



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 12:11 AM GMT

PDB ID : 3FPV
Title : Crystal Structure of HbpS
Authors : Ortiz de Orue Lucana, D.; Bogel, G.; Zou, P.; Groves, M.R.
Deposited on : 2009-01-06
Resolution : 2.20 Å(reported)

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

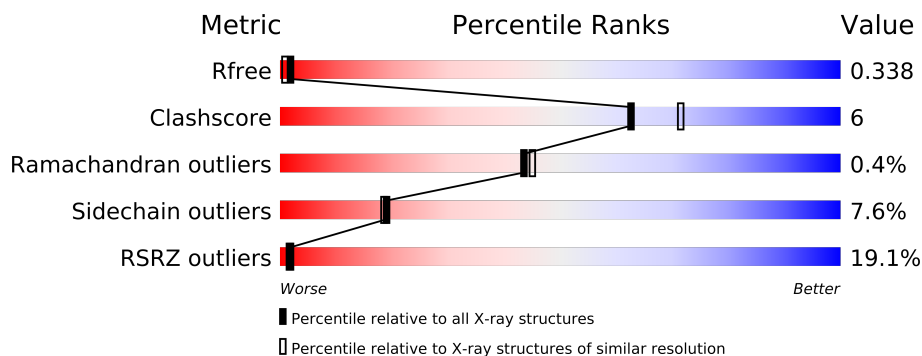
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	192	
1	B	192	
1	C	192	
1	D	192	
1	E	192	
1	F	192	
1	G	192	
1	H	192	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8497 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Extracellular haem-binding protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	B	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	C	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	D	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	E	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	F	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	G	141	Total	C	N	O	0	0	0
			997	614	185	198			
1	H	141	Total	C	N	O	0	0	0
			997	614	185	198			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
A	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
A	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
A	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
B	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
B	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
B	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
B	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
C	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
C	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
C	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
C	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
D	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
D	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
D	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
E	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
E	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
E	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
E	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
F	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
F	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
F	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
F	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
G	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
G	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
G	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
G	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2
H	-35	GLY	-	EXPRESSION TAG	UNP Q9RIM2
H	-34	ALA	-	EXPRESSION TAG	UNP Q9RIM2
H	-33	GLY	-	EXPRESSION TAG	UNP Q9RIM2
H	-32	ALA	-	EXPRESSION TAG	UNP Q9RIM2

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Fe 1 1	0	0
2	E	2	Total Fe 2 2	0	0
2	H	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	A	1	Total Fe 1 1	0	0
2	F	1	Total Fe 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0

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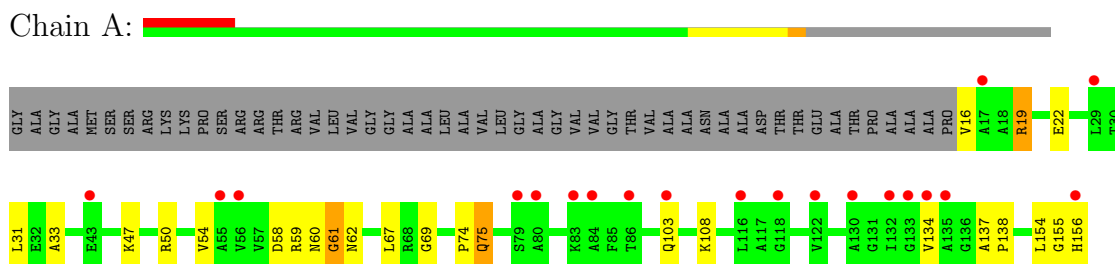
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	101	Total 101	O 101	0	0
3	C	57	Total 57	O 57	0	0
3	D	50	Total 50	O 50	0	0
3	E	35	Total 35	O 35	0	0
3	F	84	Total 84	O 84	0	0
3	G	46	Total 46	O 46	0	0
3	H	59	Total 59	O 59	0	0

