Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:53 AM GMT

PDB ID	:	2LH7
Title	:	X-RAY STRUCTURAL INVESTIGATION OF LEGHEMOGLOBIN. VI. STRUCTURE OF ACETATE-FERRILEGHEMOGLOBIN AT A RESOLUTION OF 2.0 ANGSTROMS (RUSSIAN)
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Deposited on	:	1982-04-23
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

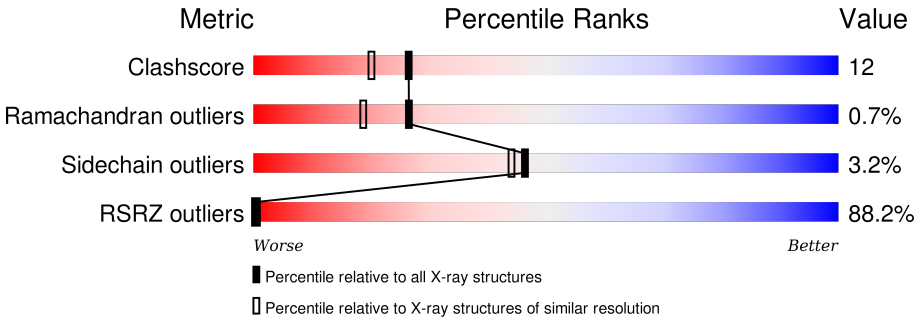
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	153	88% 24% 46% 26% .

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
3	NBE	A	155	-	-	X	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 1295 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.

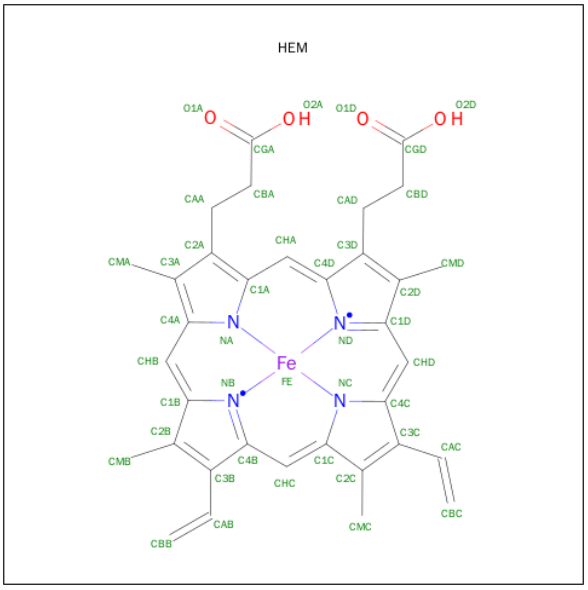
- Molecule 1 is a protein called LEGHEMOGLOBIN (NITROSOBENZENE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	153	Total	C	N	O	S	36	1	0
			1180	761	193	225	1			

There are 2 discrepancies between the modelled and reference sequences:

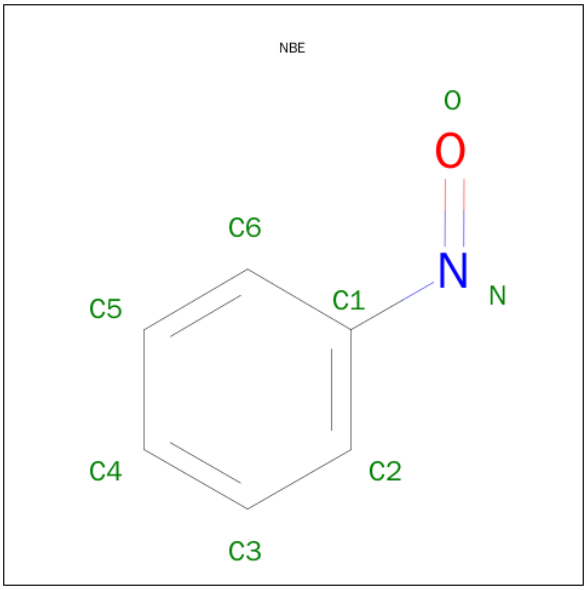
Chain	Residue	Modelled	Actual	Comment	Reference
A	79	GLU	GLN	CONFLICT	UNP P02240
A	150	ASP	ASN	CONFLICT	UNP P02240

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	3	0
			43	34	1	4	4		

- Molecule 3 is NITROSOBENZENE (three-letter code: NBE) (formula: C_6H_5NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	8	6	1	1	0	0

- Molecule 4 is water.

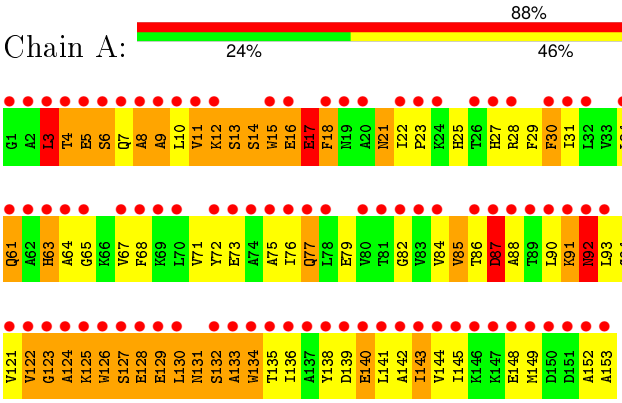
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	64	64	64	0	0

3 Residue-property plots (i)

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: LEGHEMOGLOBIN (NITROSOBENZENE)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	B 1 1 2	Depositor
Cell constants a, b, c, α, β, γ	93.23Å 38.25Å 51.88Å 90.00° 90.00° 98.70°	Depositor
Resolution (Å)	(Not available) – 2.00 9.92 – 1.98	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00) 92.3 (9.92-1.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available) 0.478 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	20.9	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.45 , 140.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[1]	$< \|L\| > = 0.39$, $< L^2 > = 0.21$	Xtriage
Outliers	0 of 11563 reflections	Xtriage
F_o,F_c correlation	0.52	EDS
Total number of atoms	1295	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: HEM, NBE

