



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:07 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 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

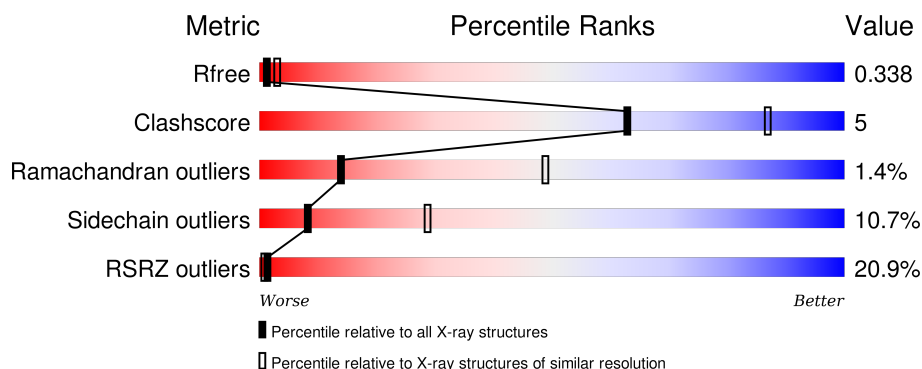
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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}	91344	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (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. 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	746	<div> <div>3%</div> <div>80%</div> <div>11%</div> <div>9%</div> </div>
1	B	746	<div> <div>6%</div> <div>78%</div> <div>12%</div> <div>9%</div> </div>
1	C	746	<div> <div>24%</div> <div>68%</div> <div>20%</div> <div>9%</div> </div>
1	D	746	<div> <div>43%</div> <div>65%</div> <div>22%</div> <div>9%</div> </div>

2 Entry composition

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

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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

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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

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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

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- Chemical structure of HEM (Heme) showing a central iron atom coordinated by four nitrogen atoms in a porphyrin-like ring, with various side chains and a central heme group.

- Molecule 3 is water.