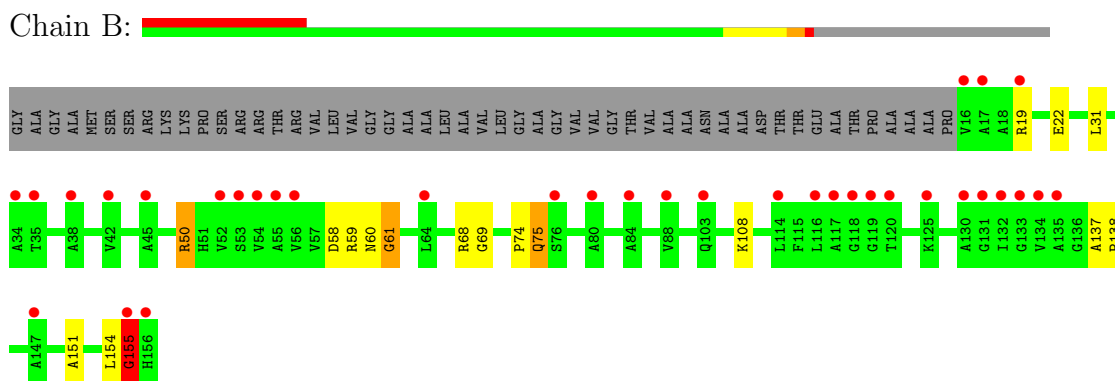
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

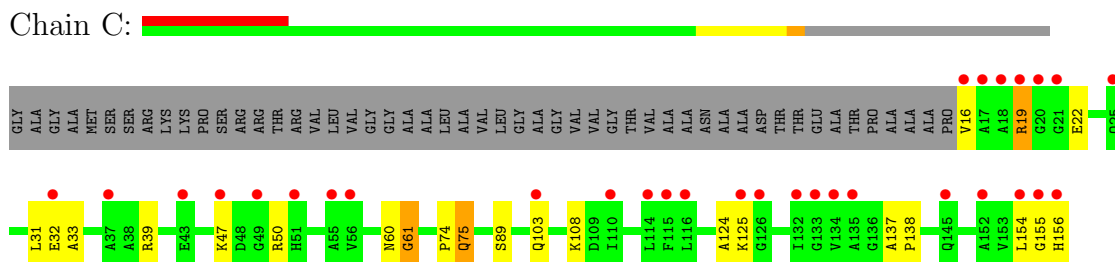
- Molecule 1: Extracellular haem-binding protein



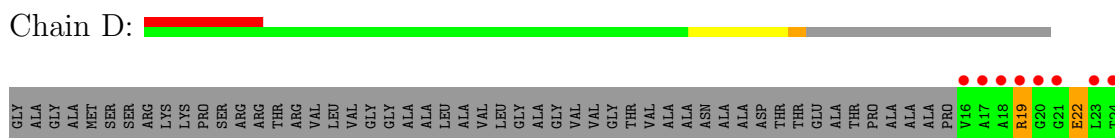
- Molecule 1: Extracellular haem-binding protein



- Molecule 1: Extracellular haem-binding protein



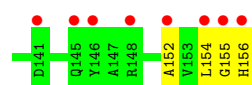
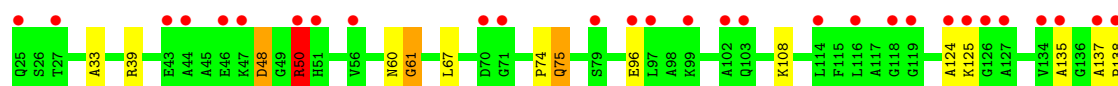
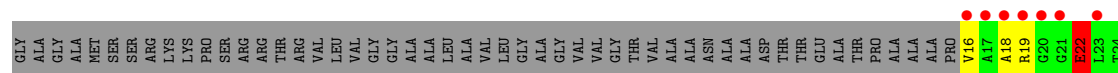
- Molecule 1: Extracellular haem-binding protein





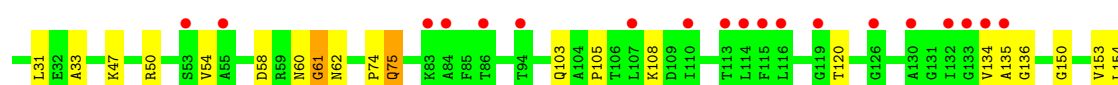
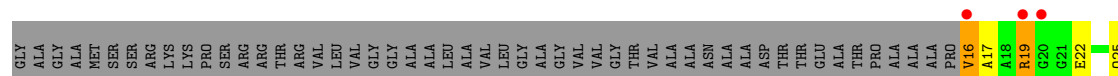
- Molecule 1: Extracellular haem-binding protein

