:C:301:HOH:O	2.19	0.51
1:E:123:ILE:O	1:E:127[A]:GLU:HG2	2.11	0.51
1:F:25[B]:TYR:N	1:F:25[B]:TYR:CD1	2.79	0.50
1:G:33[A]:LYS:HG3	3:G:466:HOH:O	2.11	0.50
1:F:93:LEU:HD11	3:F:315:HOH:O	2.11	0.50
1:B:123:ILE:O	1:B:127[B]:GLU:HG2	2.11	0.50
1:K:39[A]:ARG:HH22	1:K:133:TRP:HE1	1.60	0.50
1:B:10:TYR:OH	1:B:103[A]:GLU:HG2	2.13	0.49
1:L:42:ASP:O	1:L:46[B]:HIS:ND1	2.38	0.49
1:A:154:ILE:HD11	1:D:152:ALA:CB	2.43	0.49
1:F:139:ASP:O	1:F:143[C]:LYS:HG3	2.13	0.49
1:E:39[A]:ARG:HG3	3:E:435:HOH:O	2.13	0.49
1:D:9[B]:ASN:OD1	3:D:303:HOH:O	2.20	0.49
1:A:43:VAL:HG11	1:A:133:TRP:CE2	2.48	0.48
1:F:43:VAL:HG11	1:F:133:TRP:CE2	2.48	0.48
1:G:25[B]:TYR:CD1	1:G:25[B]:TYR:N	2.81	0.48
1:D:43:VAL:HG11	1:D:133:TRP:CE2	2.48	0.48
1:H:33[A]:LYS:HG3	3:H:448:HOH:O	2.12	0.48
1:I:43:VAL:HG11	1:I:133:TRP:CE2	2.48	0.48
1:C:10:TYR:OH	1:C:103[C]:GLU:HG2	2.14	0.48
1:D:123:ILE:O	1:D:127:GLU:HG2	2.14	0.47
1:A:123:ILE:O	1:A:127[A]:GLU:HG2	2.14	0.47
1:H:25[C]:TYR:N	1:H:25[C]:TYR:CD1	2.82	0.47
1:J:39:ARG:NH2	1:J:133:TRP:HE1	2.11	0.47
1:A:39:ARG:NH1	3:A:210:HOH:O	2.44	0.47
1:C:123:ILE:O	1:C:127:GLU:HG2	2.14	0.47
1:J:140:LEU:O	1:J:144:MET:HG2	2.15	0.47
1:B:155:ARG:O	1:E:155:ARG:NH1	2.47	0.47
1:G:43:VAL:HG11	1:G:133:TRP:CE2	2.50	0.47
1:B:43:VAL:HG11	1:B:133:TRP:CE2	2.50	0.47
2:K:201:SO4:O1	3:K:301:HOH:O	2.19	0.47
1:L:25[B]:TYR:N	1:L:25[B]:TYR:CD1	2.83	0.47
1:H:152:ALA:HB1	1:I:154:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:ILE:O	1:K:127:GLU:HG2	2.15	0.46
1:K:140:LEU:O	1:K:144:MET:HG2	2.15	0.46
1:L:43:VAL:HG11	1:L:133:TRP:CE2	2.50	0.46
1:C:43:VAL:HG11	1:C:133:TRP:CE2	2.50	0.46
1:B:39:ARG:CD	1:E:155:ARG:HH21	2.18	0.45
1:B:157:GLU:HB2	1:E:155:ARG:NE	2.32	0.45
1:F:149:PHE:O	1:F:153:GLN:HG2	2.17	0.45
1:H:20:VAL:HG13	1:H:77:LEU:CD2	2.46	0.45
1:B:42:ASP:OD2	1:B:156:GLU:HG2	2.17	0.45
1:J:43:VAL:HG11	1:J:133:TRP:CE2	2.52	0.44
1:F:155:ARG:HH11	1:F:155:ARG:HG2	1.81	0.44
1:J:123:ILE:O	1:J:127:GLU:HG2	2.17	0.44
1:H:43:VAL:HG11	1:H:133:TRP:CE2	2.53	0.44
