



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:03 PM UTC

PDB ID : 3FPV / pdb_00003fpv
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 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
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

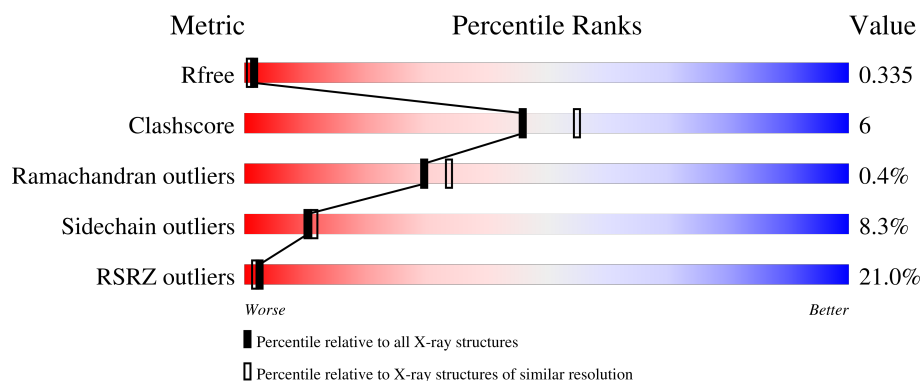
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	192	 6% 60% 12% • 27%
1	B	192	 17% 64% 8% •• 27%
1	C	192	 18% 61% 10% • 27%
1	D	192	 11% 60% 11% • 27%
1	E	192	 35% 60% 11% •• 27%

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Mol	Chain	Length	Quality of chain
1	F	192	9% 59% 11% • • 27%
1	G	192	8% 63% 9% • 27%
1	H	192	19% 62% 9% • • 27%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8497 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 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 (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	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	D	1	Total Fe 1 1	0	0
2	E	2	Total Fe 2 2	0	0
2	F	1	Total Fe 1 1	0	0
2	H	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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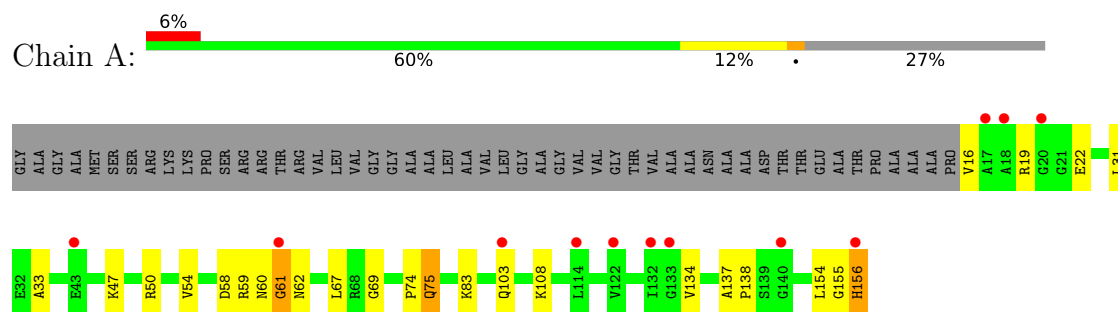
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	101	Total 101	O 101	0	0
3	C	57	Total 57	O 57	0	0
3	D	50	Total 50	O 50	0	0
3	E	35	Total 35	O 35	0	0
3	F	84	Total 84	O 84	0	0
3	G	46	Total 46	O 46	0	0
3	H	59	Total 59	O 59	0	0

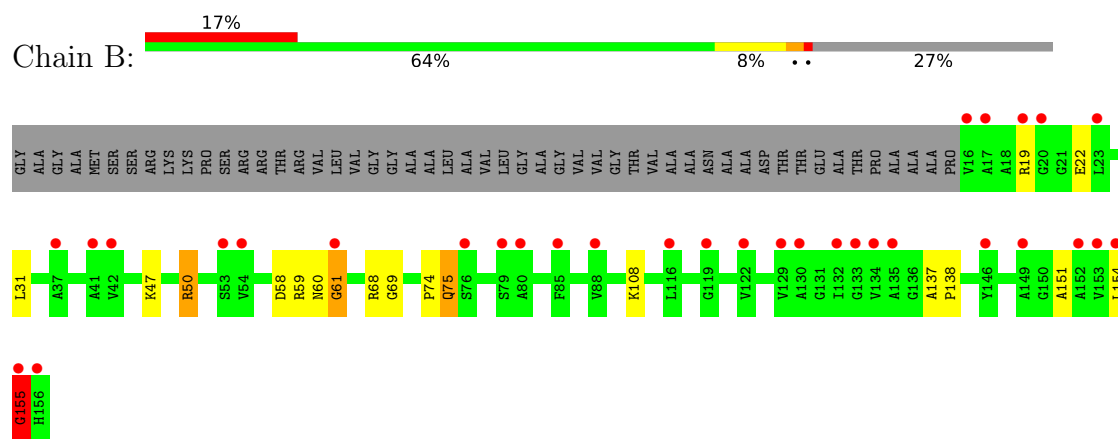
3 Residue-property plots [i](#)