Chain E:



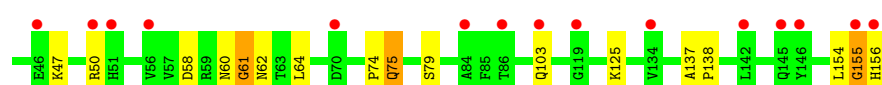
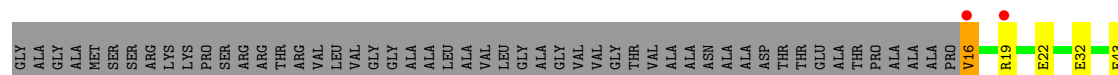
- Molecule 1: Extracellular haem-binding protein

Chain F:



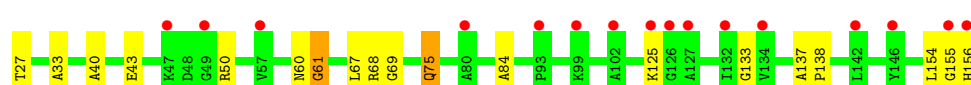
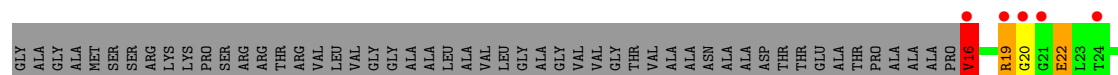
- Molecule 1: Extracellular haem-binding protein

Chain G:



- Molecule 1: Extracellular haem-binding protein

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	152.52Å 152.52Å 152.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.20 19.86 – 2.21	Depositor EDS
% Data completeness (in resolution range)	99.1 (19.86-2.20) 99.1 (19.86-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.21Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.264 0.296 , 0.338	Depositor DCC
R_{free} test set	2914 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 47.3	EDS
Estimated twinning fraction	0.033 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 58323 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8497	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE

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	0.21	0/1012	0.36	0/1376
1	B	0.21	0/1012	0.36	0/1376
1	C	0.20	0/1012	0.35	0/1376
1	D	0.20	0/1012	0.36	0/1376
1	E	0.21	0/1012	0.36	0/1376
1	F	0.21	0/1012	0.36	0/1376
1	G	0.20	0/1012	0.35	0/1376
1	H	0.20	0/1012	0.35	0/1376
All	All	0.21	0/8096	0.36	0/11008

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	6
1	D	0	8
1	E	0	10
1	F	0	8
1	G	0	4
1	H	0	6
All	All	0	51