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	3.17	130/1214 (10.7%)	2.08	36/1648 (2.2%)

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	7

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	SER	CB-OG	10.29	1.55	1.42
1	A	138	TYR	CB-CG	9.76	1.66	1.51
1	A	138	TYR	CZ-OH	9.45	1.53	1.37
1	A	15	TRP	CD2-CE2	9.35	1.52	1.41
1	A	112	GLU	CG-CD	9.15	1.65	1.51
1	A	132[A]	SER	CA-CB	8.59	1.65	1.52
1	A	132[B]	SER	CA-CB	8.59	1.65	1.52
1	A	132[C]	SER	CA-CB	8.59	1.65	1.52
1	A	72	TYR	CE1-CZ	8.56	1.49	1.38
1	A	120	GLU	CG-CD	8.51	1.64	1.51
1	A	35	GLU	CD-OE2	8.38	1.34	1.25
1	A	106	HIS	CB-CG	8.19	1.64	1.50
1	A	15	TRP	CB-CG	8.16	1.65	1.50
1	A	123	GLY	CA-C	8.15	1.64	1.51
1	A	65	GLY	C-O	8.02	1.36	1.23
1	A	13	SER	CA-CB	8.02	1.65	1.52
1	A	72	TYR	CG-CD2	8.00	1.49	1.39
1	A	18	PHE	CB-CG	7.86	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	GLY	CA-C	7.80	1.64	1.51
1	A	129	GLU	CD-OE1	7.26	1.33	1.25
1	A	5	GLU	CD-OE2	7.14	1.33	1.25
1	A	15	TRP	CZ3-CH2	7.03	1.51	1.40
1	A	138	TYR	CD2-CE2	6.99	1.49	1.39
1	A	144	VAL	CB-CG2	6.99	1.67	1.52
1	A	11	VAL	CB-CG1	6.97	1.67	1.52
1	A	140	GLU	CB-CG	6.96	1.65	1.52
1	A	44	PHE	CB-CG	6.94	1.63	1.51
1	A	102	VAL	CB-CG1	6.89	1.67	1.52
1	A	110	VAL	CB-CG2	6.89	1.67	1.52
1	A	128	GLU	CD-OE2	-6.87	1.18	1.25
1	A	46	PHE	CB-CG	6.84	1.62	1.51
1	A	27	HIS	CE1-NE2	6.78	1.48	1.32
1	A	85	VAL	CB-CG2	6.76	1.67	1.52
1	A	111	LYS	N-CA	6.75	1.59	1.46
1	A	61	GLN	C-O	6.73	1.36	1.23
1	A	104	ASP	N-CA	6.71	1.59	1.46
1	A	152	ALA	C-O	6.71	1.36	1.23
1	A	15	TRP	NE1-CE2	-6.68	1.28	1.37
1	A	72	TYR	C-O	6.67	1.36	1.23
1	A	79	GLU	CB-CG	6.59	1.64	1.52
1	A	14	SER	CB-OG	-6.58	1.33	1.42
1	A	134	TRP	N-CA	6.58	1.59	1.46
1	A	121	VAL	CB-CG2	6.57	1.66	1.52
1	A	101	GLY	CA-C	6.56	1.62	1.51
1	A	28	ARG	CZ-NH1	6.56	1.41	1.33
1	A	68	PHE	C-O	6.55	1.35	1.23
1	A	113	ALA	CA-CB	6.54	1.66	1.52
1	A	88	ALA	N-CA	6.54	1.59	1.46
1	A	35	GLU	CD-OE1	-6.50	1.18	1.25
1	A	138	TYR	CD1-CE1	6.47	1.49	1.39
1	A	73	GLU	CG-CD	6.42	1.61	1.51
1	A	13	SER	CB-OG	-6.36	1.33	1.42
1	A	124	ALA	N-CA	6.29	1.58	1.46
1	A	86	THR	N-CA	6.29	1.58	1.46
1	A	27	HIS	CG-ND1	6.27	1.52	1.38
1	A	11	VAL	N-CA	6.26	1.58	1.46
1	A	149	MET	C-O	6.24	1.35	1.23
1	A	145	ILE	N-CA	6.19	1.58	1.46
1	A	109	VAL	CA-CB	6.17	1.67	1.54
1	A	111	LYS	CD-CE	6.12	1.66	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	SER	N-CA	6.08	1.58	1.46
1	A	68	PHE	CG-CD2	6.03	1.47	1.38
1	A	6	SER	CA-CB	5.99	1.61	1.52
1	A	15	TRP	C-O	5.99	1.34	1.23
1	A	124	ALA	C-O	5.98	1.34	1.23
1	A	16	GLU	CG-CD	5.96	1.60	1.51
1	A	97	HIS	CA-CB	5.96	1.67	1.53
1	A	148	GLU	CB-CG	5.93	1.63	1.52
1	A	63	HIS	CB-CG	5.92	1.60	1.50
1	A	40	ALA	CA-CB	5.92	1.64	1.52
1	A	99	SER	N-CA	5.91	1.58	1.46
1	A	122	VAL	N-CA	5.91	1.58	1.46
1	A	55	GLN	C-O	5.88	1.34	1.23
1	A	68	PHE	CE1-CZ	5.87	1.48	1.37
1	A	67	VAL	CB-CG2	5.86	1.65	1.52
1	A	75	ALA	N-CA	5.86	1.58	1.46
1	A	97	HIS	CG-CD2	-5.82	1.25	1.35
1	A	52	GLU	CG-CD	-5.79	1.43	1.51
1	A	45	SER	CB-OG	5.76	1.49	1.42
1	A	15	TRP	CD1-NE1	5.75	1.47	1.38
1	A	152	ALA	N-CA	5.75	1.57	1.46
1	A	102	VAL	N-CA	5.73	1.57	1.46
1	A	84	VAL	CB-CG1	5.69	1.64	1.52
1	A	77	GLN	CG-CD	5.67	1.64	1.51
1	A	8	ALA	C-O	5.65	1.34	1.23
1	A	82	GLY	CA-C	5.65	1.60	1.51
1	A	90	LEU	CA-CB	5.61	1.66	1.53
1	A	120	GLU	CA-CB	5.59	1.66	1.53
1	A	18	PHE	N-CA	5.56	1.57	1.46
1	A	111	LYS	CB-CG	5.55	1.67	1.52
1	A	58	PRO	N-CD	5.52	1.55	1.47
1	A	53	VAL	CA-CB	5.49	1.66	1.54
1	A	115	LEU	N-CA	5.49	1.57	1.46
1	A	16	GLU	CD-OE1	5.45	1.31	1.25
1	A	125	LYS	CD-CE	5.42	1.64	1.51
1	A	9	ALA	CA-CB	5.41	1.63	1.52
1	A	92	ASN	CB-CG	5.41	1.63	1.51
1	A	76	ILE	C-O	5.38	1.33	1.23
1	A	99	SER	C-O	5.37	1.33	1.23
1	A	71	VAL	CB-CG1	5.37	1.64	1.52
1	A	153	ALA	C-OXT	5.36	1.33	1.23
1	A	59	GLU	CD-OE2	5.34	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	VAL	CB-CG1	5.33	1.64	1.52
1	A	140	GLU	CD-OE2	5.32	1.31	1.25
1	A	75	ALA	C-O	5.32	1.33	1.23
1	A	98	VAL	CB-CG2	5.32	1.64	1.52
1	A	45	SER	N-CA	5.28	1.56	1.46
1	A	92	ASN	C-O	5.27	1.33	1.23
1	A	79	GLU	C-O	5.23	1.33	1.23
1	A	106	HIS	ND1-CE1	5.23	1.47	1.34
1	A	4	THR	C-O	5.22	1.33	1.23
1	A	63	HIS	CE1-NE2	5.20	1.44	1.32
1	A	15	TRP	N-CA	5.18	1.56	1.46
1	A	3	LEU	CA-CB	5.16	1.65	1.53
1	A	148	GLU	CG-CD	-5.15	1.44	1.51
1	A	91	LYS	CD-CE	5.15	1.64	1.51
1	A	43	LEU	CA-CB	5.13	1.65	1.53
1	A	141	LEU	N-CA	5.12	1.56	1.46
1	A	68	PHE	N-CA	5.12	1.56	1.46
1	A	133	ALA	CA-C	5.10	1.66	1.52
1	A	143	ILE	CA-CB	5.09	1.66	1.54
1	A	138	TYR	N-CA	5.08	1.56	1.46
1	A	127	SER	C-O	5.06	1.32	1.23
1	A	38	PRO	N-CA	5.05	1.55	1.47
1	A	130	LEU	N-CA	5.05	1.56	1.46
1	A	52	GLU	N-CA	5.03	1.56	1.46
1	A	84	VAL	N-CA	5.02	1.56	1.46
1	A	64	ALA	N-CA	5.02	1.56	1.46
1	A	85	VAL	CA-C	5.01	1.66	1.52
1	A	134	TRP	CD2-CE2	-5.01	1.35	1.41