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.

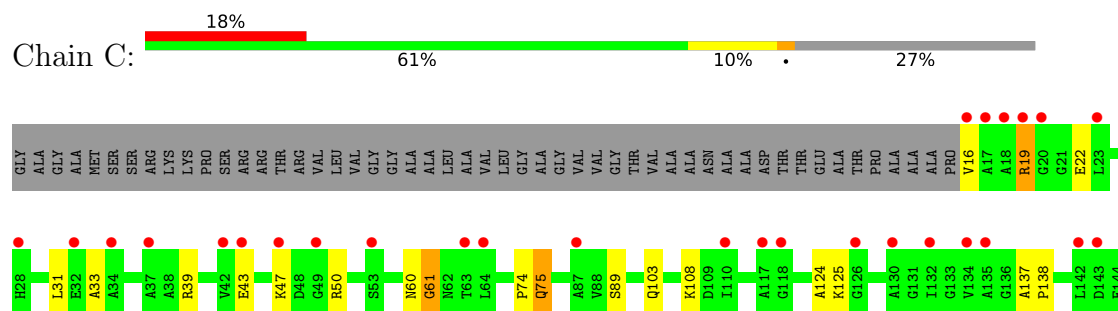
- Molecule 1: Extracellular haem-binding protein

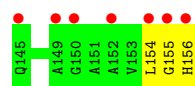


- Molecule 1: Extracellular haem-binding protein

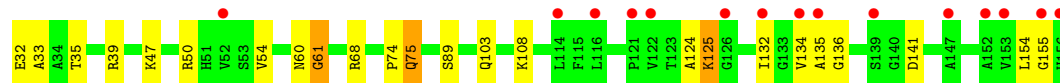
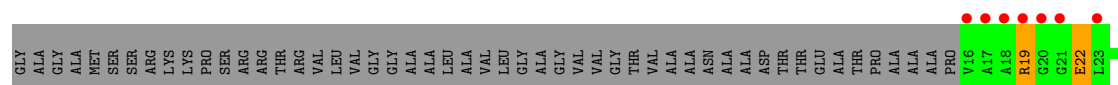


- Molecule 1: Extracellular haem-binding protein

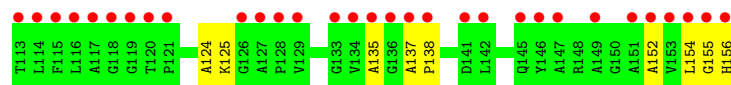
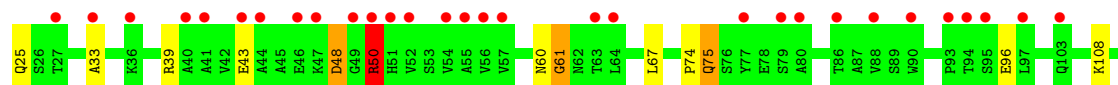
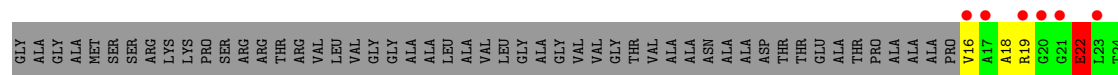




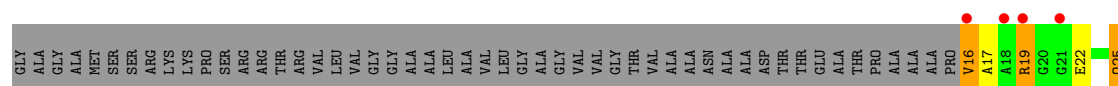
- Molecule 1: Extracellular haem-binding protein