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	LEU	Peptide
1	A	19	ARG	Peptide
1	A	60	ASN	Peptide
1	A	61	GLY	Peptide
1	B	154	LEU	Peptide
1	B	155	GLY	Peptide
1	B	19	ARG	Peptide
1	B	60	ASN	Peptide
1	B	61	GLY	Peptide
1	C	124	ALA	Peptide
1	C	154	LEU	Peptide
1	C	155	GLY	Peptide
1	C	19	ARG	Peptide
1	C	60	ASN	Peptide
1	C	61	GLY	Peptide
1	D	124	ALA	Peptide
1	D	135	ALA	Peptide
1	D	136	GLY	Peptide
1	D	154	LEU	Peptide
1	D	155	GLY	Peptide
1	D	19	ARG	Peptide
1	D	60	ASN	Peptide
1	D	61	GLY	Peptide
1	E	124	ALA	Peptide
1	E	135	ALA	Peptide
1	E	154	LEU	Peptide
1	E	16	VAL	Peptide
1	E	18	ALA	Peptide
1	E	19	ARG	Peptide
1	E	22	GLU	Peptide
1	E	50	ARG	Peptide
1	E	60	ASN	Peptide
1	E	61	GLY	Peptide
1	F	135	ALA	Peptide
1	F	136	GLY	Peptide
1	F	154	LEU	Peptide
1	F	155	GLY	Peptide
1	F	16	VAL	Peptide
1	F	19	ARG	Peptide
1	F	60	ASN	Peptide
1	F	61	GLY	Peptide
1	G	155	GLY	Peptide
1	G	19	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	G	60	ASN	Peptide
1	G	61	GLY	Peptide
1	H	154	LEU	Peptide
1	H	155	GLY	Peptide
1	H	16	VAL	Peptide
1	H	19	ARG	Peptide
1	H	60	ASN	Peptide
1	H	61	GLY	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	997	0	996	20	0
1	B	997	0	996	17	0
1	C	997	0	996	11	0
1	D	997	0	996	14	0
1	E	997	0	996	15	0
1	F	997	0	996	22	0
1	G	997	0	996	12	0
1	H	997	0	996	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
3	A	81	0	0	0	0
3	B	101	0	0	1	0
3	C	57	0	0	0	0
3	D	50	0	0	0	0
3	E	35	0	0	0	0
3	F	84	0	0	2	0
3	G	46	0	0	0	0
3	H	59	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	8497	0	7968	90	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (90) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:22:GLU:HB2	1:H:33:ALA:HB2	1.56	0.85
1:A:155:GLY:HA2	1:F:22:GLU:OE1	1.80	0.82
1:A:33:ALA:HB2	1:F:22:GLU:HB3	1.65	0.77
1:C:33:ALA:HB2	1:H:22:GLU:HB2	1.69	0.75
1:A:155:GLY:N	1:A:156:HIS:HA	2.02	0.74
1:D:22:GLU:HB2	1:E:33:ALA:HB2	1.69	0.74
1:B:155:GLY:HA2	1:G:22:GLU:OE1	1.91	0.70
1:A:22:GLU:HB3	1:F:33:ALA:HB2	1.74	0.68
1:H:19:ARG:HG3	1:H:20:GLY:H	1.60	0.66
1:H:19:ARG:HG3	1:H:20:GLY:N	2.13	0.63
1:D:33:ALA:HB2	1:E:22:GLU:HG3	1.79	0.62
1:B:137:ALA:HB1	1:B:138:PRO:HD2	1.81	0.62
1:A:33:ALA:CB	1:F:22:GLU:HB3	2.30	0.60
1:B:61:GLY:H	1:D:74:PRO:HB3	1.65	0.60
1:C:31:LEU:HD11	1:E:67:LEU:HB3	1.83	0.60
1:E:61:GLY:H	1:G:74:PRO:HB3	1.67	0.59
1:A:75:GLN:NE2	1:A:75:GLN:H	2.01	0.59
1:D:75:GLN:H	1:D:75:GLN:NE2	1.99	0.58
1:D:33:ALA:CB	1:E:22:GLU:HG3	2.32	0.58
1:B:75:GLN:H	1:B:75:GLN:HE21	1.53	0.57
1:B:75:GLN:H	1:B:75:GLN:NE2	2.02	0.57
1:B:58:ASP:O	1:B:61:GLY:HA2	2.05	0.57
1:A:75:GLN:HE21	1:A:75:GLN:H	1.53	0.55
1:A:22:GLU:OE1	1:F:155:GLY:HA2	2.08	0.54
1:F:31:LEU:HD11	1:H:67:LEU:HB3	1.89	0.54
1:F:75:GLN:NE2	1:F:75:GLN:H	2.06	0.54
1:A:22:GLU:HB3	1:F:33:ALA:CB	2.38	0.53
1:F:17:ALA:HB1	3:F:1210:HOH:O	2.07	0.53
1:H:16:VAL:N	3:H:1176:HOH:O	2.42	0.53
1:E:48:ASP:N	1:E:48:ASP:OD1	2.42	0.53
1:A:69:GLY:HA2	1:B:31:LEU:HD22	1.91	0.53
1:A:74:PRO:HB3	1:G:61:GLY:H	1.74	0.52
1:H:137:ALA:HB1	1:H:138:PRO:HD2	1.90	0.52
1:B:151:ALA:HB1	1:G:16:VAL:HG21	1.90	0.52
1:C:75:GLN:H	1:C:75:GLN:NE2	2.07	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:75:GLN:HE21	1:D:75:GLN:H	1.57	0.51
1:B:137:ALA:HB1	1:B:138:PRO:CD	2.40	0.51