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

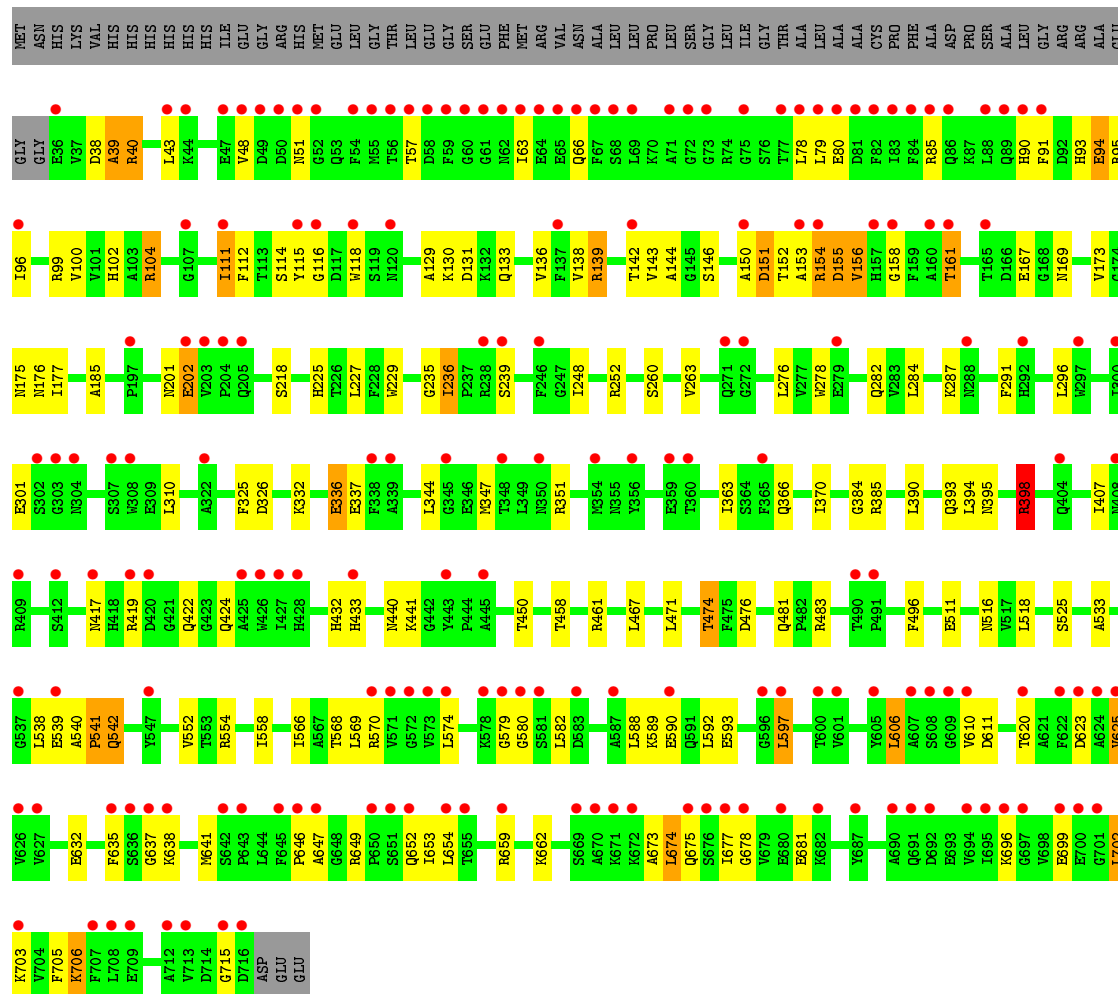


WORLD WIDE
PDB
PROTEIN DATA BANK

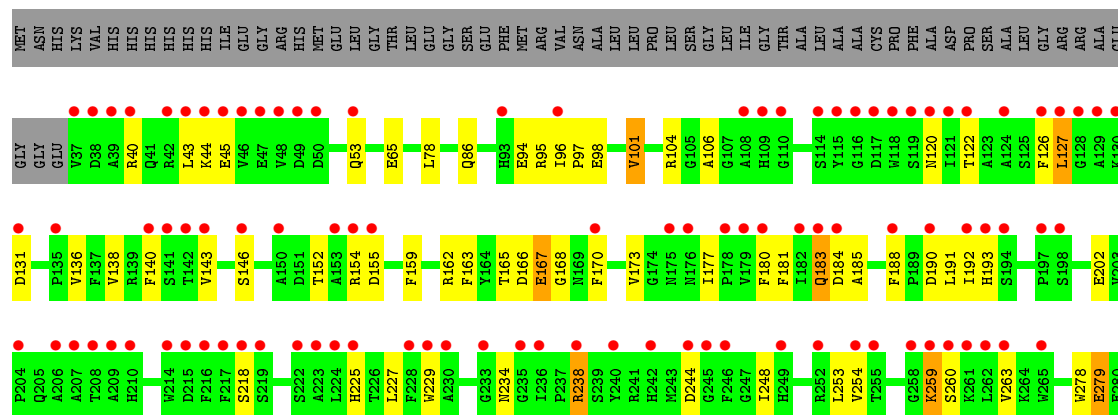
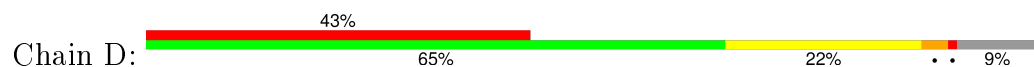
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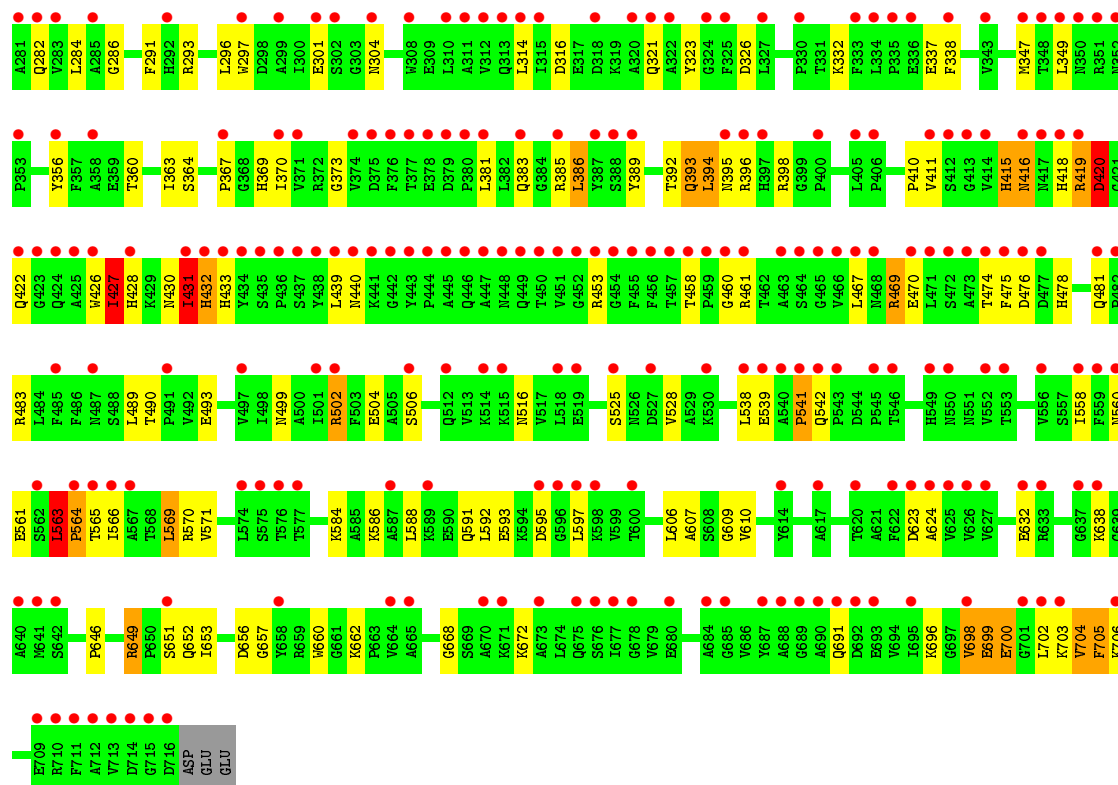
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	97	Total	O	0	0
			97	97		