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	TYR	CB-CG-CD1	-10.23	114.86	121.00
1	A	28	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	112	GLU	OE1-CD-OE2	-8.78	112.77	123.30
1	A	15	TRP	CG-CD2-CE3	-7.64	127.03	133.90
1	A	16	GLU	OE1-CD-OE2	-7.38	114.45	123.30
1	A	73	GLU	OE1-CD-OE2	-7.26	114.59	123.30
1	A	138	TYR	CB-CG-CD2	7.16	125.30	121.00
1	A	128	GLU	OE1-CD-OE2	-6.95	114.95	123.30
1	A	108	PRO	N-CA-CB	6.93	111.62	103.30
1	A	29	PHE	CB-CG-CD1	-6.82	116.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	17	GLU	OE1-CD-OE2	-6.78	115.16	123.30
1	A	30	PHE	CB-CG-CD2	-6.57	116.20	120.80
1	A	46	PHE	CB-CG-CD2	6.56	125.39	120.80
1	A	54	PRO	N-CA-CB	6.56	111.17	103.30
1	A	23	PRO	N-CA-CB	6.51	111.11	103.30
1	A	120	GLU	OE1-CD-OE2	-6.40	115.62	123.30
1	A	29	PHE	CD1-CG-CD2	6.15	126.29	118.30
1	A	72	TYR	CG-CD1-CE1	-6.13	116.39	121.30
1	A	15	TRP	CH2-CZ2-CE2	-6.07	111.33	117.40
1	A	126	TRP	CE2-CD2-CG	-5.91	102.57	107.30
1	A	134	TRP	CG-CD1-NE1	-5.84	104.26	110.10
1	A	15	TRP	CD2-CE3-CZ3	-5.77	111.30	118.80
1	A	68	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	A	5	GLU	OE1-CD-OE2	-5.66	116.50	123.30
1	A	48	LYS	CB-CA-C	-5.66	99.08	110.40
1	A	138	TYR	CD1-CE1-CZ	5.64	124.88	119.80
1	A	142	ALA	O-C-N	5.62	131.69	122.70
1	A	12	LYS	O-C-N	5.53	131.54	122.70
1	A	87	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	A	126	TRP	NE1-CE2-CD2	5.43	112.73	107.30
1	A	131	ASN	O-C-N	5.37	131.29	122.70
1	A	149	MET	O-C-N	5.37	131.28	122.70
1	A	15	TRP	NE1-CE2-CZ2	-5.33	124.53	130.40
1	A	15	TRP	CD1-NE1-CE2	-5.33	104.21	109.00
1	A	8	ALA	O-C-N	5.28	131.14	122.70
1	A	124	ALA	CB-CA-C	-5.16	102.36	110.10

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	17	GLU	Sidechain
1	A	42	ASP	Sidechain
1	A	55	GLN	Sidechain
1	A	56	ASN	Sidechain
1	A	61	GLN	Sidechain
1	A	87	ASP	Sidechain
1	A	92	ASN	Sidechain