1:K:29:ALA:HB2	1:K:44[B]:GLU:HB3	1.98	0.44
1:H:123:ILE:O	1:H:127:GLU:HG2	2.17	0.44
1:E:10:TYR:OH	1:E:103[B]:GLU:HG2	2.18	0.43
1:G:155:ARG:NH2	1:L:155:ARG:O	2.51	0.43
1:E:43:VAL:HG11	1:E:133:TRP:CE2	2.53	0.43
1:F:155:ARG:O	3:F:302:HOH:O	2.21	0.43
1:G:140:LEU:O	1:G:144:MET:HG2	2.18	0.43
1:D:43:VAL:O	1:D:47[A]:GLU:HG3	2.18	0.43
1:G:96:ASP:OD1	3:G:305:HOH:O	2.21	0.43
1:F:123:ILE:O	1:F:127:GLU:HG2	2.19	0.42
1:H:43:VAL:HG11	1:H:133:TRP:CZ2	2.54	0.42
1:A:105:ILE:HG23	1:A:117:ARG:HG3	2.01	0.42
1:D:38:LYS:NZ	1:D:154:ILE:O	2.52	0.42
1:J:151:GLN:O	1:J:154:ILE:HG12	2.19	0.42
1:C:154:ILE:HD11	1:F:152:ALA:CB	2.49	0.42
1:A:39:ARG:NH2	1:A:157:GLU:OE1	2.34	0.42
1:B:155:ARG:NH2	3:B:305:HOH:O	2.45	0.42
1:G:149:PHE:O	1:G:153:GLN:HG2	2.19	0.42
1:F:151:GLN:O	1:F:154:ILE:HG12	2.19	0.42
1:B:20:VAL:HG13	1:B:77:LEU:CD2	2.48	0.42
1:H:84:GLU:O	1:H:88:ARG:HG3	2.18	0.42
1:G:154:ILE:HD11	1:L:152:ALA:CB	2.50	0.42
1:I:112[A]:HIS:CE1	1:I:114:TYR:HH	2.38	0.42
1:G:154:ILE:HD11	1:L:152:ALA:HB1	2.01	0.42
1:I:140:LEU:O	1:I:144:MET:HG2	2.20	0.42
1:A:43:VAL:HG11	1:A:133:TRP:CZ2	2.55	0.42
1:B:157:GLU:HG2	1:B:157:GLU:O	2.20	0.41
1:L:140:LEU:O	1:L:144:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:GLY:N	3:B:314:HOH:O	2.53	0.41
1:G:137:GLU:OE2	3:G:306:HOH:O	2.22	0.41
1:C:22:ILE:HD11	1:C:52:MET:HA	2.03	0.41
1:D:154:ILE:HD11	1:K:152:ALA:HB1	2.02	0.41
1:C:154:ILE:HD11	1:F:152:ALA:HB1	2.02	0.41
1:I:39[B]:ARG:NH2	3:I:214:HOH:O	2.48	0.41
1:A:38:LYS:HE3	3:A:369:HOH:O	2.20	0.41
1:J:43:VAL:HG11	1:J:133:TRP:CZ2	2.56	0.41
1:C:38[A]:LYS:NZ	1:C:154:ILE:O	2.39	0.41
1:H:10:TYR:OH	1:H:103[B]:GLU:HG2	2.20	0.41
1:F:20:VAL:HG13	1:F:77:LEU:HD23	2.02	0.41
1:E:139:ASP:O	1:E:143:LYS:HG3	2.21	0.41
1:L:123:ILE:O	1:L:127:GLU:HG2	2.21	0.41
1:E:151:GLN:O	1:E:154:ILE:HG12	2.21	0.40
1:H:130:HIS:HB3	3:H:301:HOH:O	2.21	0.40
1:H:152:ALA:CB	1:I:154:ILE:HD11	2.51	0.40
1:D:29:ALA:HB2	1:D:44[B]:GLU:HB3	2.03	0.40
1:G:20:VAL:HG13	1:G:77:LEU:HD23	2.03	0.40
1:G:155:ARG:NH2	1:L:39:ARG:HB2	2.37	0.40