1:G:58:ASP:O	1:G:61:GLY:HA2	2.11	0.51
1:E:74:PRO:HB3	1:H:61:GLY:H	1.75	0.51
1:H:75:GLN:H	1:H:75:GLN:HE21	1.58	0.51
1:C:74:PRO:HB3	1:D:61:GLY:H	1.76	0.51
1:H:75:GLN:NE2	1:H:75:GLN:H	2.08	0.50
1:E:75:GLN:H	1:E:75:GLN:HE21	1.59	0.50
1:F:75:GLN:HE21	1:F:75:GLN:H	1.58	0.50
1:G:75:GLN:H	1:G:75:GLN:NE2	2.08	0.50
1:D:54:VAL:HG22	1:D:134:VAL:HG22	1.93	0.50
1:F:31:LEU:HD22	1:H:69:GLY:HA2	1.94	0.49
1:B:59:ARG:O	1:B:59:ARG:HG3	2.12	0.49
1:D:39:ARG:NH2	1:G:32:GLU:OE1	2.44	0.49
1:G:137:ALA:HB1	1:G:138:PRO:HD2	1.94	0.49
1:A:62:ASN:HB3	1:B:68:ARG:CZ	2.42	0.49
1:C:137:ALA:HB1	1:C:138:PRO:HD2	1.95	0.49
1:A:137:ALA:HB1	1:A:138:PRO:HD2	1.95	0.49
1:E:155:GLY:HA3	1:E:156:HIS:HA	1.53	0.48
1:F:58:ASP:O	1:F:61:GLY:CA	2.61	0.48
1:B:58:ASP:O	1:B:61:GLY:CA	2.61	0.48
1:F:54:VAL:HG22	1:F:134:VAL:HG22	1.94	0.48
1:C:75:GLN:NE2	1:D:89:SER:HB3	2.29	0.47
1:A:58:ASP:O	1:A:61:GLY:HA2	2.15	0.47
1:C:39:ARG:HH11	1:E:39:ARG:HH11	1.63	0.47
1:F:62:ASN:HB3	1:H:68:ARG:CZ	2.45	0.47
1:D:33:ALA:HB2	1:E:22:GLU:CG	2.44	0.46
1:C:33:ALA:CB	1:H:22:GLU:HB2	2.44	0.46
1:H:137:ALA:HB1	1:H:138:PRO:CD	2.45	0.46
1:F:58:ASP:O	1:F:61:GLY:HA2	2.16	0.45
1:A:54:VAL:HG22	1:A:134:VAL:HG22	1.98	0.45
1:A:58:ASP:O	1:A:61:GLY:CA	2.64	0.45
1:E:152:ALA:O	1:E:156:HIS:NE2	2.50	0.45
1:A:31:LEU:HD22	1:B:69:GLY:HA2	1.98	0.45
1:G:125:LYS:HD2	1:G:125:LYS:HA	1.79	0.45
1:A:67:LEU:HB3	1:B:31:LEU:HD11	1.99	0.44
1:D:33:ALA:HB2	1:E:22:GLU:HB2	2.00	0.44
1:B:50:ARG:HD3	3:B:717:HOH:O	2.16	0.44
1:A:137:ALA:HB1	1:A:138:PRO:CD	2.48	0.44
1:B:74:PRO:HB3	1:F:61:GLY:H	1.81	0.44
1:C:61:GLY:H	1:F:74:PRO:HB3	1.81	0.44
1:E:137:ALA:HB1	1:E:138:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:22:GLU:OE1	1:G:155:GLY:HA2	2.18	0.44
1:E:50:ARG:HG2	1:E:138:PRO:HD3	2.00	0.43
1:G:58:ASP:HB2	1:G:64:LEU:HD21	2.01	0.43
1:F:155:GLY:C	1:F:156:HIS:CG	2.92	0.43
1:C:89:SER:HB3	1:F:75:GLN:NE2	2.34	0.42
1:A:59:ARG:O	1:A:59:ARG:HG3	2.18	0.42
1:F:105:PRO:O	1:F:108:LYS:HG2	2.20	0.42
1:F:25:GLN:HG2	3:F:1209:HOH:O	2.19	0.42
1:D:35:THR:O	1:D:39:ARG:HG3	2.20	0.42
1:F:150:GLY:O	1:F:153:VAL:HG22	2.19	0.42
1:H:84:ALA:HB2	1:H:133:GLY:N	2.36	0.41
1:H:40:ALA:HA	1:H:43:GLU:HB3	2.03	0.41
1:D:68:ARG:CZ	1:G:62:ASN:HB3	2.51	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	139/192 (72%)	136 (98%)	3 (2%)	0	100	100
1	B	139/192 (72%)	137 (99%)	1 (1%)	1 (1%)	30	28
1	C	139/192 (72%)	134 (96%)	4 (3%)	1 (1%)	30	28
1	D	139/192 (72%)	132 (95%)	6 (4%)	1 (1%)	30	28
1	E	139/192 (72%)	134 (96%)	4 (3%)	1 (1%)	30	28
1	F	139/192 (72%)	136 (98%)	2 (1%)	1 (1%)	30	28
1	G	139/192 (72%)	138 (99%)	1 (1%)	0	100	100
1	H	139/192 (72%)	135 (97%)	4 (3%)	0	100	100
All	All	1112/1536 (72%)	1082 (97%)	25 (2%)	5 (0%)	43	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	125	LYS
1	D	125	LYS
1	E	125	LYS
1	F	155	GLY
1	B	155	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	95/125 (76%)	88 (93%)	7 (7%)	20	19
1	B	95/125 (76%)	92 (97%)	3 (3%)	51	62
1	C	95/125 (76%)	86 (90%)	9 (10%)	12	11
1	D	95/125 (76%)	86 (90%)	9 (10%)	12	11
1	E	95/125 (76%)	89 (94%)	6 (6%)	25	27
1	F	95/125 (76%)	87 (92%)	8 (8%)	16	15
1	G	95/125 (76%)	86 (90%)	9 (10%)	12	11
1	H	95/125 (76%)	88 (93%)	7 (7%)	20	19
All	All	760/1000 (76%)	702 (92%)	58 (8%)	19	18

