



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:44 PM GMT

PDB ID : 4BIM
Title : CATALASE 3 FROM NEUROSPORA CRASSA IN TETRAGONAL FORM
EXPOSES A MODIFIED TETRAMERIC ORGANIZATION
Authors : Zarate-Romero, A.; Rudino-Pinera, E.
Deposited on : 2013-04-11
Resolution : 2.95 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>

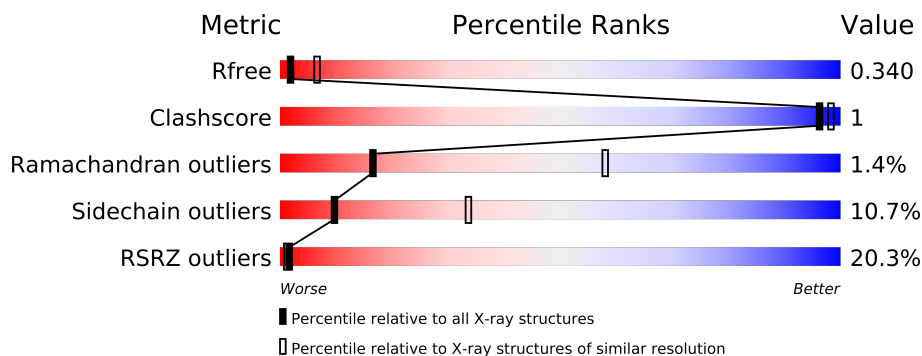
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.95 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	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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	746	
1	B	746	
1	C	746	
1	D	746	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21809 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 CATALASE 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	681	Total	C	N	O	S	0	0	0
			5340	3381	941	1012	6			
1	B	679	Total	C	N	O	S	0	0	0
			5324	3371	939	1008	6			
1	C	681	Total	C	N	O	S	0	0	0
			5340	3381	941	1012	6			
1	D	680	Total	C	N	O	S	0	0	0
			5331	3376	940	1009	6			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	EXPRESSION TAG	UNP Q9C169
A	-25	ASN	-	EXPRESSION TAG	UNP Q9C169
A	-24	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-23	LYS	-	EXPRESSION TAG	UNP Q9C169
A	-22	VAL	-	EXPRESSION TAG	UNP Q9C169
A	-21	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-20	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-19	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-18	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-17	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-16	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-15	ILE	-	EXPRESSION TAG	UNP Q9C169
A	-14	GLU	-	EXPRESSION TAG	UNP Q9C169
A	-13	GLY	-	EXPRESSION TAG	UNP Q9C169
A	-12	ARG	-	EXPRESSION TAG	UNP Q9C169
A	-11	HIS	-	EXPRESSION TAG	UNP Q9C169
A	-10	MET	-	EXPRESSION TAG	UNP Q9C169
A	-9	GLU	-	EXPRESSION TAG	UNP Q9C169
A	-8	LEU	-	EXPRESSION TAG	UNP Q9C169
A	-7	GLY	-	EXPRESSION TAG	UNP Q9C169
A	-6	THR	-	EXPRESSION TAG	UNP Q9C169

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	EXPRESSION TAG	UNP Q9C169
A	-4	GLU	-	EXPRESSION TAG	UNP Q9C169
A	-3	GLY	-	EXPRESSION TAG	UNP Q9C169
A	-2	SER	-	EXPRESSION TAG	UNP Q9C169
A	-1	GLU	-	EXPRESSION TAG	UNP Q9C169
A	0	PHE	-	EXPRESSION TAG	UNP Q9C169
B	-26	MET	-	EXPRESSION TAG	UNP Q9C169
B	-25	ASN	-	EXPRESSION TAG	UNP Q9C169
B	-24	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-23	LYS	-	EXPRESSION TAG	UNP Q9C169
B	-22	VAL	-	EXPRESSION TAG	UNP Q9C169
B	-21	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-20	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-19	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-18	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-17	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-16	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-15	ILE	-	EXPRESSION TAG	UNP Q9C169
B	-14	GLU	-	EXPRESSION TAG	UNP Q9C169
B	-13	GLY	-	EXPRESSION TAG	UNP Q9C169
B	-12	ARG	-	EXPRESSION TAG	UNP Q9C169
B	-11	HIS	-	EXPRESSION TAG	UNP Q9C169
B	-10	MET	-	EXPRESSION TAG	UNP Q9C169
B	-9	GLU	-	EXPRESSION TAG	UNP Q9C169
B	-8	LEU	-	EXPRESSION TAG	UNP Q9C169
B	-7	GLY	-	EXPRESSION TAG	UNP Q9C169
B	-6	THR	-	EXPRESSION TAG	UNP Q9C169
B	-5	LEU	-	EXPRESSION TAG	UNP Q9C169
B	-4	GLU	-	EXPRESSION TAG	UNP Q9C169
B	-3	GLY	-	EXPRESSION TAG	UNP Q9C169
B	-2	SER	-	EXPRESSION TAG	UNP Q9C169
B	-1	GLU	-	EXPRESSION TAG	UNP Q9C169
B	0	PHE	-	EXPRESSION TAG	UNP Q9C169
C	-26	MET	-	EXPRESSION TAG	UNP Q9C169
C	-25	ASN	-	EXPRESSION TAG	UNP Q9C169
C	-24	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-23	LYS	-	EXPRESSION TAG	UNP Q9C169
C	-22	VAL	-	EXPRESSION TAG	UNP Q9C169
C	-21	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-20	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-19	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-18	HIS	-	EXPRESSION TAG	UNP Q9C169

Continued on next page...

Continued from previous page...