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	1180	0	1200	24	200
2	A	43	0	30	7	0
3	A	8	0	5	12	0
4	A	64	0	0	0	27
All	All	1295	0	1235	29	201

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 12.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:PHE:HZ	3:A:155:NBE:H5	1.25	0.96
1:A:30:PHE:CZ	3:A:155:NBE:H5	2.17	0.76
1:A:63:HIS:HB3	3:A:155:NBE:H3	1.72	0.71
1:A:63:HIS:HB3	3:A:155:NBE:C3	2.24	0.68
2:A:154:HEM:NA	3:A:155:NBE:H2	2.10	0.67
1:A:92:ASN:O	1:A:96:VAL:HG12	2.01	0.60
1:A:63:HIS:HB3	3:A:155:NBE:C4	2.32	0.60
1:A:77:GLN:NE2	1:A:85:VAL:H	2.03	0.56
1:A:18:PHE:CE1	1:A:25:HIS:HB3	2.40	0.56
1:A:30:PHE:HZ	3:A:155:NBE:C5	2.08	0.56
2:A:154:HEM:C4A	3:A:155:NBE:H2	2.43	0.54
1:A:63:HIS:HB3	3:A:155:NBE:H4	1.89	0.54
1:A:21:ASN:C	1:A:21:ASN:HD22	2.11	0.51
1:A:102:VAL:HG13	2:A:154:HEM:HAC	1.95	0.49
1:A:139:ASP:O	1:A:143:ILE:HG13	2.13	0.49
1:A:103:ALA:O	1:A:106:HIS:HB2	2.14	0.47
2:A:154:HEM:C1A	3:A:155:NBE:H2	2.50	0.47
1:A:54:PRO:HB2	1:A:57:ASN:HB2	1.95	0.46
1:A:87:ASP:O	1:A:91:LYS:HG3	2.16	0.46
2:A:154:HEM:C1A	3:A:155:NBE:C2	2.99	0.45
1:A:31:ILE:O	1:A:35:GLU:HG3	2.16	0.45
1:A:93:LEU:HA	1:A:93:LEU:HD23	1.59	0.44
2:A:154:HEM:NA	3:A:155:NBE:C2	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HG3	2:A:154:HEM:HAD2	2.01	0.43
1:A:21:ASN:C	1:A:21:ASN:ND2	2.72	0.42
1:A:17:GLU:OE2	1:A:122:VAL:HG12	2.20	0.41
1:A:136:ILE:O	1:A:140:GLU:HG2	2.21	0.41
1:A:22:ILE:HA	1:A:22:ILE:HD13	1.81	0.40