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	19	ARG
1	A	47	LYS
1	A	50	ARG
1	A	75	GLN
1	A	103	GLN
1	A	108	LYS
1	B	50	ARG
1	B	75	GLN
1	B	108	LYS
1	C	16	VAL
1	C	19	ARG
1	C	32	GLU

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Mol	Chain	Res	Type
1	C	47	LYS
1	C	50	ARG
1	C	75	GLN
1	C	103	GLN
1	C	108	LYS
1	C	156	HIS
1	D	19	ARG
1	D	22	GLU
1	D	32	GLU
1	D	47	LYS
1	D	50	ARG
1	D	75	GLN
1	D	108	LYS
1	D	132	ILE
1	D	141	ASP
1	E	22	GLU
1	E	48	ASP
1	E	50	ARG
1	E	75	GLN
1	E	96	GLU
1	E	108	LYS
1	F	16	VAL
1	F	19	ARG
1	F	47	LYS
1	F	50	ARG
1	F	75	GLN
1	F	103	GLN
1	F	120	THR
1	F	156	HIS
1	G	16	VAL
1	G	43	GLU
1	G	47	LYS
1	G	50	ARG
1	G	75	GLN
1	G	79	SER
1	G	103	GLN
1	G	154	LEU
1	G	156	HIS
1	H	16	VAL
1	H	22	GLU
1	H	27	THR
1	H	50	ARG

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Mol	Chain	Res	Type
1	H	75	GLN
1	H	125	LYS
1	H	156	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	75	GLN
1	A	156	HIS
1	B	75	GLN
1	C	25	GLN
1	C	75	GLN
1	D	75	GLN
1	D	145	GLN
1	E	25	GLN
1	E	75	GLN
1	F	25	GLN
1	F	75	GLN
1	G	25	GLN
1	G	75	GLN
1	H	75	GLN
1	H	156	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	141/192 (73%)	0.92	20 (14%) 3 3	64, 67, 77, 80	0
1	B	141/192 (73%)	1.23	35 (24%) 1 1	63, 68, 77, 82	0
1	C	141/192 (73%)	1.17	31 (21%) 1 1	64, 67, 76, 79	0
1	D	141/192 (73%)	1.08	24 (17%) 2 2	64, 67, 76, 78	0
1	E	141/192 (73%)	1.67	44 (31%) 1 1	64, 70, 74, 77	0
1	F	141/192 (73%)	1.02	24 (17%) 2 2	63, 68, 77, 82	0
1	G	141/192 (73%)	0.93	17 (12%) 5 4	64, 67, 76, 82	0
1	H	141/192 (73%)	1.19	21 (14%) 3 3	62, 66, 75, 79	0
All	All	1128/1536 (73%)	1.15	216 (19%) 2 2	62, 68, 76, 82	0