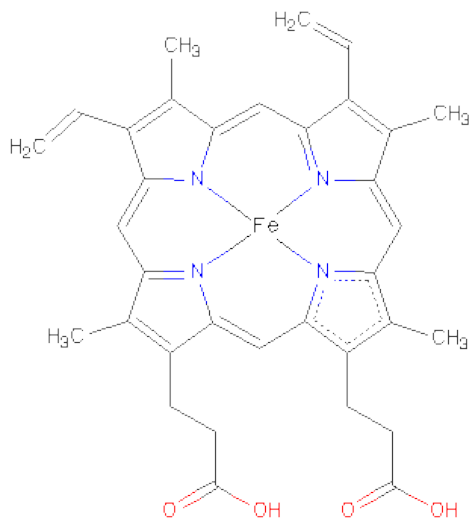
Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-16	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-15	ILE	-	EXPRESSION TAG	UNP Q9C169
C	-14	GLU	-	EXPRESSION TAG	UNP Q9C169
C	-13	GLY	-	EXPRESSION TAG	UNP Q9C169
C	-12	ARG	-	EXPRESSION TAG	UNP Q9C169
C	-11	HIS	-	EXPRESSION TAG	UNP Q9C169
C	-10	MET	-	EXPRESSION TAG	UNP Q9C169
C	-9	GLU	-	EXPRESSION TAG	UNP Q9C169
C	-8	LEU	-	EXPRESSION TAG	UNP Q9C169
C	-7	GLY	-	EXPRESSION TAG	UNP Q9C169
C	-6	THR	-	EXPRESSION TAG	UNP Q9C169
C	-5	LEU	-	EXPRESSION TAG	UNP Q9C169
C	-4	GLU	-	EXPRESSION TAG	UNP Q9C169
C	-3	GLY	-	EXPRESSION TAG	UNP Q9C169
C	-2	SER	-	EXPRESSION TAG	UNP Q9C169
C	-1	GLU	-	EXPRESSION TAG	UNP Q9C169
C	0	PHE	-	EXPRESSION TAG	UNP Q9C169
D	-26	MET	-	EXPRESSION TAG	UNP Q9C169
D	-25	ASN	-	EXPRESSION TAG	UNP Q9C169
D	-24	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-23	LYS	-	EXPRESSION TAG	UNP Q9C169
D	-22	VAL	-	EXPRESSION TAG	UNP Q9C169
D	-21	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-20	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-19	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-18	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-17	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-16	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-15	ILE	-	EXPRESSION TAG	UNP Q9C169
D	-14	GLU	-	EXPRESSION TAG	UNP Q9C169
D	-13	GLY	-	EXPRESSION TAG	UNP Q9C169
D	-12	ARG	-	EXPRESSION TAG	UNP Q9C169
D	-11	HIS	-	EXPRESSION TAG	UNP Q9C169
D	-10	MET	-	EXPRESSION TAG	UNP Q9C169
D	-9	GLU	-	EXPRESSION TAG	UNP Q9C169
D	-8	LEU	-	EXPRESSION TAG	UNP Q9C169
D	-7	GLY	-	EXPRESSION TAG	UNP Q9C169
D	-6	THR	-	EXPRESSION TAG	UNP Q9C169
D	-5	LEU	-	EXPRESSION TAG	UNP Q9C169
D	-4	GLU	-	EXPRESSION TAG	UNP Q9C169
D	-3	GLY	-	EXPRESSION TAG	UNP Q9C169

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	EXPRESSION TAG	UNP Q9C169
D	-1	GLU	-	EXPRESSION TAG	UNP Q9C169
D	0	PHE	-	EXPRESSION TAG	UNP Q9C169

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	90	Total	O	0	0
			90	90		
3	B	61	Total	O	0	0
			61	61		
3	C	54	Total	O	0	0
			54	54		

Continued on next page...

Continued from previous page...

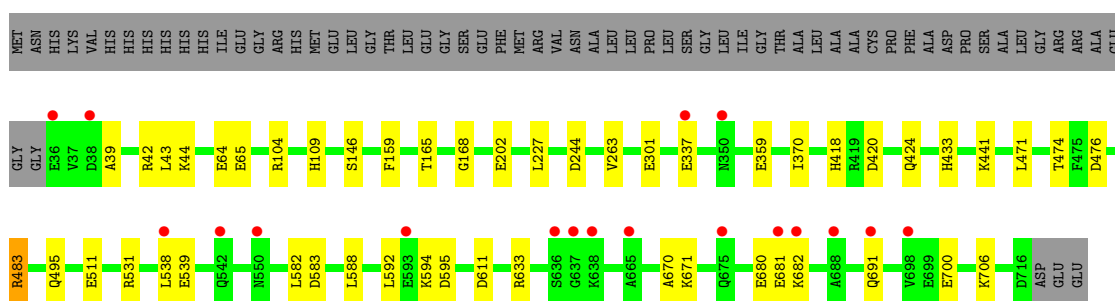
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total	O	0	0
			97	97		

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.

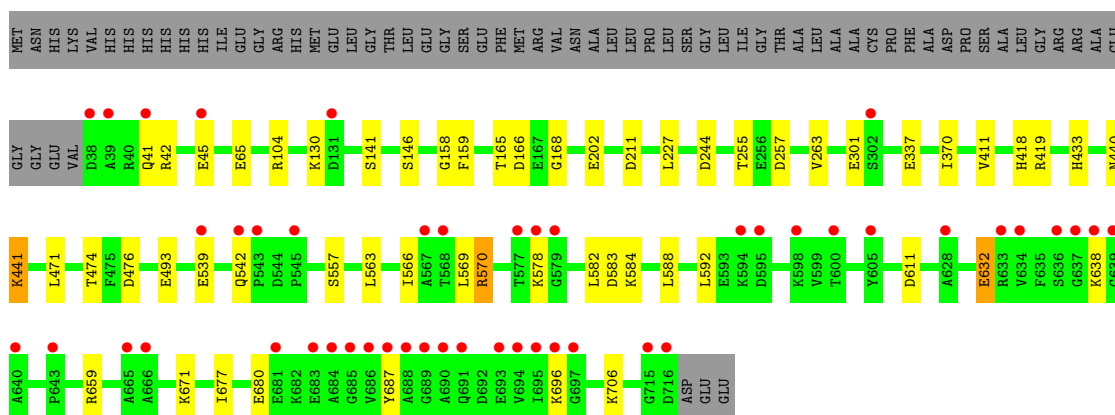
• Molecule 1: CATALASE 3

Chain A:



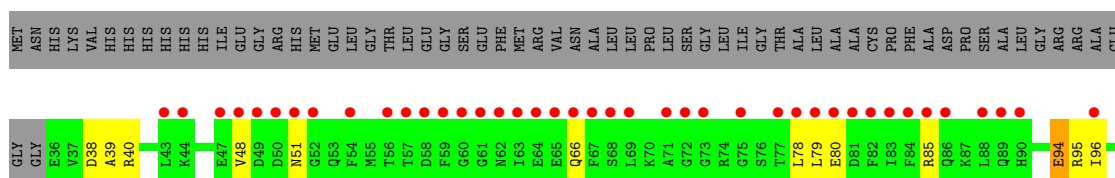
• Molecule 1: CATALASE 3

Chain B:

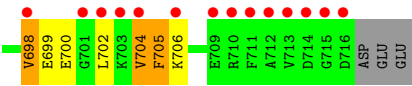


• Molecule 1: CATALASE 3

Chain C:







4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.51Å 207.51Å 137.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.30 – 2.95 29.30 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.30-2.95) 98.9 (29.30-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.95Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.255 , 0.304 0.285 , 0.340	Depositor DCC
R_{free} test set	3166 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 62443 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	21809	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: HEM

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	0.45	0/5473	0.64	0/7424
1	B	0.45	0/5457	0.65	2/7402 (0.0%)
1	C	0.47	0/5473	0.70	4/7424 (0.1%)
1	D	0.48	0/5464	0.73	2/7412 (0.0%)
All	All	0.46	0/21867	0.68	8/29662 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	541	PRO	C-N-CA	7.57	140.63	121.70
1	B	632	GLU	C-N-CA	6.37	137.63	121.70
1	C	702	LEU	C-N-CA	5.85	136.31	121.70
1	C	39	ALA	C-N-CA	5.37	135.13	121.70
1	C	150	ALA	C-N-CA	5.32	134.99	121.70
1	D	698	VAL	C-N-CA	5.24	134.79	121.70
1	D	609	GLY	C-N-CA	5.13	134.53	121.70
1	B	566	ILE	C-N-CA	5.09	134.43	121.70

There are no chirality outliers.

There are no planarity outliers.

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	5340	0	0	7	0
1	B	5324	0	0	4	0
1	C	5340	0	0	6	0
1	D	5331	0	0	8	0
2	A	43	0	0	0	0
2	B	43	0	0	0	0
2	C	43	0	0	0	0
2	D	43	0	0	0	0
3	A	90	0	0	2	0
3	B	61	0	0	0	0
3	C	54	0	0	0	0
3	D	97	0	0	0	1
All	All	21809	0	0	24	1

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 1.

All (24) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:483:ARG:NH2	3:A:2070:HOH:O	2.30	0.63
1:A:495:GLN:OE1	1:A:531:ARG:NH2	2.37	0.56
1:C:157:HIS:O	1:C:176:ASN:N	2.39	0.56
1:D:165:THR:OG1	1:D:168:GLY:O	2.25	0.55
1:C:153:ALA:CB	1:C:154:ARG:CA	2.91	0.48
1:C:94:GLU:O	1:C:95:ARG:NH1	2.46	0.48
1:D:704:VAL:CA	1:D:705:PHE:CB	2.92	0.47
1:D:254:VAL:N	1:D:373:GLY:O	2.47	0.47
1:D:652:GLN:NE2	1:D:656:ASP:OD2	2.46	0.47
1:B:255:THR:OG1	1:B:257:ASP:OD1	2.33	0.47
1:C:102:HIS:CA	1:C:142:THR:O	2.63	0.46
1:D:141:SER:O	1:D:158:GLY:N	2.49	0.45
1:C:652:GLN:NE2	1:D:652:GLN:OE1	2.52	0.43
1:B:493:GLU:OE1	1:B:557:SER:OG	2.35	0.43
1:B:165:THR:OG1	1:B:168:GLY:O	2.37	0.43
1:A:39:ALA:O	1:A:42:ARG:NH1	2.52	0.42
1:A:420:ASP:O	1:A:424:GLN:NE2	2.52	0.42
1:C:495:GLN:NE2	1:C:499:ASN:OD1	2.52	0.42
1:D:162:ARG:NH2	1:D:369:HIS:CE1	2.87	0.42
1:A:165:THR:OG1	1:A:168:GLY:O	2.37	0.41
1:A:42:ARG:NH2	3:A:2002:HOH:O	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:SER:O	1:B:158:GLY:N	2.54	0.40
1:D:653:ILE:O	1:D:656:ASP:O	2.39	0.40
1:A:109:HIS:NE2	1:A:359:GLU:OE1	2.55	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	Distance(Å)	Clash(Å)
3:D:2016:HOH:O	3:D:2016:HOH:O[8_554]	2.19	0.01

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	679/746 (91%)	640 (94%)	38 (6%)	1 (0%)	59 93
1	B	677/746 (91%)	628 (93%)	46 (7%)	3 (0%)	43 85
1	C	679/746 (91%)	619 (91%)	49 (7%)	11 (2%)	14 54
1	D	678/746 (91%)	585 (86%)	70 (10%)	23 (3%)	6 28
All	All	2713/2984 (91%)	2472 (91%)	203 (8%)	38 (1%)	16 58

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	161	THR
1	C	568	THR
1	D	427	ILE
1	D	563	LEU
1	D	564	PRO
1	D	705	PHE
1	B	632	GLU
1	C	152	THR
1	C	398	ARG
1	C	678	GLY
1	D	94	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	259	LYS
1	D	411	VAL
1	D	415	HIS
1	D	428	HIS
1	D	541	PRO
1	B	570	ARG
1	C	40	ARG
1	C	169	ASN
1	D	143	VAL
1	D	410	PRO
1	D	469	ARG
1	D	699	GLU
1	D	704	VAL
1	A	670	ALA
1	B	441	LYS
1	D	127	LEU
1	D	607	ALA
1	D	610	VAL
1	C	38	ASP
1	C	129	ALA
1	C	542	GLN
1	D	167	GLU
1	C	715	GLY
1	D	419	ARG
1	D	420	ASP
1	D	431	ILE
1	D	460	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	559/609 (92%)	520 (93%)	39 (7%)	21	60
1	B	557/609 (92%)	511 (92%)	46 (8%)	16	50
1	C	559/609 (92%)	491 (88%)	68 (12%)	7	27
1	D	558/609 (92%)	472 (85%)	86 (15%)	4	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	2233/2436 (92%)	1994 (89%)	239 (11%)	10	33