All (201) 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)
1:A:126:TRP:CD1	1:A:128:GLU:C[2_675]	0.34	1.86
1:A:4:THR:OG1	1:A:17:GLU:CB[2_675]	0.47	1.73
1:A:127:SER:N	1:A:131:ASN:CA[2_675]	0.51	1.69
1:A:6:SER:O	1:A:14:SER:N[2_675]	0.53	1.67
1:A:8:ALA:CA	1:A:13:SER:OG[2_675]	0.54	1.66
1:A:6:SER:OG	1:A:14:SER:O[2_675]	0.57	1.63
1:A:10:LEU:CA	1:A:10:LEU:C[2_675]	0.59	1.61
1:A:126:TRP:NE1	1:A:128:GLU:CA[2_675]	0.66	1.54
1:A:9:ALA:CB	1:A:12:LYS:C[2_675]	0.69	1.51
1:A:119:LYS:CD	1:A:128:GLU:OE2[2_675]	0.76	1.44
1:A:126:TRP:C	1:A:131:ASN:C[2_675]	0.80	1.40
1:A:126:TRP:CG	1:A:128:GLU:O[2_675]	0.84	1.36
1:A:126:TRP:C	1:A:131:ASN:CA[2_675]	0.90	1.30
1:A:8:ALA:C	1:A:13:SER:CB[2_675]	0.90	1.30
1:A:134:TRP:N	4:A:215:HOH:O[2_675]	0.91	1.29
1:A:9:ALA:N	1:A:13:SER:CA[2_675]	0.95	1.25
1:A:10:LEU:O	1:A:10:LEU:CB[2_675]	0.96	1.24
1:A:126:TRP:NE1	1:A:128:GLU:N[2_675]	0.98	1.22
1:A:119:LYS:CE	1:A:128:GLU:CG[2_675]	1.01	1.19
1:A:130:LEU:N	1:A:130:LEU:CD2[2_675]	1.04	1.16
1:A:8:ALA:N	1:A:13:SER:OG[2_675]	1.05	1.15
1:A:127:SER:N	1:A:131:ASN:N[2_675]	1.09	1.11
1:A:10:LEU:CA	1:A:10:LEU:O[2_675]	1.09	1.11
1:A:7:GLN:CB	4:A:201:HOH:O[2_675]	1.09	1.11
1:A:9:ALA:CA	1:A:13:SER:N[2_675]	1.10	1.10
1:A:4:THR:CB	1:A:17:GLU:CB[2_675]	1.11	1.09
1:A:125:LYS:C	1:A:133:ALA:N[2_675]	1.13	1.07
1:A:130:LEU:O	4:A:190:HOH:O[2_675]	1.13	1.07
1:A:7:GLN:CA	4:A:201:HOH:O[2_675]	1.15	1.05
1:A:126:TRP:O	1:A:131:ASN:C[2_675]	1.19	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:CD1	1:A:128:GLU:O[2_675]	1.21	0.99
1:A:7:GLN:OE1	1:A:17:GLU:OE2[2_675]	1.23	0.97
1:A:6:SER:C	1:A:14:SER:N[2_675]	1.24	0.96
1:A:9:ALA:O	1:A:9:ALA:O[2_675]	1.26	0.94
1:A:126:TRP:CE2	1:A:128:GLU:CA[2_675]	1.26	0.94
1:A:9:ALA:CB	1:A:12:LYS:CA[2_675]	1.26	0.94
1:A:123:GLY:O	1:A:132[B]:SER:OG[2_675]	1.28	0.92
1:A:7:GLN:OE1	1:A:17:GLU:OE1[2_675]	1.28	0.92
1:A:125:LYS:CB	1:A:133:ALA:CA[2_675]	1.29	0.91
1:A:119:LYS:O	4:A:181:HOH:O[2_675]	1.29	0.91
1:A:126:TRP:O	1:A:131:ASN:O[2_675]	1.30	0.90
1:A:10:LEU:CD1	1:A:14:SER:OG[2_675]	1.30	0.90
1:A:7:GLN:NE2	1:A:122:VAL:CA[2_675]	1.30	0.90
1:A:17:GLU:C	4:A:219:HOH:O[2_675]	1.31	0.89
1:A:9:ALA:N	1:A:13:SER:CB[2_675]	1.31	0.89
1:A:125:LYS:O	1:A:133:ALA:N[2_675]	1.31	0.89
1:A:7:GLN:OE1	1:A:17:GLU:CD[2_675]	1.32	0.88
1:A:4:THR:O	4:A:204:HOH:O[2_675]	1.32	0.88
1:A:6:SER:C	1:A:14:SER:CA[2_675]	1.33	0.87
1:A:9:ALA:N	1:A:13:SER:N[2_675]	1.34	0.86
1:A:7:GLN:CG	1:A:17:GLU:OE2[2_675]	1.35	0.85
1:A:7:GLN:CD	1:A:17:GLU:OE2[2_675]	1.35	0.85
1:A:9:ALA:CB	1:A:13:SER:N[2_675]	1.35	0.85
1:A:8:ALA:CA	1:A:13:SER:CB[2_675]	1.36	0.84
1:A:6:SER:CB	1:A:14:SER:O[2_675]	1.39	0.81
1:A:126:TRP:CB	1:A:128:GLU:O[2_675]	1.39	0.81
1:A:126:TRP:CD1	1:A:128:GLU:CA[2_675]	1.41	0.79
1:A:7:GLN:C	4:A:201:HOH:O[2_675]	1.42	0.78
1:A:6:SER:C	1:A:13:SER:C[2_675]	1.42	0.78
1:A:119:LYS:CD	1:A:128:GLU:CD[2_675]	1.42	0.78
1:A:4:THR:CA	1:A:17:GLU:CG[2_675]	1.44	0.76
1:A:4:THR:N	1:A:17:GLU:CG[2_675]	1.44	0.76
1:A:6:SER:O	1:A:14:SER:CA[2_675]	1.44	0.76
1:A:4:THR:CB	1:A:17:GLU:CA[2_675]	1.45	0.75
1:A:134:TRP:CA	4:A:215:HOH:O[2_675]	1.45	0.75
1:A:126:TRP:NE1	1:A:128:GLU:C[2_675]	1.50	0.70
1:A:10:LEU:CA	1:A:10:LEU:CA[2_675]	1.50	0.70
1:A:6:SER:C	1:A:13:SER:O[2_675]	1.52	0.68
1:A:10:LEU:CD2	1:A:11:VAL:CA[2_675]	1.53	0.67
1:A:4:THR:OG1	1:A:17:GLU:CG[2_675]	1.53	0.67
1:A:130:LEU:CA	1:A:130:LEU:CD2[2_675]	1.53	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLN:N	1:A:13:SER:O[2_675]	1.53	0.67
1:A:122:VAL:N	1:A:129:GLU:OE2[2_675]	1.54	0.66
1:A:5:GLU:CB	1:A:16:GLU:CB[2_675]	1.54	0.66
1:A:5:GLU:C	1:A:16:GLU:CB[2_675]	1.55	0.65
1:A:126:TRP:CG	1:A:128:GLU:C[2_675]	1.55	0.65
1:A:6:SER:CB	1:A:14:SER:C[2_675]	1.56	0.64
1:A:126:TRP:CD1	1:A:129:GLU:N[2_675]	1.56	0.64
1:A:127:SER:CA	1:A:131:ASN:CA[2_675]	1.56	0.64
1:A:9:ALA:C	1:A:9:ALA:O[2_675]	1.57	0.63
1:A:6:SER:O	1:A:13:SER:C[2_675]	1.57	0.63
1:A:10:LEU:N	1:A:10:LEU:O[2_675]	1.58	0.62
1:A:56:ASN:OD1	4:A:171:HOH:O[1_545]	1.58	0.62
1:A:10:LEU:CG	1:A:14:SER:OG[2_675]	1.58	0.62
1:A:127:SER:N	1:A:131:ASN:CB[2_675]	1.58	0.62
1:A:7:GLN:N	1:A:14:SER:CA[2_675]	1.60	0.60
1:A:10:LEU:C	1:A:10:LEU:CB[2_675]	1.60	0.60
1:A:130:LEU:CB	1:A:130:LEU:CG[2_675]	1.60	0.60
1:A:125:LYS:CA	1:A:133:ALA:N[2_675]	1.61	0.59
1:A:6:SER:CB	1:A:15:TRP:N[2_675]	1.62	0.58
1:A:118:ILE:O	1:A:129:GLU:OE2[2_675]	1.62	0.58
1:A:126:TRP:C	1:A:131:ASN:CB[2_675]	1.63	0.57
1:A:129:GLU:C	1:A:130:LEU:CD2[2_675]	1.63	0.57
1:A:4:THR:OG1	1:A:17:GLU:CA[2_675]	1.64	0.56
1:A:6:SER:CB	1:A:15:TRP:CA[2_675]	1.64	0.56
1:A:4:THR:CB	1:A:17:GLU:CG[2_675]	1.65	0.55
1:A:6:SER:N	1:A:17:GLU:N[2_675]	1.66	0.54
1:A:130:LEU:CA	1:A:130:LEU:CB[2_675]	1.67	0.53
1:A:18:PHE:N	4:A:219:HOH:O[2_675]	1.68	0.52
1:A:126:TRP:CA	1:A:131:ASN:C[2_675]	1.68	0.52
1:A:6:SER:OG	1:A:14:SER:C[2_675]	1.68	0.52