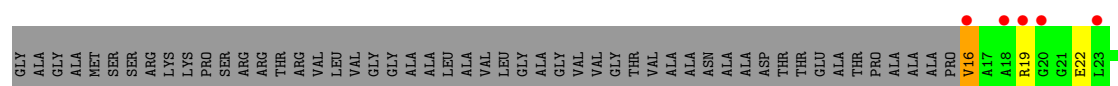
- Molecule 1: Extracellular haem-binding protein



- Molecule 1: Extracellular haem-binding protein

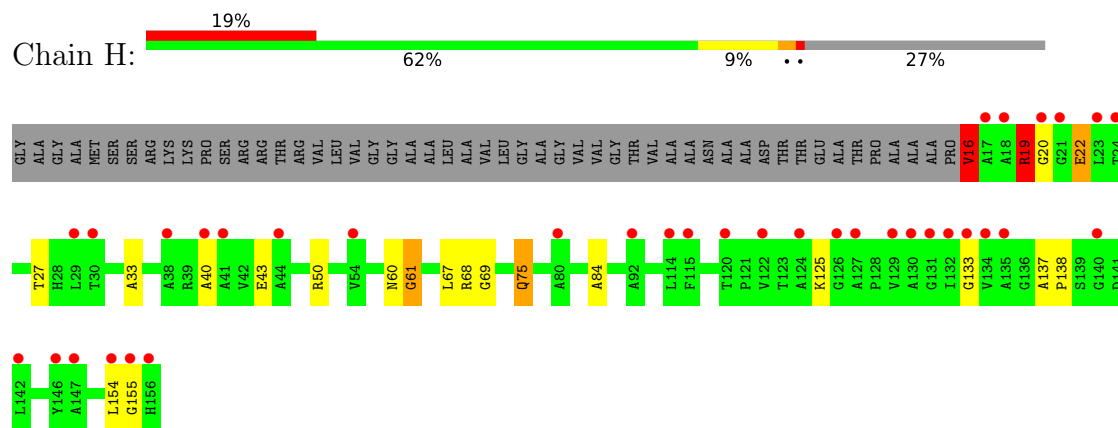


- Molecule 1: Extracellular haem-binding protein



- 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) 98.9 (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 0.295 , 0.335	Depositor DCC
R_{free} test set	2915 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.033 for l,-k,h	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.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.31	0/1012	0.67	0/1376
1	B	0.31	0/1012	0.66	0/1376
1	C	0.30	0/1012	0.67	0/1376
1	D	0.30	0/1012	0.70	0/1376
1	E	0.31	0/1012	0.71	0/1376
1	F	0.31	0/1012	0.68	0/1376
1	G	0.30	0/1012	0.68	0/1376
1	H	0.30	0/1012	0.68	0/1376
All	All	0.30	0/8096	0.68	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 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	997	0	996	21	0
1	B	997	0	996	18	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	13	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	1	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
All	All	8497	0	7968	92	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 (92) 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: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:NE2	1:D:75:GLN:H	1.99	0.58
1:D:33:ALA:CB	1:E:22:GLU:HG3	2.32	0.58
1:B:75:GLN:HE21	1:B:75:GLN:H	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:H	1:A:75:GLN:HE21	1.53	0.55
1:A:83:LYS:NZ	3:A:385:HOH:O	2.39	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:NE2	1:C:75:GLN:H	2.07	0.52
1:D:75:GLN:H	1:D:75:GLN:HE21	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ALA:HB1	1:B:138:PRO:CD	2.40	0.51
1:E:74:PRO:HB3	1:H:61:GLY:H	1.75	0.51
1:G:58:ASP:O	1:G:61:GLY:HA2	2.11	0.51
1:H:75:GLN:HE21	1:H:75:GLN:H	1.58	0.51
1:C:74:PRO:HB3	1:D:61:GLY:H	1.76	0.51
1:H:75:GLN:H	1:H:75:GLN:NE2	2.08	0.50
1:E:75:GLN:HE21	1:E:75:GLN:H	1.59	0.50
1:F:75:GLN:H	1:F:75:GLN:HE21	1.58	0.50
1:G:75:GLN:NE2	1:G:75:GLN:H	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:F:155:GLY:C	1:F:156:HIS:CG	2.92	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:B:50:ARG:HD3	3:B:717:HOH:O	2.16	0.44
1:D:33:ALA:HB2	1:E:22:GLU:HB2	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE1	1:G:155:GLY:HA2	2.18	0.44
1:E:137:ALA:HB1	1:E:138:PRO:CD	2.48	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: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:B:155:GLY:HA2	1:G:22:GLU:CD	2.45	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:40:ALA:HA	1:H:43:GLU:HB3	2.03	0.41
1:H:84:ALA:HB2	1:H:133:GLY:N	2.36	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%)	18	19
1	C	139/192 (72%)	134 (96%)	4 (3%)	1 (1%)	18	19
1	D	139/192 (72%)	132 (95%)	6 (4%)	1 (1%)	18	19
1	E	139/192 (72%)	134 (96%)	4 (3%)	1 (1%)	18	19
1	F	139/192 (72%)	136 (98%)	2 (1%)	1 (1%)	18	19
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%)	30	34