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	44	LYS
1	A	64	GLU
1	A	65	GLU
1	A	104	ARG
1	A	146	SER
1	A	159	PHE
1	A	202	GLU
1	A	227	LEU
1	A	244	ASP
1	A	263	VAL
1	A	301	GLU
1	A	337	GLU
1	A	370	ILE
1	A	418	HIS
1	A	433	HIS
1	A	441	LYS
1	A	471	LEU
1	A	474	THR
1	A	476	ASP
1	A	483	ARG
1	A	511	GLU
1	A	538	LEU
1	A	539	GLU
1	A	582	LEU
1	A	583	ASP
1	A	588	LEU
1	A	592	LEU
1	A	594	LYS
1	A	595	ASP
1	A	611	ASP
1	A	633	ARG
1	A	671	LYS
1	A	680	GLU
1	A	681	GLU
1	A	682	LYS
1	A	691	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	700	GLU
1	A	706	LYS
1	B	41	GLN
1	B	42	ARG
1	B	45	GLU
1	B	65	GLU
1	B	104	ARG
1	B	130	LYS
1	B	146	SER
1	B	159	PHE
1	B	166	ASP
1	B	202	GLU
1	B	211	ASP
1	B	227	LEU
1	B	244	ASP
1	B	263	VAL
1	B	301	GLU
1	B	337	GLU
1	B	370	ILE
1	B	411	VAL
1	B	418	HIS
1	B	419	ARG
1	B	433	HIS
1	B	440	ASN
1	B	441	LYS
1	B	471	LEU
1	B	474	THR
1	B	476	ASP
1	B	539	GLU
1	B	542	GLN
1	B	563	LEU
1	B	569	LEU
1	B	570	ARG
1	B	578	LYS
1	B	582	LEU
1	B	583	ASP
1	B	584	LYS
1	B	588	LEU
1	B	592	LEU
1	B	611	ASP
1	B	638	LYS
1	B	659	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	671	LYS
1	B	677	ILE
1	B	680	GLU
1	B	687	TYR
1	B	696	LYS
1	B	706	LYS
1	C	48	VAL
1	C	51	ASN
1	C	66	GLN
1	C	78	LEU
1	C	79	LEU
1	C	80	GLU
1	C	85	ARG
1	C	94	GLU
1	C	96	ILE
1	C	99	ARG
1	C	104	ARG
1	C	111	ILE
1	C	114	SER
1	C	131	ASP
1	C	139	ARG
1	C	146	SER
1	C	151	ASP
1	C	154	ARG
1	C	155	ASP
1	C	156	VAL
1	C	167	GLU
1	C	176	ASN
1	C	202	GLU
1	C	227	LEU
1	C	236	ILE
1	C	239	SER
1	C	263	VAL
1	C	296	LEU
1	C	301	GLU
1	C	336	GLU
1	C	337	GLU
1	C	370	ILE
1	C	393	GLN
1	C	395	ASN
1	C	398	ARG
1	C	419	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	422	GLN
1	C	424	GLN
1	C	441	LYS
1	C	450	THR
1	C	471	LEU
1	C	474	THR
1	C	476	ASP
1	C	511	GLU
1	C	538	LEU
1	C	542	GLN
1	C	552	VAL
1	C	554	ARG
1	C	558	ILE
1	C	570	ARG
1	C	582	LEU
1	C	588	LEU
1	C	590	GLU
1	C	592	LEU
1	C	597	LEU
1	C	606	LEU
1	C	611	ASP
1	C	625	VAL
1	C	638	LYS
1	C	659	ARG
1	C	662	LYS
1	C	674	LEU
1	C	675	GLN
1	C	677	ILE
1	C	681	GLU
1	C	696	LYS
1	C	703	LYS
1	C	706	LYS
1	D	40	ARG
1	D	43	LEU
1	D	44	LYS
1	D	45	GLU
1	D	53	GLN
1	D	65	GLU
1	D	86	GLN
1	D	96	ILE
1	D	101	VAL
1	D	104	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	120	ASN
1	D	126	PHE
1	D	127	LEU
1	D	131	ASP
1	D	146	SER
1	D	155	ASP
1	D	166	ASP
1	D	167	GLU
1	D	183	GLN
1	D	184	ASP
1	D	190	ASP
1	D	193	HIS
1	D	202	GLU
1	D	227	LEU
1	D	238	ARG
1	D	244	ASP
1	D	259	LYS
1	D	263	VAL
1	D	279	GLU
1	D	296	LEU
1	D	301	GLU
1	D	304	ASN
1	D	316	ASP
1	D	321	GLN
1	D	332	LYS
1	D	337	GLU
1	D	370	ILE
1	D	386	LEU
1	D	393	GLN
1	D	394	LEU
1	D	416	ASN
1	D	420	ASP
1	D	422	GLN
1	D	427	ILE
1	D	431	ILE
1	D	432	HIS
1	D	433	HIS
1	D	439	LEU
1	D	440	ASN
1	D	453	ARG
1	D	461	ARG
1	D	467	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	469	ARG
1	D	470	GLU
1	D	476	ASP
1	D	478	HIS
1	D	502	ARG
1	D	528	VAL
1	D	538	LEU
1	D	539	GLU
1	D	560	ASN
1	D	561	GLU
1	D	563	LEU
1	D	565	THR
1	D	566	ILE
1	D	569	LEU
1	D	570	ARG
1	D	584	LYS
1	D	586	LYS
1	D	588	LEU
1	D	591	GLN
1	D	592	LEU
1	D	593	GLU
1	D	595	ASP
1	D	597	LEU
1	D	606	LEU
1	D	632	GLU
1	D	638	LYS
1	D	649	ARG
1	D	651	SER
1	D	672	LYS
1	D	691	GLN
1	D	698	VAL
1	D	700	GLU
1	D	702	LEU
1	D	706	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

4 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	4000	1	49,50,50	2.78	13 (26%)	46,82,82	1.71	10 (21%)
2	HEM	B	4000	1	49,50,50	4.38	13 (26%)	46,82,82	1.66	11 (23%)
2	HEM	C	4000	1	49,50,50	3.52	13 (26%)	46,82,82	1.77	9 (19%)
2	HEM	D	4000	-	49,50,50	5.06	12 (24%)	46,82,82	1.73	11 (23%)

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	4000	1	-	0/14/114/114	0/0/8/8
2	HEM	B	4000	1	-	0/14/114/114	0/0/8/8
2	HEM	C	4000	1	-	0/14/114/114	0/0/8/8
2	HEM	D	4000	-	-	0/14/114/114	0/0/8/8