1:A:5:GLU:CA	1:A:16:GLU:CB[2_675]	1.69	0.51
1:A:126:TRP:O	1:A:131:ASN:CA[2_675]	1.69	0.51
1:A:122:VAL:O	1:A:132[C]:SER:OG[2_675]	1.70	0.50
1:A:56:ASN:CB	4:A:187:HOH:O[1_545]	1.70	0.50
1:A:126:TRP:NE1	1:A:127:SER:C[2_675]	1.71	0.49
1:A:7:GLN:CB	1:A:17:GLU:OE2[2_675]	1.71	0.49
1:A:17:GLU:O	4:A:219:HOH:O[2_675]	1.72	0.48
1:A:8:ALA:C	1:A:13:SER:OG[2_675]	1.73	0.47
1:A:6:SER:CB	1:A:15:TRP:C[2_675]	1.73	0.47
1:A:15:TRP:CB	4:A:218:HOH:O[2_675]	1.73	0.47
1:A:6:SER:CA	1:A:16:GLU:N[2_675]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LYS:CB	1:A:133:ALA:N[2_675]	1.75	0.45
1:A:6:SER:N	1:A:16:GLU:N[2_675]	1.76	0.44
1:A:10:LEU:O	1:A:10:LEU:CG[2_675]	1.77	0.43
1:A:56:ASN:OD1	4:A:170:HOH:O[1_545]	1.78	0.42
1:A:118:ILE:O	1:A:129:GLU:CD[2_675]	1.80	0.40
1:A:133:ALA:C	4:A:215:HOH:O[2_675]	1.80	0.40
1:A:5:GLU:CG	1:A:16:GLU:CG[2_675]	1.81	0.39
1:A:118:ILE:CG2	1:A:129:GLU:CB[2_675]	1.81	0.39
1:A:126:TRP:CH2	1:A:126:TRP:CH2[2_675]	1.81	0.39
1:A:130:LEU:CA	1:A:130:LEU:CG[2_675]	1.81	0.39
1:A:8:ALA:N	1:A:13:SER:CB[2_675]	1.81	0.39
1:A:5:GLU:CG	1:A:16:GLU:CB[2_675]	1.81	0.39
1:A:10:LEU:N	1:A:10:LEU:C[2_675]	1.82	0.38
1:A:11:VAL:O	4:A:218:HOH:O[2_675]	1.82	0.38
1:A:122:VAL:CG2	1:A:132[A]:SER:OG[2_675]	1.82	0.38
1:A:127:SER:N	1:A:131:ASN:C[2_675]	1.83	0.37
1:A:126:TRP:CE2	1:A:128:GLU:N[2_675]	1.83	0.37
1:A:9:ALA:CB	1:A:12:LYS:O[2_675]	1.83	0.37
1:A:6:SER:CA	1:A:15:TRP:N[2_675]	1.84	0.36
1:A:4:THR:N	1:A:17:GLU:CD[2_675]	1.84	0.36
1:A:7:GLN:NE2	1:A:122:VAL:CB[2_675]	1.84	0.36
1:A:15:TRP:N	4:A:218:HOH:O[2_675]	1.85	0.35
1:A:10:LEU:CD1	1:A:14:SER:CB[2_675]	1.85	0.35
1:A:126:TRP:O	1:A:131:ASN:CG[2_675]	1.87	0.33
1:A:126:TRP:CB	1:A:132[B]:SER:OG[2_675]	1.87	0.33
1:A:9:ALA:CB	1:A:12:LYS:CB[2_675]	1.87	0.33
1:A:6:SER:C	1:A:14:SER:C[2_675]	1.88	0.32
1:A:7:GLN:N	1:A:14:SER:N[2_675]	1.88	0.32
1:A:8:ALA:CB	1:A:13:SER:OG[2_675]	1.88	0.32
1:A:7:GLN:N	1:A:13:SER:C[2_675]	1.88	0.32
1:A:119:LYS:CG	1:A:128:GLU:CB[2_675]	1.88	0.32
1:A:4:THR:CG2	1:A:17:GLU:CB[2_675]	1.89	0.31
1:A:126:TRP:C	1:A:131:ASN:N[2_675]	1.90	0.30
1:A:7:GLN:CG	1:A:122:VAL:CG1[2_675]	1.91	0.29
1:A:125:LYS:O	1:A:130:LEU:O[2_675]	1.92	0.28
1:A:7:GLN:C	1:A:13:SER:OG[2_675]	1.94	0.26
1:A:6:SER:CA	1:A:14:SER:C[2_675]	1.95	0.25
1:A:10:LEU:C	1:A:10:LEU:C[2_675]	1.95	0.25
1:A:7:GLN:NE2	1:A:122:VAL:C[2_675]	1.95	0.25
1:A:4:THR:C	4:A:204:HOH:O[2_675]	1.95	0.25
1:A:9:ALA:C	1:A:13:SER:N[2_675]	1.96	0.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:N	1:A:16:GLU:CA[2_675]	1.96	0.24
1:A:122:VAL:CG2	1:A:129:GLU:CA[2_675]	1.97	0.23
4:A:159:HOH:O	4:A:176:HOH:O[2_675]	1.97	0.23
1:A:126:TRP:C	1:A:131:ASN:O[2_675]	1.97	0.23
1:A:130:LEU:N	1:A:130:LEU:CG[2_675]	1.98	0.22
1:A:126:TRP:N	1:A:131:ASN:C[2_675]	1.98	0.22
1:A:122:VAL:CG2	1:A:129:GLU:O[2_675]	1.99	0.21
1:A:9:ALA:CA	1:A:13:SER:CA[2_675]	2.00	0.20
1:A:124:ALA:O	1:A:135:THR:CB[2_675]	2.01	0.19
1:A:6:SER:N	1:A:13:SER:O[2_675]	2.01	0.19
1:A:126:TRP:CB	4:A:189:HOH:O[2_675]	2.02	0.18
1:A:16:GLU:O	4:A:219:HOH:O[2_675]	2.03	0.17
1:A:8:ALA:O	1:A:13:SER:CB[2_675]	2.03	0.17
1:A:128:GLU:N	4:A:210:HOH:O[2_675]	2.03	0.17
1:A:127:SER:CA	1:A:131:ASN:CB[2_675]	2.04	0.16
1:A:126:TRP:CG	1:A:128:GLU:CA[2_675]	2.04	0.16
1:A:126:TRP:CD2	1:A:128:GLU:CA[2_675]	2.05	0.15
1:A:9:ALA:CA	1:A:12:LYS:C[2_675]	2.05	0.15
1:A:6:SER:CA	1:A:13:SER:O[2_675]	2.05	0.15
1:A:122:VAL:C	1:A:132[C]:SER:OG[2_675]	2.05	0.15
1:A:122:VAL:CG1	1:A:129:GLU:CG[2_675]	2.05	0.15
1:A:126:TRP:O	1:A:131:ASN:CB[2_675]	2.06	0.14
1:A:8:ALA:C	1:A:13:SER:CA[2_675]	2.06	0.14
1:A:119:LYS:CG	1:A:128:GLU:OE2[2_675]	2.06	0.14
1:A:119:LYS:NZ	1:A:128:GLU:CG[2_675]	2.07	0.13
1:A:119:LYS:CD	1:A:128:GLU:CG[2_675]	2.07	0.13
1:A:56:ASN:N	4:A:170:HOH:O[1_545]	2.07	0.13
1:A:123:GLY:O	1:A:132[C]:SER:OG[2_675]	2.08	0.12
1:A:125:LYS:O	1:A:133:ALA:CA[2_675]	2.08	0.12
1:A:4:THR:C	1:A:17:GLU:CG[2_675]	2.08	0.12
1:A:119:LYS:CE	1:A:128:GLU:CB[2_675]	2.09	0.11
1:A:5:GLU:O	1:A:16:GLU:CB[2_675]	2.09	0.11
1:A:6:SER:CB	1:A:16:GLU:N[2_675]	2.10	0.10
1:A:6:SER:N	1:A:16:GLU:C[2_675]	2.11	0.09
1:A:123:GLY:C	1:A:132[C]:SER:OG[2_675]	2.11	0.09
1:A:15:TRP:CA	4:A:218:HOH:O[2_675]	2.12	0.08
1:A:130:LEU:C	4:A:190:HOH:O[2_675]	2.12	0.08
1:A:5:GLU:CG	1:A:16:GLU:CD[2_675]	2.13	0.07
1:A:7:GLN:NE2	1:A:122:VAL:O[2_675]	2.14	0.06
1:A:118:ILE:CG2	1:A:129:GLU:CG[2_675]	2.16	0.04
1:A:126:TRP:N	1:A:133:ALA:N[2_675]	2.17	0.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:GLU:C	1:A:13:SER:O[2_675]	2.17	0.03
1:A:126:TRP:NE1	1:A:128:GLU:CB[2_675]	2.17	0.03
1:A:125:LYS:CA	1:A:133:ALA:CA[2_675]	2.18	0.02
1:A:119:LYS:C	4:A:181:HOH:O[2_675]	2.18	0.02
1:A:7:GLN:CA	1:A:14:SER:CA[2_675]	2.18	0.02
1:A:5:GLU:C	1:A:16:GLU:CA[2_675]	2.18	0.02
1:A:122:VAL:CG2	1:A:129:GLU:C[2_675]	2.18	0.02