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	156	HIS	7.8
1	E	50	ARG	6.6
1	E	156	HIS	6.4
1	F	156	HIS	6.4
1	D	19	ARG	6.3
1	E	126	GLY	6.3
1	E	19	ARG	6.1
1	D	20	GLY	5.9
1	E	152	ALA	5.9
1	C	126	GLY	5.6
1	D	17	ALA	5.6
1	B	134	VAL	5.4
1	G	156	HIS	5.0
1	D	126	GLY	5.0
1	E	20	GLY	4.8
1	E	51	HIS	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	133	GLY	4.7
1	E	47	LYS	4.6
1	E	145	GLN	4.6
1	B	135	ALA	4.6
1	D	152	ALA	4.6
1	E	155	GLY	4.5
1	C	19	ARG	4.5
1	C	125	LYS	4.5
1	F	19	ARG	4.4
1	B	156	HIS	4.4
1	A	134	VAL	4.3
1	H	19	ARG	4.3
1	B	132	ILE	4.2
1	A	156	HIS	4.1
1	G	19	ARG	4.1
1	E	146	TYR	4.1
1	C	49	GLY	4.1
1	H	47	LYS	4.0
1	D	156	HIS	4.0
1	H	21	GLY	4.0
1	B	53	SER	4.0
1	F	155	GLY	3.9
1	A	132	ILE	3.8
1	D	25	GLN	3.8
1	H	80	ALA	3.8
1	B	54	VAL	3.8
1	E	125	LYS	3.7
1	B	80	ALA	3.7
1	E	127	ALA	3.6
1	F	16	VAL	3.6
1	B	55	ALA	3.6
1	A	84	ALA	3.6
1	H	102	ALA	3.6
1	H	16	VAL	3.5
1	E	46	GLU	3.5
1	B	131	GLY	3.5
1	H	155	GLY	3.5
1	D	23	LEU	3.5
1	E	43	GLU	3.5
1	C	155	GLY	3.5
1	B	19	ARG	3.4
1	G	50	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	G	103	GLN	3.4
1	G	155	GLY	3.4
1	E	137	ALA	3.4
1	D	114	LEU	3.4
1	E	23	LEU	3.3
1	B	84	ALA	3.3
1	C	156	HIS	3.3
1	E	17	ALA	3.3
1	B	116	LEU	3.3
1	G	51	HIS	3.3
1	E	124	ALA	3.3
1	A	133	GLY	3.2
1	H	20	GLY	3.2
1	C	55	ALA	3.2
1	B	56	VAL	3.2
1	E	25	GLN	3.1
1	D	134	VAL	3.1
1	C	20	GLY	3.1
1	D	125	LYS	3.1
1	C	32	GLU	3.1
1	E	135	ALA	3.1
1	F	114	LEU	3.1
1	B	42	VAL	3.1
1	D	116	LEU	3.1
1	H	134	VAL	3.0
1	B	34	ALA	3.0
1	G	146	TYR	3.0
1	E	21	GLY	3.0
1	A	103	GLN	3.0
1	D	155	GLY	3.0
1	G	142	LEU	2.9
1	D	21	GLY	2.9
1	E	134	VAL	2.9
1	F	86	THR	2.9
1	H	24	THR	2.9
1	C	43	GLU	2.8
1	F	126	GLY	2.8
1	F	134	VAL	2.8
1	E	148	ARG	2.8
1	E	27	THR	2.8
1	E	103	GLN	2.8
1	A	83	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	146	TYR	2.7
1	F	83	LYS	2.7
1	H	126	GLY	2.7
1	C	132	ILE	2.7
1	D	132	ILE	2.7
1	A	118	GLY	2.7
1	B	17	ALA	2.7
1	C	17	ALA	2.7
1	D	24	THR	2.6
1	F	119	GLY	2.6
1	E	70	ASP	2.6
1	E	102	ALA	2.6
1	G	84	ALA	2.6
1	C	154	LEU	2.6
1	G	46	GLU	2.6
1	H	99	LYS	2.6
1	C	110	ILE	2.6
1	H	132	ILE	2.6