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4000	HEM	C3D-C4D	23.79	1.50	1.44
2	D	4000	HEM	C2D-C1D	21.58	1.49	1.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	HEM	C2D-C1D	19.36	1.49	1.44
2	B	4000	HEM	C3D-C4D	18.98	1.49	1.44
2	C	4000	HEM	C3D-C4D	14.74	1.48	1.44
2	C	4000	HEM	C2D-C1D	12.88	1.47	1.44
2	A	4000	HEM	C2D-C1D	8.83	1.46	1.44
2	A	4000	HEM	C3D-C4D	7.79	1.46	1.44
2	B	4000	HEM	C3D-C2D	-7.68	1.30	1.43
2	A	4000	HEM	C3D-C2D	-7.65	1.30	1.43
2	A	4000	HEM	C2B-C1B	-7.47	1.42	1.44
2	C	4000	HEM	C3D-C2D	-6.87	1.31	1.43
2	C	4000	HEM	C2B-C1B	-6.68	1.42	1.44
2	D	4000	HEM	C3B-C2B	-6.68	1.32	1.43
2	D	4000	HEM	C3D-C2D	-6.00	1.33	1.43
2	B	4000	HEM	C2B-C1B	-5.00	1.43	1.44
2	C	4000	HEM	C3B-C2B	-4.92	1.35	1.43
2	D	4000	HEM	C3B-C4B	4.83	1.50	1.44
2	B	4000	HEM	C3B-C2B	-4.79	1.35	1.43
2	D	4000	HEM	C2B-C1B	4.72	1.45	1.44
2	A	4000	HEM	C3B-C2B	-4.48	1.35	1.43
2	A	4000	HEM	C3B-C4B	4.48	1.49	1.44
2	A	4000	HEM	C3C-CAC	3.99	1.52	1.40
2	D	4000	HEM	O1D-CGD	3.96	1.36	1.22
2	C	4000	HEM	C3B-C4B	3.91	1.49	1.44
2	B	4000	HEM	C3C-CAC	3.51	1.51	1.40
2	C	4000	HEM	C3C-C2C	-3.47	1.37	1.43
2	A	4000	HEM	C4D-ND	-3.28	1.32	1.39
2	C	4000	HEM	C3C-CAC	3.22	1.50	1.40
2	D	4000	HEM	C3C-C2C	-3.16	1.38	1.43
2	C	4000	HEM	C4D-ND	-3.08	1.33	1.39
2	B	4000	HEM	C3C-C2C	-3.03	1.38	1.43
2	B	4000	HEM	C4D-ND	-2.93	1.33	1.39
2	A	4000	HEM	C3B-CAB	2.89	1.49	1.40
2	B	4000	HEM	C3B-C4B	2.87	1.47	1.44
2	C	4000	HEM	CHA-C4D	2.82	1.39	1.35
2	D	4000	HEM	C3B-CAB	2.80	1.49	1.40
2	C	4000	HEM	C1B-NB	-2.77	1.33	1.39
2	C	4000	HEM	CAA-C2A	-2.69	1.47	1.52
2	B	4000	HEM	C3B-CAB	2.63	1.48	1.40
2	B	4000	HEM	CHB-C1B	2.62	1.39	1.35
2	B	4000	HEM	C1B-NB	-2.58	1.34	1.39
2	A	4000	HEM	C3C-C2C	-2.54	1.39	1.43
2	D	4000	HEM	O2D-CGD	-2.48	1.21	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4000	HEM	C1B-NB	-2.47	1.34	1.39
2	C	4000	HEM	C3B-CAB	2.42	1.47	1.40
2	D	4000	HEM	CHB-C1B	2.37	1.39	1.35
2	D	4000	HEM	C1B-NB	-2.35	1.34	1.39
2	A	4000	HEM	CHA-C4D	2.35	1.39	1.35
2	B	4000	HEM	CHA-C4D	2.32	1.39	1.35
2	A	4000	HEM	CHB-C1B	2.26	1.39	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4000	HEM	CBD-CAD-C3D	-4.28	105.02	114.37
2	C	4000	HEM	CBD-CAD-C3D	-4.12	105.37	114.37
2	C	4000	HEM	C3B-C4B-NB	-4.11	111.06	114.00
2	A	4000	HEM	CBD-CAD-C3D	-3.97	105.70	114.37
2	D	4000	HEM	C3B-C4B-NB	-3.92	111.19	114.00
2	D	4000	HEM	CMA-C3A-C4A	-3.90	122.62	128.62
2	D	4000	HEM	CAD-CBD-CGD	-3.88	101.39	113.48
2	C	4000	HEM	C3A-C4A-NA	3.85	112.32	109.41
2	D	4000	HEM	C3A-C4A-NA	3.62	112.15	109.41
2	B	4000	HEM	C4A-CHB-C1B	-3.62	122.71	127.47
2	A	4000	HEM	C3A-C4A-NA	3.61	112.13	109.41
2	A	4000	HEM	C3B-C4B-NB	-3.47	111.52	114.00
2	A	4000	HEM	C4A-CHB-C1B	-3.46	122.92	127.47
2	A	4000	HEM	CMA-C3A-C4A	-3.42	123.36	128.62
2	D	4000	HEM	CMA-C3A-C2A	3.22	131.02	124.94
2	A	4000	HEM	CMA-C3A-C2A	3.21	131.00	124.94
2	A	4000	HEM	CHC-C4B-NB	3.21	127.25	124.58
2	C	4000	HEM	C4A-CHB-C1B	-3.17	123.30	127.47
2	C	4000	HEM	CMA-C3A-C2A	3.15	130.89	124.94
2	C	4000	HEM	CHD-C1D-ND	3.12	127.18	124.58
2	B	4000	HEM	CHD-C1D-ND	3.12	127.18	124.58
2	B	4000	HEM	CMA-C3A-C4A	-3.08	123.88	128.62
2	B	4000	HEM	CMA-C3A-C2A	3.08	130.74	124.94
2	B	4000	HEM	C3A-C4A-NA	3.01	111.68	109.41
2	C	4000	HEM	CMA-C3A-C4A	-2.98	124.03	128.62
2	D	4000	HEM	C4A-NA-C1A	-2.95	102.87	106.76
2	B	4000	HEM	C3B-C4B-NB	-2.90	111.92	114.00
2	C	4000	HEM	C4A-C3A-C2A	-2.83	105.02	107.00
2	C	4000	HEM	CHC-C4B-NB	2.66	126.80	124.58
2	D	4000	HEM	C1A-CHA-C4D	-2.63	124.01	127.47
2	D	4000	HEM	CHC-C4B-NB	2.52	126.68	124.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4000	HEM	C4D-ND-C1D	-2.47	102.63	105.16
2	B	4000	HEM	C4A-C3A-C2A	-2.34	105.37	107.00
2	B	4000	HEM	CHC-C4B-NB	2.23	126.44	124.58
2	A	4000	HEM	C1A-CHA-C4D	-2.17	124.62	127.47
2	A	4000	HEM	CHD-C1D-ND	2.16	126.38	124.58
2	B	4000	HEM	O2D-CGD-CBD	2.15	121.81	114.22
2	B	4000	HEM	C1D-CHD-C4C	-2.13	120.97	126.57
2	D	4000	HEM	C2A-C1A-NA	2.10	112.65	109.73
2	A	4000	HEM	C4A-C3A-C2A	-2.01	105.60	107.00
2	D	4000	HEM	C1D-CHD-C4C	-2.01	121.28	126.57