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%)	13	14
1	B	95/125 (76%)	91 (96%)	4 (4%)	26	36
1	C	95/125 (76%)	86 (90%)	9 (10%)	8	8
1	D	95/125 (76%)	84 (88%)	11 (12%)	5	5
1	E	95/125 (76%)	87 (92%)	8 (8%)	10	11
1	F	95/125 (76%)	86 (90%)	9 (10%)	8	8
1	G	95/125 (76%)	87 (92%)	8 (8%)	10	11
1	H	95/125 (76%)	88 (93%)	7 (7%)	13	14
All	All	760/1000 (76%)	697 (92%)	63 (8%)	10	11

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	47	LYS
1	A	50	ARG
1	A	75	GLN
1	A	103	GLN
1	A	108	LYS
1	A	156	HIS
1	B	47	LYS
1	B	50	ARG

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	108	LYS
1	C	16	VAL
1	C	19	ARG
1	C	43	GLU
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	103	GLN
1	D	108	LYS
1	D	125	LYS
1	D	132	ILE
1	D	141	ASP
1	E	22	GLU
1	E	25	GLN
1	E	43	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	25	GLN
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	47	LYS
1	G	75	GLN

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Mol	Chain	Res	Type
1	G	79	SER
1	G	99	LYS
1	G	103	GLN
1	G	154	LEU
1	G	156	HIS
1	H	16	VAL
1	H	19	ARG
1	H	22	GLU
1	H	27	THR
1	H	50	ARG
1	H	75	GLN
1	H	125	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	75	GLN
1	A	156	HIS
1	B	51	HIS
1	B	75	GLN
1	C	25	GLN
1	C	51	HIS
1	C	75	GLN
1	D	75	GLN
1	D	145	GLN
1	D	156	HIS
1	E	75	GLN
1	E	91	ASN
1	F	51	HIS
1	F	75	GLN
1	F	91	ASN
1	G	51	HIS
1	G	75	GLN
1	H	51	HIS
1	H	75	GLN
1	H	156	HIS

5.3.3 RNA ⓘ

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](#)

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.

No monomer is involved in short contacts.