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	153/153 (100%)	150 (98%)	2 (1%)	1 (1%)	26 19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	LEU

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	127/125 (102%)	123 (97%)	4 (3%)	47 46

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	21	ASN
1	A	34	LEU
1	A	96	VAL

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

Mol	Chain	Res	Type
1	A	21	ASN
1	A	25	HIS
1	A	61	GLN
1	A	77	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 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	HEM	A	154	1,3	30,50,50	4.19	22 (73%)	24,82,82	2.78	11 (45%)
3	NBE	A	155	2	8,8,8	0.60	0	9,9,9	0.94	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	154	1,3	-	0/10/54/54	0/0/8/8
3	NBE	A	155	2	-	0/2/2/2	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	154	HEM	C2D-C3D	-6.05	1.36	1.54
2	A	154	HEM	C2C-C1C	-3.11	1.46	1.52
2	A	154	HEM	C2D-C1D	2.17	1.59	1.51
2	A	154	HEM	CMC-C2C	2.64	1.59	1.53
2	A	154	HEM	CMB-C2B	2.86	1.59	1.53
2	A	154	HEM	CMA-C3A	2.93	1.57	1.51
2	A	154	HEM	CMD-C2D	3.17	1.60	1.53
2	A	154	HEM	C1A-CHA	3.25	1.48	1.39
2	A	154	HEM	C2A-C3A	3.32	1.47	1.37
2	A	154	HEM	C3C-CAC	3.38	1.57	1.51
2	A	154	HEM	FE-ND	3.76	2.17	1.97
2	A	154	HEM	C3D-C4D	3.83	1.56	1.51
2	A	154	HEM	C4A-CHB	3.84	1.50	1.39
2	A	154	HEM	CAD-C3D	5.11	1.64	1.54
2	A	154	HEM	CHC-C1C	5.26	1.48	1.36
2	A	154	HEM	CAA-C2A	5.37	1.61	1.52
2	A	154	HEM	CHD-C4C	5.95	1.50	1.36
2	A	154	HEM	C3B-C4B	6.36	1.57	1.51
2	A	154	HEM	FE-NB	6.48	2.31	1.97
2	A	154	HEM	C4C-NC	6.51	1.44	1.36
2	A	154	HEM	C3B-CAB	6.92	1.64	1.51
2	A	154	HEM	C1C-NC	8.07	1.46	1.36