1	A	130	ALA	2.6
1	C	25	GLN	2.6
1	G	134	VAL	2.6
1	G	145	GLN	2.6
1	H	49	GLY	2.6
1	G	56	VAL	2.6
1	F	130	ALA	2.5
1	H	127	ALA	2.5
1	B	117	ALA	2.5
1	D	18	ALA	2.5
1	C	103	GLN	2.5
1	E	118	GLY	2.5
1	E	154	LEU	2.5
1	F	84	ALA	2.5
1	A	122	VAL	2.5
1	F	116	LEU	2.5
1	C	135	ALA	2.5
1	B	130	ALA	2.5
1	B	155	GLY	2.4
1	H	125	LYS	2.4
1	E	56	VAL	2.4
1	B	16	VAL	2.4
1	B	52	VAL	2.4
1	D	135	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	141	ASP	2.4
1	C	134	VAL	2.4
1	C	145	GLN	2.4
1	C	133	GLY	2.4
1	G	16	VAL	2.4
1	C	21	GLY	2.4
1	C	47	LYS	2.4
1	D	38	ALA	2.4
1	F	55	ALA	2.4
1	B	35	THR	2.4
1	F	113	THR	2.4
1	A	116	LEU	2.3
1	E	116	LEU	2.3
1	H	142	LEU	2.3
1	D	16	VAL	2.3
1	F	94	THR	2.3
1	F	20	GLY	2.3
1	E	99	LYS	2.3
1	A	79	SER	2.3
1	B	88	VAL	2.3
1	A	80	ALA	2.3
1	E	18	ALA	2.3
1	B	125	LYS	2.3
1	A	29	LEU	2.3
1	A	43	GLU	2.3
1	B	114	LEU	2.3
1	C	37	ALA	2.3
1	E	138	PRO	2.3
1	B	118	GLY	2.3
1	B	119	GLY	2.3
1	B	147	ALA	2.3
1	F	135	ALA	2.3
1	H	93	PRO	2.3
1	F	133	GLY	2.2
1	E	96	GLU	2.2
1	F	132	ILE	2.2
1	A	135	ALA	2.2
1	B	120	THR	2.2
1	D	133	GLY	2.2
1	D	50	ARG	2.2
1	C	116	LEU	2.2
1	E	114	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	56	VAL	2.2
1	G	86	THR	2.2
1	F	115	PHE	2.2
1	C	51	HIS	2.2
1	E	71	GLY	2.1
1	C	115	PHE	2.1
1	A	86	THR	2.1
1	B	76	SER	2.1
1	F	53	SER	2.1
1	D	32	GLU	2.1
1	E	16	VAL	2.1
1	B	38	ALA	2.1
1	A	55	ALA	2.1
1	C	18	ALA	2.1
1	E	79	SER	2.1
1	C	152	ALA	2.1
1	B	64	LEU	2.1
1	C	16	VAL	2.1
1	B	103	GLN	2.1
1	F	110	ILE	2.1
1	B	45	ALA	2.1
1	E	44	ALA	2.1
1	G	70	ASP	2.1
1	E	119	GLY	2.1
1	F	107	LEU	2.1
1	A	56	VAL	2.1
1	G	119	GLY	2.0
1	C	114	LEU	2.0
1	H	57	VAL	2.0
1	D	79	SER	2.0
1	A	17	ALA	2.0
1	E	97	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FE	E	157	1/1	0.30	1.70	132,132,132,132	0
2	FE	E	158	1/1	0.18	-0.25	99,99,99,99	0
2	FE	F	157	1/1	0.12	-2.00	69,69,69,69	0
2	FE	A	157	1/1	0.09	-2.32	72,72,72,72	0
2	FE	B	157	1/1	0.13	-2.42	55,55,55,55	0
2	FE	C	157	1/1	0.06	-2.64	77,77,77,77	0
2	FE	D	157	1/1	0.07	-2.91	72,72,72,72	0
2	FE	H	157	1/1	0.09	-3.13	80,80,80,80	0

6.5 Other polymers

There are no such residues in this entry.