All (1) 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:B:418:HOH:O	3:H:486:HOH:O[6_465]	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	172/158 (109%)	171 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	172/158 (109%)	172 (100%)	0	0	100	100
1	C	170/158 (108%)	168 (99%)	2 (1%)	0	100	100
1	D	168/158 (106%)	167 (99%)	1 (1%)	0	100	100
1	E	169/158 (107%)	167 (99%)	2 (1%)	0	100	100
1	F	171/158 (108%)	171 (100%)	0	0	100	100
1	G	172/158 (109%)	172 (100%)	0	0	100	100
1	H	169/158 (107%)	168 (99%)	1 (1%)	0	100	100
1	I	170/158 (108%)	170 (100%)	0	0	100	100
1	J	164/158 (104%)	163 (99%)	1 (1%)	0	100	100
1	K	166/158 (105%)	166 (100%)	0	0	100	100
1	L	167/158 (106%)	167 (100%)	0	0	100	100
All	All	2030/1896 (107%)	2022 (100%)	8 (0%)	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	153/139 (110%)	153 (100%)	0	100	100
1	B	153/139 (110%)	153 (100%)	0	100	100
1	C	150/139 (108%)	150 (100%)	0	100	100
1	D	148/139 (106%)	146 (99%)	2 (1%)	67	58
1	E	151/139 (109%)	151 (100%)	0	100	100
1	F	152/139 (109%)	151 (99%)	1 (1%)	84	80
1	G	152/139 (109%)	152 (100%)	0	100	100
1	H	149/139 (107%)	149 (100%)	0	100	100
1	I	151/139 (109%)	151 (100%)	0	100	100
1	J	146/139 (105%)	143 (98%)	3 (2%)	53	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	147/139 (106%)	147 (100%)	0	100 100
1	L	149/139 (107%)	149 (100%)	0	100 100
All	All	1801/1668 (108%)	1795 (100%)	6 (0%)	93 91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	39[A]	ARG
1	D	39[B]	ARG
1	F	155	ARG
1	J	50[A]	ASP
1	J	50[B]	ASP
1	J	156	GLU