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	681/746 (91%)	-0.07	18 (2%) 53 24	15, 51, 103, 141	0
1	B	679/746 (91%)	0.23	48 (7%) 16 9	19, 63, 154, 227	0
1	C	681/746 (91%)	1.32	169 (24%) 1 1	32, 79, 138, 169	0
1	D	680/746 (91%)	2.19	317 (46%) 1 0	32, 94, 149, 188	0
All	All	2721/2984 (91%)	0.92	552 (20%) 1 1	15, 75, 140, 227	0

All (552) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	446	GLN	10.3
1	D	443	TYR	10.2
1	D	445	ALA	9.3
1	C	708	LEU	9.1
1	D	127	LEU	8.9
1	C	605	TYR	8.8
1	D	444	PRO	8.4
1	C	579	GLY	8.3
1	C	66	GLN	8.2
1	D	120	ASN	8.1
1	D	314	LEU	7.6
1	D	447	ALA	7.4
1	D	455	PHE	7.2
1	B	687	TYR	7.0
1	B	633	ARG	7.0
1	D	388	SER	7.0
1	D	466	VAL	6.9
1	C	428	HIS	6.8
1	D	315	ILE	6.7
1	C	60	GLY	6.7
1	D	126	PHE	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	215	ASP	6.6
1	D	690	ALA	6.4
1	D	128	GLY	6.3
1	B	691	GLN	6.2
1	D	641	MET	6.1
1	B	568	THR	6.1
1	D	473	ALA	6.0
1	D	687	TYR	6.0
1	D	150	ALA	5.9
1	D	678	GLY	5.9
1	D	468	ASN	5.9
1	D	552	VAL	5.8
1	C	645	PHE	5.8
1	D	715	GLY	5.8
1	D	434	TYR	5.8
1	D	311	ALA	5.8
1	D	37	VAL	5.7
1	D	324	GLY	5.7
1	C	651	SER	5.7
1	D	442	GLY	5.6
1	C	637	GLY	5.5
1	D	322	ALA	5.5
1	C	360	THR	5.5
1	D	417	ASN	5.5
1	B	688	ALA	5.5
1	C	572	GLY	5.4
1	C	635	PHE	5.3
1	D	559	PHE	5.3
1	D	491	PRO	5.3
1	C	643	PRO	5.3
1	D	412	SER	5.3
1	C	345	GLY	5.3
1	D	321	GLN	5.2
1	D	206	ALA	5.2
1	C	609	GLY	5.2
1	C	84	PHE	5.1
1	D	414	VAL	5.1
1	D	689	GLY	5.1
1	D	418	HIS	5.0
1	D	433	HIS	5.0
1	D	416	ASN	5.0
1	D	566	ILE	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	684	ALA	4.9
1	D	688	ALA	4.9
1	D	545	PRO	4.9
1	C	427	ILE	4.9
1	C	642	SER	4.9
1	C	623	ASP	4.9
1	D	325	PHE	4.9
1	D	450	THR	4.8
1	D	675	GLN	4.8
1	D	370	ILE	4.8
1	D	121	ILE	4.8
1	D	449	GLN	4.8
1	C	63	ILE	4.8
1	C	67	PHE	4.8
1	B	545	PRO	4.8
1	C	691	GLN	4.8
1	D	436	PRO	4.7
1	C	59	PHE	4.7
1	B	39	ALA	4.7
1	C	75	GLY	4.7
1	D	441	LYS	4.7
1	D	677	ILE	4.7
1	C	687	TYR	4.7
1	C	624	ALA	4.6
1	C	573	VAL	4.6
1	D	456	PHE	4.6
1	D	665	ALA	4.6
1	D	482	PRO	4.6
1	C	625	VAL	4.6
1	C	659	ARG	4.6
1	D	435	SER	4.5
1	D	400	PRO	4.5
1	C	52	GLY	4.5
1	D	53	GLN	4.5
1	D	664	VAL	4.5
1	D	713	VAL	4.5
1	B	686	VAL	4.5
1	D	223	ALA	4.4
1	C	636	SER	4.4
1	D	110	GLY	4.3
1	D	190	ASP	4.3
1	C	607	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	685	GLY	4.3
1	C	73	GLY	4.2
1	D	464	SER	4.2
1	D	285	ALA	4.2
1	D	352	ASN	4.2
1	C	676	SER	4.2
1	D	338	PHE	4.2
1	D	39	ALA	4.2
1	D	376	PHE	4.2
1	C	65	GLU	4.2
1	C	116	GLY	4.1
1	C	49	ASP	4.1
1	D	38	ASP	4.1
1	D	454	GLY	4.1
1	C	655	THR	4.1
1	D	565	THR	4.0
1	C	590	GLU	4.0
1	D	193	HIS	4.0
1	D	562	SER	4.0
1	C	83	ILE	4.0
1	C	672	LYS	4.0
1	D	283	VAL	4.0
1	D	313	GLN	4.0
1	C	713	VAL	3.9
1	D	377	THR	3.9
1	D	353	PRO	3.9
1	C	69	LEU	3.9
1	D	625	VAL	3.9
1	A	538	LEU	3.9
1	D	439	LEU	3.9
1	C	581	SER	3.9
1	D	238	ARG	3.8
1	D	438	TYR	3.8
1	D	207	ALA	3.8
1	D	638	LYS	3.8
1	C	88	LEU	3.8
1	D	225	HIS	3.8
1	D	242	HIS	3.8
1	D	709	GLU	3.8
1	D	623	ASP	3.8
1	D	115	TYR	3.8
1	C	712	ALA	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	281	ALA	3.8
1	D	297	TRP	3.8
1	D	432	HIS	3.8
1	C	158	GLY	3.8
1	D	423	GLY	3.8
1	D	541	PRO	3.7
1	B	689	GLY	3.7
1	C	638	LYS	3.7
1	D	214	TRP	3.7
1	D	519	GLU	3.7
1	D	453	ARG	3.7
1	D	153	ALA	3.7
1	C	239	SER	3.7
1	C	610	VAL	3.7
1	C	68	SER	3.7
1	C	80	GLU	3.7
1	D	304	ASN	3.7
1	C	90	HIS	3.7
1	D	49	ASP	3.7
1	D	389	TYR	3.7
1	D	426	TRP	3.7
1	A	637	GLY	3.6
1	C	50	ASP	3.6
1	C	79	LEU	3.6
1	D	525	SER	3.6
1	C	699	GLU	3.6
1	D	374	VAL	3.6