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	154	HEM	CAA-C2A-C1A	-5.23	121.33	127.01
2	A	154	HEM	CMA-C3A-C4A	-4.94	120.19	128.36
2	A	154	HEM	CAA-CBA-CGA	-3.04	107.18	112.75
2	A	154	HEM	C2C-C1C-NC	-2.56	105.89	110.21
2	A	154	HEM	C3B-C4B-CHC	2.02	126.00	123.16
2	A	154	HEM	CMA-C3A-C2A	2.33	130.11	125.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	154	HEM	CMD-C2D-C3D	2.37	124.84	114.35
2	A	154	HEM	CMB-C2B-C3B	4.12	126.81	116.53
2	A	154	HEM	CAD-C3D-C2D	4.44	125.98	113.22
2	A	154	HEM	CAD-C3D-C4D	4.81	129.43	112.47
2	A	154	HEM	CMC-C2C-C3C	5.17	129.42	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	154	HEM	7	0
3	A	155	NBE	12	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, 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	153/153 (100%)	4.34	135 (88%)	0 0	8, 18, 49, 64	19 (12%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	ALA	25.4
1	A	3	LEU	16.8
1	A	49	GLY	14.3
1	A	48	LYS	13.1
1	A	1	GLY	12.8
1	A	51	SER	12.5
1	A	47	LEU	10.4
1	A	50	THR	10.2
1	A	153	ALA	9.0
1	A	83	VAL	8.3
1	A	130	LEU	8.2
1	A	87	ASP	7.8
1	A	150	ASP	7.3
1	A	40	ALA	7.2
1	A	55	GLN	7.1
1	A	20	ALA	7.0
1	A	5	GLU	6.9
1	A	136	ILE	6.9
1	A	58	PRO	6.9
1	A	60	LEU	6.5
1	A	53	VAL	6.4
1	A	46	PHE	6.4
1	A	15	TRP	6.3
1	A	32	LEU	6.1
1	A	45	SER	6.1
1	A	151	ASP	6.1
1	A	81	THR	6.1

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Mol	Chain	Res	Type	RSRZ
1	A	143	ILE	6.0
1	A	93	LEU	5.7
1	A	86	THR	5.6
1	A	102	VAL	5.6
1	A	44	PHE	5.6
1	A	88	ALA	5.4
1	A	82	GLY	5.4
1	A	89	THR	5.3
1	A	144	VAL	5.3
1	A	152	ALA	5.3
1	A	26	THR	5.2
1	A	122	VAL	5.2
1	A	145	ILE	5.2
1	A	101	GLY	5.0
1	A	92	ASN	4.9
1	A	31	ILE	4.9
1	A	124	ALA	4.9
1	A	10	LEU	4.9
1	A	19	ASN	4.7
1	A	54	PRO	4.5
1	A	11	VAL	4.5
1	A	126	TRP	4.4
1	A	127	SER	4.4
1	A	99	SER	4.3
1	A	30	PHE	4.3
1	A	72	TYR	4.2
1	A	125	LYS	4.2
1	A	42	ASP	4.2
1	A	123	GLY	4.1
1	A	114	ILE	4.0
1	A	69	LYS	4.0
1	A	23	PRO	4.0
1	A	80	VAL	4.0
1	A	16	GLU	4.0
1	A	7	GLN	4.0
1	A	147	LYS	3.9
1	A	141	LEU	3.9
1	A	8	ALA	3.9
1	A	56	ASN	3.9
1	A	43	LEU	3.9
1	A	68	PHE	3.9
1	A	115	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	121	VAL	3.8
1	A	149	MET	3.8
1	A	98	VAL	3.7
1	A	73	GLU	3.7
1	A	90	LEU	3.7
1	A	129	GLU	3.7
1	A	67	VAL	3.6
1	A	18	PHE	3.4
1	A	116	LYS	3.4
1	A	84	VAL	3.4
1	A	140	GLU	3.4
1	A	108	PRO	3.4
1	A	95	SER	3.4
1	A	57	ASN	3.3
1	A	39	ALA	3.3
1	A	138	TYR	3.3
1	A	9	ALA	3.3
1	A	142	ALA	3.3
1	A	62	ALA	3.2
1	A	137	ALA	3.2
1	A	65	GLY	3.2
1	A	75	ALA	3.1
1	A	104	ASP	3.1
1	A	105	ALA	3.1
1	A	59	GLU	3.1
1	A	6	SER	3.1
1	A	64	ALA	3.0
1	A	96	VAL	3.0
1	A	118	ILE	3.0
1	A	78	LEU	3.0
1	A	41	LYS	3.0
1	A	100	LYS	2.9
1	A	35	GLU	2.9
1	A	61	GLN	2.9
1	A	109	VAL	2.8
1	A	113	ALA	2.8
1	A	139	ASP	2.7
1	A	148	GLU	2.7
1	A	24	LYS	2.7
1	A	97	HIS	2.7
1	A	36	ILE	2.7
1	A	27	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	2.7
1	A	135	THR	2.7
1	A	28	ARG	2.6
1	A	22	ILE	2.6
1	A	63	HIS	2.5
1	A	132[A]	SER	2.5
1	A	119	LYS	2.5
1	A	110	VAL	2.5
1	A	133	ALA	2.5
1	A	70	LEU	2.4
1	A	74	ALA	2.4
1	A	38	PRO	2.4
1	A	107	PHE	2.3
1	A	111	LYS	2.3
1	A	76	ILE	2.3
1	A	120	GLU	2.2
1	A	4	THR	2.2
1	A	117	THR	2.2
1	A	128	GLU	2.2
1	A	134	TRP	2.1
1	A	77	GLN	2.1
1	A	91	LYS	2.1
1	A	146	LYS	2.0
1	A	12	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 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NBE	A	155	8/8	0.77	0.50	3.34	19,33,53,58	0
2	HEM	A	154	43/43	0.72	0.32	-0.03	0,18,43,56	3

6.5 Other polymers (i)

There are no such residues in this entry.