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

Mol	Chain	Res	Type
1	E	17	ASN
1	E	100	ASN
1	L	17	ASN
1	L	100	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

13 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	L	201	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	F	201	-	4,4,4	0.14	0	6,6,6	0.08	0
2	SO4	K	201	-	4,4,4	0.17	0	6,6,6	0.12	0
2	SO4	H	201	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	C	203	-	4,4,4	0.18	0	6,6,6	0.14	0
2	SO4	H	202	-	4,4,4	0.19	0	6,6,6	0.10	0
2	SO4	C	202	-	4,4,4	0.13	0	6,6,6	0.06	0
2	SO4	E	201	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	B	201	-	4,4,4	0.15	0	6,6,6	0.06	0
2	SO4	G	201	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	D	201	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	C	201	-	4,4,4	0.14	0	6,6,6	0.15	0
2	SO4	J	201	-	4,4,4	0.18	0	6,6,6	0.08	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	201	SO4	1	0
2	G	201	SO4	1	0
2	J	201	SO4	1	0

5.7 Other polymers (i)

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, 95^{th} 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%)	-0.43	3 (1%)	66	63	4, 9, 22, 77	0
1	B	158/158 (100%)	-0.55	5 (3%)	47	42	4, 9, 22, 78	0
1	C	158/158 (100%)	-0.51	4 (2%)	57	52	4, 9, 21, 77	0
1	D	158/158 (100%)	-0.50	3 (1%)	66	63	4, 9, 22, 86	0
1	E	158/158 (100%)	-0.46	5 (3%)	47	42	4, 9, 23, 83	0
1	F	158/158 (100%)	-0.45	4 (2%)	57	52	4, 9, 21, 81	0
1	G	158/158 (100%)	-0.48	5 (3%)	47	42	4, 9, 21, 79	0
1	H	158/158 (100%)	-0.53	3 (1%)	66	63	4, 9, 22, 82	0
1	I	158/158 (100%)	-0.55	4 (2%)	57	52	4, 9, 22, 76	0
1	J	158/158 (100%)	-0.47	3 (1%)	66	63	4, 10, 22, 80	0
1	K	158/158 (100%)	-0.50	3 (1%)	66	63	4, 10, 22, 80	0
1	L	158/158 (100%)	-0.56	4 (2%)	57	52	4, 9, 22, 80	0
All	All	1896/1896 (100%)	-0.50	46 (2%)	59	54	4, 9, 22, 86	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	158	GLY	18.6
1	A	158	GLY	16.2
1	E	158	GLY	14.4
1	H	158	GLY	12.4
1	G	158	GLY	11.5
1	J	158	GLY	9.4
1	D	158	GLY	7.7
1	A	157	GLU	6.5
1	K	158	GLY	6.5
1	G	157	GLU	6.1
1	F	157	GLU	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	157	GLU	5.6
1	I	158	GLY	5.4
1	K	157	GLU	5.4
1	C	158	GLY	5.0
1	E	157	GLU	4.9
1	B	158	GLY	4.9
1	C	157	GLU	4.7
1	I	157	GLU	4.4
1	J	157	GLU	4.4
1	L	158	GLY	4.4
1	L	157	GLU	4.3
1	B	157	GLU	4.1
1	K	156	GLU	3.8
1	H	157	GLU	3.6
1	L	156	GLU	3.6
1	E	156	GLU	3.5
1	C	155	ARG	3.5
1	G	155	ARG	3.5
1	I	156[A]	GLU	3.4
1	A	156[A]	GLU	3.4
1	L	155	ARG	3.1
1	C	156	GLU	3.1
1	D	156	GLU	2.9
1	I	155	ARG	2.7
1	E	142	GLN	2.7
1	J	156	GLU	2.6
1	G	156	GLU	2.5
1	B	156	GLU	2.3
1	F	156	GLU	2.3
1	B	39	ARG	2.2
1	B	155	ARG	2.2
1	H	155	ARG	2.2
1	E	99	LYS	2.1
1	G	39	ARG	2.0
1	F	155	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 carbohydrates 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, 95^{th} 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
2	SO4	J	201	5/5	0.54	0.46	38,44,48,51	0
2	SO4	C	202	5/5	0.85	0.30	72,76,77,81	0
2	SO4	H	202	5/5	0.94	0.20	44,47,52,52	0
2	SO4	D	201	5/5	0.95	0.25	40,45,48,54	0
2	SO4	L	201	5/5	0.96	0.26	41,43,46,48	0
2	SO4	F	201	5/5	0.96	0.24	46,52,53,58	0
2	SO4	G	201	5/5	0.96	0.26	44,49,56,61	0
2	SO4	K	201	5/5	0.96	0.27	39,40,45,50	0
2	SO4	C	203	5/5	0.96	0.22	45,46,47,51	0
2	SO4	E	201	5/5	0.99	0.05	11,12,14,16	0
2	SO4	B	201	5/5	1.00	0.05	8,10,12,13	0
2	SO4	C	201	5/5	1.00	0.05	10,11,11,12	0
2	SO4	H	201	5/5	1.00	0.04	10,10,11,12	0

6.5 Other polymers (i)

There are no such residues in this entry.