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	141/192 (73%)	1.27	12 (8%) 16 14	64, 67, 77, 80	0
1	B	141/192 (73%)	1.51	32 (22%) 2 1	63, 68, 77, 82	0
1	C	141/192 (73%)	1.54	35 (24%) 2 1	64, 67, 76, 79	0
1	D	141/192 (73%)	1.39	22 (15%) 5 4	64, 67, 76, 78	0
1	E	141/192 (73%)	1.98	67 (47%) 0 0	64, 70, 74, 77	0
1	F	141/192 (73%)	1.39	17 (12%) 8 6	63, 68, 77, 82	0
1	G	141/192 (73%)	1.29	16 (11%) 10 8	64, 67, 76, 82	0
1	H	141/192 (73%)	1.58	36 (25%) 1 1	62, 66, 75, 79	0
All	All	1128/1536 (73%)	1.49	237 (21%) 2 2	62, 68, 76, 82	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	156	HIS	4.6
1	F	155	GLY	4.5
1	D	17	ALA	4.5
1	E	152	ALA	4.1
1	F	156	HIS	4.0
1	D	16	VAL	3.9
1	E	135	ALA	3.9
1	D	20	GLY	3.9
1	H	155	GLY	3.8
1	B	134	VAL	3.8
1	E	117	ALA	3.7
1	F	126	GLY	3.7
1	E	134	VAL	3.6
1	F	19	ARG	3.6
1	B	156	HIS	3.5
1	C	126	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	126	GLY	3.5
1	C	16	VAL	3.4
1	B	17	ALA	3.4
1	F	16	VAL	3.4
1	E	40	ALA	3.4
1	E	50	ARG	3.4
1	H	130	ALA	3.4
1	H	20	GLY	3.3
1	B	23	LEU	3.3
1	E	155	GLY	3.3
1	B	135	ALA	3.2
1	G	16	VAL	3.3
1	C	132	ILE	3.2
1	A	17	ALA	3.2
1	D	19	ARG	3.2
1	B	155	GLY	3.2
1	E	146	TYR	3.2
1	G	146	TYR	3.2
1	A	156	HIS	3.2
1	C	43	GLU	3.1
1	D	152	ALA	3.1
1	D	155	GLY	3.1
1	H	142	LEU	3.1
1	B	16	VAL	3.1
1	E	145	GLN	3.1
1	E	147	ALA	3.1
1	F	153	VAL	3.1
1	C	118	GLY	3.0
1	E	126	GLY	3.0
1	E	20	GLY	3.0
1	E	16	VAL	2.9
1	E	52	VAL	2.9
1	C	18	ALA	2.9
1	E	51	HIS	2.9
1	C	155	GLY	2.9
1	E	118	GLY	2.9
1	G	23	LEU	2.9
1	G	134	VAL	2.9
1	C	20	GLY	2.9
1	B	41	ALA	2.9
1	C	17	ALA	2.9
1	B	20	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	149	ALA	2.8
1	E	156	HIS	2.8
1	E	17	ALA	2.8
1	E	137	ALA	2.8
1	E	54	VAL	2.8
1	C	19	ARG	2.8
1	H	29	LEU	2.8
1	B	152	ALA	2.8
1	E	44	ALA	2.8
1	E	115	PHE	2.8
1	F	37	ALA	2.8
1	H	120	THR	2.7
1	D	135	ALA	2.7
1	H	146	TYR	2.7
1	H	115	PHE	2.7
1	E	128	PRO	2.7
1	E	114	LEU	2.7
1	B	154	LEU	2.7
1	H	127	ALA	2.7
1	E	116	LEU	2.7
1	B	42	VAL	2.6
1	C	154	LEU	2.6
1	A	133	GLY	2.6
1	E	127	ALA	2.6
1	F	34	ALA	2.6
1	G	19	ARG	2.6
1	E	63	THR	2.6
1	C	110	ILE	2.6
1	H	132	ILE	2.6
1	H	114	LEU	2.6
1	F	18	ALA	2.6
1	G	135	ALA	2.6
1	C	63	THR	2.6
1	H	126	GLY	2.6
1	D	156	HIS	2.6
1	D	23	LEU	2.5
1	B	19	ARG	2.5
1	A	20	GLY	2.5
1	E	138	PRO	2.5
1	E	151	ALA	2.5
1	H	21	GLY	2.5
1	B	53	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	134	VAL	2.5
1	G	56	VAL	2.5
1	E	46	GLU	2.5
1	G	118	GLY	2.5
1	B	85	PHE	2.5
1	C	53	SER	2.5
1	E	43	GLU	2.5
1	G	132	ILE	2.5
1	C	142	LEU	2.5
1	D	114	LEU	2.5
1	E	154	LEU	2.5
1	H	23	LEU	2.5