1	C	491	PRO	3.6
1	C	707	PHE	3.6
1	C	426	TRP	3.6
1	D	633	ARG	3.6
1	C	62	ASN	3.5
1	D	155	ASP	3.5
1	B	638	LYS	3.5
1	D	587	ALA	3.5
1	B	578	LYS	3.5
1	D	543	PRO	3.5
1	D	122	THR	3.5
1	C	443	TYR	3.5
1	B	695	ILE	3.5
1	B	639	GLY	3.5
1	C	96	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	246	PHE	3.4
1	B	38	ASP	3.4
1	C	627	VAL	3.4
1	C	412	SER	3.4
1	D	463	ALA	3.4
1	D	333	PHE	3.4
1	D	459	PRO	3.4
1	A	542	GLN	3.4
1	B	696	LYS	3.4
1	C	338	PHE	3.4
1	D	691	GLN	3.4
1	D	716	ASP	3.4
1	B	579	GLY	3.4
1	C	51	ASN	3.4
1	C	696	LYS	3.4
1	D	673	ALA	3.4
1	D	458	THR	3.3
1	C	72	GLY	3.3
1	C	570	ARG	3.3
1	D	600	THR	3.3
1	D	431	ILE	3.3
1	D	451	VAL	3.3
1	D	252	ARG	3.3
1	D	676	SER	3.3
1	D	116	GLY	3.3
1	D	129	ALA	3.3
1	C	56	THR	3.3
1	D	371	VAL	3.3
1	C	160	ALA	3.3
1	D	183	GLN	3.3
1	D	334	LEU	3.3
1	D	335	PRO	3.2
1	B	665	ALA	3.2
1	C	539	GLU	3.2
1	D	680	GLU	3.2
1	C	608	SER	3.2
1	B	643	PRO	3.2
1	C	626	VAL	3.2
1	D	460	GLY	3.2
1	C	157	HIS	3.2
1	D	343	VAL	3.2
1	C	47	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	45	GLU	3.2
1	C	716	ASP	3.2
1	D	260	SER	3.2
1	D	422	GLN	3.2
1	C	161	THR	3.2
1	D	249	HIS	3.2
1	B	567	ALA	3.2
1	C	71	ALA	3.2
1	B	637	GLY	3.2
1	D	471	LEU	3.2
1	D	219	SER	3.1
1	D	437	SER	3.1
1	A	698	VAL	3.1
1	D	560	ASN	3.1
1	C	682	LYS	3.1
1	D	658	TYR	3.1
1	B	684	ALA	3.1
1	D	224	LEU	3.1
1	D	472	SER	3.1
1	D	240	TYR	3.1
1	C	58	ASP	3.1
1	D	539	GLU	3.1
1	D	413	GLY	3.1
1	D	182	ILE	3.1
1	D	109	HIS	3.1
1	D	282	GLN	3.1
1	D	502	ARG	3.1
1	D	47	GLU	3.1
1	D	406	PRO	3.1
1	D	299	ALA	3.1
1	C	580	GLY	3.0
1	C	490	THR	3.0
1	D	142	THR	3.0
1	D	378	GLU	3.0
1	C	115	TYR	3.0
1	C	425	ALA	3.0
1	B	693	GLU	3.0
1	C	81	ASP	3.0
1	A	682	LYS	3.0
1	D	312	VAL	3.0
1	D	236	ILE	3.0
1	D	114	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	575	SER	2.9
1	B	595	ASP	2.9
1	D	358	ALA	2.9
1	D	624	ALA	2.9
1	D	118	TRP	2.9
1	D	461	ARG	2.9
1	C	578	LYS	2.9
1	D	50	ASP	2.9
1	D	230	ALA	2.9
1	D	698	VAL	2.9
1	B	683	GLU	2.9
1	D	550	ASN	2.9
1	D	701	GLY	2.9
1	B	715	GLY	2.9
1	C	700	GLU	2.9
1	D	512	GLN	2.9
1	D	485	PHE	2.9
1	D	542	GLN	2.9
1	C	82	PHE	2.9
1	D	380	PRO	2.9
1	B	539	GLU	2.8
1	D	176	ASN	2.8
1	C	64	GLU	2.8
1	C	647	ALA	2.8
1	D	538	LEU	2.8
1	D	117	ASP	2.8
1	D	194	SER	2.8
1	D	198	SER	2.8
1	C	675	GLN	2.8
1	B	577	THR	2.8
1	D	348	THR	2.8
1	D	457	THR	2.8
1	D	131	ASP	2.8
1	C	78	LEU	2.8
1	B	716	ASP	2.8
1	B	681	GLU	2.8
1	C	107	GLY	2.8
1	D	204	PRO	2.8
1	C	86	GLN	2.8
1	D	597	LEU	2.8
1	D	130	LYS	2.7
1	D	448	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	452	GLY	2.7
1	A	681	GLU	2.7
1	C	622	PHE	2.7
1	D	477	ASP	2.7
1	D	263	VAL	2.7
1	D	595	ASP	2.7
1	C	288	ASN	2.7
1	D	693	GLU	2.7
1	C	596	GLY	2.7
1	C	61	GLY	2.7
1	D	476	ASP	2.7
1	D	527	ASP	2.7
1	B	594	LYS	2.7
1	C	667	VAL	2.7
1	D	310	LEU	2.7
1	D	170	PHE	2.7
1	D	244	ASP	2.7
1	D	514	LYS	2.7
1	C	118	TRP	2.7
1	C	419	ARG	2.7
1	D	46	VAL	2.7
1	D	518	LEU	2.7
1	C	715	GLY	2.7
1	D	387	TYR	2.7
1	B	694	VAL	2.6
1	C	571	VAL	2.6
1	D	556	VAL	2.6
1	D	135	PRO	2.6
1	D	703	LYS	2.6
1	A	36	GLU	2.6
1	C	680	GLU	2.6
1	B	690	ALA	2.6
1	D	217	PHE	2.6
1	D	259	LYS	2.6
1	D	292	HIS	2.6
1	D	671	LYS	2.6
1	D	402	PHE	2.6
1	C	458	THR	2.6
1	C	43	LEU	2.6
1	B	598	LYS	2.6
1	C	356	TYR	2.6
1	C	120	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	411	VAL	2.6
1	D	467	LEU	2.6
1	D	564	PRO	2.6
1	C	694	VAL	2.6
1	D	695	ILE	2.5
1	D	375	ASP	2.5
1	C	272	GLY	2.5
1	D	396	ARG	2.5
1	D	490	THR	2.5
1	D	40	ARG	2.5
1	C	48	VAL	2.5
1	D	692	ASP	2.5
1	D	261	LYS	2.5
1	D	558	ILE	2.5
1	D	146	SER	2.5
1	D	405	LEU	2.5
1	D	44	LYS	2.5
1	D	465	GLY	2.5
1	B	302	SER	2.5
1	D	470	GLU	2.5
1	A	350	ASN	2.5
1	A	550	ASN	2.5
1	D	367	PRO	2.5
1	D	501	ILE	2.5
1	C	344	LEU	2.5
1	C	106	ALA	2.4
1	D	710	ARG	2.4
1	D	712	ALA	2.4
1	B	45	GLU	2.4
1	D	301	GLU	2.4
1	D	93	HIS	2.4
1	D	540	ALA	2.4
1	C	57	THR	2.4
1	D	327	LEU	2.4
1	A	638	LYS	2.4
1	B	542	GLN	2.4
1	B	640	ALA	2.4
1	D	627	VAL	2.4
1	D	270	LYS	2.4
1	D	553	THR	2.4
1	C	695	ILE	2.4
1	D	419	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	202	GLU	2.4
1	C	77	THR	2.4
1	C	292	HIS	2.4
1	D	228	PHE	2.4
1	D	596	GLY	2.4
1	D	154	ARG	2.4
1	A	691	GLN	2.4
1	C	322	ALA	2.4
1	C	408	ASN	2.4
1	D	136	VAL	2.4
1	D	577	THR	2.4
1	D	469	ARG	2.4
1	C	583	ASP	2.4
1	C	688	ALA	2.4
1	D	356	TYR	2.4
1	D	48	VAL	2.4
1	D	233	GLY	2.4
1	B	666	ALA	2.4
1	C	354	MET	2.4
1	C	684	ALA	2.4
1	D	103	ALA	2.4
1	D	320	ALA	2.4
1	D	702	LEU	2.3
1	C	671	LYS	2.3
1	D	397	HIS	2.3
1	C	44	LYS	2.3
1	B	634	VAL	2.3
1	C	154	ARG	2.3
1	A	593	GLU	2.3
1	C	669	SER	2.3
1	C	271	GLN	2.3
1	D	143	VAL	2.3
1	D	679	VAL	2.3
1	C	303	GLY	2.3
1	C	561	GLU	2.3
1	D	222	SER	2.3
1	D	549	HIS	2.3
1	D	390	LEU	2.3
1	C	404	GLN	2.3
1	D	349	LEU	2.3
1	C	620	THR	2.3
1	D	383	GLN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	286	GLY	2.3
1	D	637	GLY	2.3
1	D	140	PHE	2.3
1	C	111	ILE	2.3
1	C	646	PRO	2.3
1	D	589	LYS	2.3
1	A	665	ALA	2.3
1	C	547	TYR	2.3
1	D	704	VAL	2.3
1	D	188	PHE	2.3
1	B	131	ASP	2.3
1	C	302	SER	2.3
1	D	43	LEU	2.3
1	D	210	HIS	2.3
1	D	208	THR	2.3
1	C	265	TRP	2.3
1	D	440	ASN	2.3
1	C	703	LYS	2.3
1	C	654	LEU	2.3
1	C	445	ALA	2.3
1	C	142	THR	2.3
1	D	546	THR	2.3
1	D	645	PHE	2.3
1	A	38	ASP	2.2
1	D	379	ASP	2.2
1	D	266	HIS	2.2
1	D	481	GLN	2.2
1	D	179	VAL	2.2
1	D	216	PHE	2.2
1	D	428	HIS	2.2
1	B	543	PRO	2.2
1	C	85	ARG	2.2
1	D	245	GLY	2.2
1	C	644	LEU	2.2
1	D	381	LEU	2.2
1	D	424	GLN	2.2
1	C	153	ALA	2.2
1	D	640	ALA	2.2
1	A	675	GLN	2.2
1	D	265	TRP	2.2
1	B	697	GLY	2.2
1	C	652	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	672	LYS	2.2
1	B	636	SER	2.2
1	C	137	PHE	2.2
1	D	132	LYS	2.2
1	D	714	ASP	2.2
1	C	165	THR	2.2
1	D	632	GLU	2.2
1	D	670	ALA	2.2
1	D	395	ASN	2.2
1	D	620	THR	2.2
1	C	203	VAL	2.2
1	C	574	LEU	2.2
1	D	192	ILE	2.2
1	D	524	ILE	2.2
1	D	706	LYS	2.2
1	D	642	SER	2.1
1	C	89	GLN	2.1
1	D	711	PHE	2.1
1	C	204	PRO	2.1
1	D	598	LYS	2.1
1	D	567	ALA	2.1
1	C	304	ASN	2.1
1	D	407	ILE	2.1
1	C	130	LYS	2.1
1	C	690	ALA	2.1
1	D	368	GLY	2.1
1	C	238	ARG	2.1
1	D	137	PHE	2.1
1	D	226	THR	2.1
1	D	347	MET	2.1
1	C	247	GLY	2.1
1	C	585	ALA	2.1
1	D	365	PHE	2.1
1	D	474	THR	2.1
1	D	351	ARG	2.1
1	C	108	ALA	2.1
1	D	533	ALA	2.1
1	C	54	PHE	2.1
1	B	600	THR	2.1
1	C	237	PRO	2.1
1	C	650	PRO	2.1
1	A	688	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	709	GLU	2.1
1	D	119	SER	2.1
1	D	588	LEU	2.1
1	D	425	ALA	2.1
1	D	619	ALA	2.1
1	B	41	GLN	2.1
1	D	229	TRP	2.1
1	D	520	GLN	2.1
1	D	622	PHE	2.1
1	D	644	LEU	2.1
1	D	650	PRO	2.0
1	C	348	THR	2.0
1	D	308	TRP	2.0
1	A	337	GLU	2.0
1	C	537	GLY	2.0
1	D	255	THR	2.0
1	B	628	ALA	2.0
1	C	677	ILE	2.0
1	D	124	ALA	2.0
1	D	323	TYR	2.0
1	D	614	TYR	2.0
1	C	283	VAL	2.0
1	D	618	ASP	2.0
1	D	617	ALA	2.0
1	A	636	SER	2.0
1	D	626	VAL	2.0
1	B	605	TYR	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	HEM	D	4000	43/43	0.34	-0.11	92,93,97,101	0
2	HEM	B	4000	43/43	0.14	-0.16	43,46,50,59	0
2	HEM	A	4000	43/43	0.14	-0.26	31,34,38,40	0
2	HEM	C	4000	43/43	0.18	-0.82	60,62,68,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.