1	D	147	ALA	2.5
1	E	33	ALA	2.5
1	H	80	ALA	2.5
1	H	133	GLY	2.5
1	E	95	SER	2.4
1	B	132	ILE	2.4
1	E	56	VAL	2.4
1	B	37	ALA	2.4
1	B	80	ALA	2.4
1	H	135	ALA	2.4
1	C	32	GLU	2.4
1	D	132	ILE	2.4
1	E	64	LEU	2.4
1	E	141	ASP	2.4
1	E	55	ALA	2.4
1	B	88	VAL	2.4
1	C	134	VAL	2.4
1	E	57	VAL	2.4
1	C	23	LEU	2.4
1	B	149	ALA	2.4
1	F	41	ALA	2.4
1	B	153	VAL	2.4
1	H	134	VAL	2.4
1	A	103	GLN	2.4
1	B	61	GLY	2.3
1	A	18	ALA	2.3
1	B	130	ALA	2.3
1	C	47	LYS	2.3
1	G	18	ALA	2.3
1	C	42	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	19	ARG	2.3
1	B	116	LEU	2.3
1	C	145	GLN	2.3
1	E	97	LEU	2.3
1	E	103	GLN	2.3
1	E	142	LEU	2.3
1	F	114	LEU	2.3
1	B	119	GLY	2.3
1	F	136	GLY	2.3
1	C	149	ALA	2.3
1	C	152	ALA	2.3
1	H	17	ALA	2.3
1	H	92	ALA	2.3
1	H	147	ALA	2.3
1	G	51	HIS	2.3
1	C	117	ALA	2.3
1	D	153	VAL	2.3
1	E	153	VAL	2.3
1	E	133	GLY	2.3
1	F	49	GLY	2.3
1	D	18	ALA	2.3
1	H	44	ALA	2.3
1	C	156	HIS	2.3
1	E	129	VAL	2.3
1	H	122	VAL	2.3
1	A	61	GLY	2.2
1	E	21	GLY	2.2
1	E	119	GLY	2.2
1	H	140	GLY	2.2
1	C	87	ALA	2.2
1	E	80	ALA	2.2
1	E	94	THR	2.2
1	H	24	THR	2.2
1	F	21	GLY	2.2
1	C	135	ALA	2.2
1	E	41	ALA	2.2
1	H	18	ALA	2.2
1	H	124	ALA	2.2
1	B	76	SER	2.2
1	E	77	TYR	2.2
1	D	116	LEU	2.2
1	H	129	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	143	ASP	2.2
1	E	49	GLY	2.2
1	G	20	GLY	2.2
1	A	43	GLU	2.2
1	C	130	ALA	2.2
1	E	120	THR	2.2
1	E	23	LEU	2.2
1	B	129	VAL	2.2
1	D	52	VAL	2.2
1	F	42	VAL	2.2
1	H	54	VAL	2.2
1	E	93	PRO	2.2
1	E	47	LYS	2.2
1	D	21	GLY	2.2
1	C	34	ALA	2.2
1	E	79	SER	2.2
1	G	147	ALA	2.2
1	H	38	ALA	2.2
1	C	64	LEU	2.1
1	D	121	PRO	2.1
1	B	133	GLY	2.1
1	H	40	ALA	2.1
1	H	41	ALA	2.1
1	E	88	VAL	2.1
1	E	90	TRP	2.1
1	E	121	PRO	2.1
1	A	140	GLY	2.1
1	C	150	GLY	2.1
1	E	27	THR	2.1
1	C	37	ALA	2.1
1	A	114	LEU	2.1
1	C	28	HIS	2.1
1	A	122	VAL	2.1
1	E	136	GLY	2.1
1	H	131	GLY	2.1
1	E	86	THR	2.1
1	G	142	LEU	2.1
1	G	156	HIS	2.1
1	D	122	VAL	2.1
1	C	49	GLY	2.1
1	B	79	SER	2.0
1	D	139	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	40	ALA	2.0
1	F	132	ILE	2.0
1	B	146	TYR	2.0
1	B	54	VAL	2.0
1	B	122	VAL	2.0
1	E	113	THR	2.0
1	H	30	THR	2.0
1	F	44	ALA	2.0
1	H	154	LEU	2.0
1	A	132	ILE	2.0
1	E	36	LYS	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
2	FE	E	157	1/1	0.75	0.23	132,132,132,132	0
2	FE	E	158	1/1	0.82	0.20	99,99,99,99	0
2	FE	H	157	1/1	0.93	0.15	80,80,80,80	0
2	FE	C	157	1/1	0.94	0.10	77,77,77,77	0
2	FE	F	157	1/1	0.95	0.19	69,69,69,69	0
2	FE	D	157	1/1	0.95	0.11	72,72,72,72	0
2	FE	A	157	1/1	0.98	0.17	72,72,72,72	0
2	FE	B	157	1/1	0.99	0.18	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.