• Molecule 1: CATALASE 3



• Molecule 1: CATALASE 3





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 , 0.338	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)	0.27 , 68.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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 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	5340	0	5156	33	0
1	B	5324	0	5141	33	0
1	C	5340	0	5156	85	0
1	D	5331	0	5151	88	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0
2	D	43	0	30	1	0
3	A	90	0	0	1	0
3	B	61	0	0	1	0
3	C	54	0	0	0	0
3	D	97	0	0	2	1
All	All	21809	0	20724	223	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (223) 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:D:704:VAL:HA	1:D:705:PHE:HB3	1.17	1.13
1:C:153:ALA:HB1	1:C:154:ARG:HA	1.22	1.10
1:D:415:HIS:HB2	1:D:416:ASN:HA	1.34	1.09
1:C:102:HIS:HA	1:C:142:THR:O	1.69	0.92
1:D:431:ILE:HD13	1:D:432:HIS:H	1.35	0.91
1:C:646:PRO:HB3	1:D:279:GLU:HG2	1.63	0.79
1:C:39:ALA:HB1	1:C:351:ARG:HG3	1.64	0.79
1:D:152:THR:HG21	1:D:284:LEU:HG	1.67	0.76
1:D:704:VAL:CA	1:D:705:PHE:HB3	2.09	0.75
1:C:153:ALA:HB1	1:C:154:ARG:CA	2.13	0.73
1:D:699:GLU:HG3	1:D:700:GLU:HG2	1.75	0.69
1:C:654:LEU:HB3	1:C:674:LEU:HD13	1.74	0.68
1:B:655:THR:O	1:B:659:ARG:HG2	1.93	0.68
1:D:426:TRP:HA	1:D:427:ILE:HB	1.75	0.68
1:C:287:LYS:HE2	1:D:282:GLN:HG3	1.76	0.68
1:C:158:GLY:HA2	1:C:175:ASN:HA	1.77	0.67
1:C:104:ARG:HE	1:C:151:ASP:HB2	1.58	0.67
1:B:593:GLU:HB3	1:C:580:GLY:HA3	1.77	0.67
1:C:91:PHE:O	1:C:94:GLU:HB2	1.95	0.67
1:C:332:LYS:HG2	1:C:481:GLN:HG3	1.76	0.66
1:D:180:PHE:HB2	1:D:248:ILE:HD13	1.78	0.65
1:C:646:PRO:HG3	1:C:649:ARG:HE	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:138:VAL:HG11	1:D:349:LEU:HD11	1.78	0.65
1:D:385:ARG:HG2	1:D:389:TYR:HE1	1.62	0.65
1:A:248:ILE:HD13	2:A:4000:HEM:HMB1	1.80	0.64
1:D:238:ARG:HH22	1:D:291:PHE:HZ	1.44	0.64
1:D:431:ILE:CD1	1:D:432:HIS:H	2.10	0.64
1:C:278:TRP:H	1:C:496:PHE:HE1	1.45	0.64
1:A:483:ARG:NH2	3:A:2070:HOH:O	2.30	0.63
1:D:260:SER:HB3	1:D:458:THR:HG21	1.80	0.63
1:D:563:LEU:HB3	1:D:564:PRO:HA	1.80	0.63
1:D:704:VAL:HA	1:D:705:PHE:CB	2.08	0.63
1:A:571:VAL:HG11	1:A:592:LEU:HD22	1.81	0.62
1:C:625:VAL:HB	1:C:654:LEU:HD12	1.81	0.62
1:C:606:LEU:HD21	1:D:506:SER:HB2	1.80	0.62
1:D:563:LEU:H	1:D:703:LYS:HG2	1.64	0.62
1:C:248:ILE:HD13	2:C:4000:HEM:HMB1	1.82	0.61
1:B:248:ILE:HD13	2:B:4000:HEM:HMB1	1.82	0.61
1:C:417:ASN:HB3	1:C:433:HIS:O	2.01	0.61
1:D:419:ARG:HE	1:D:420:ASP:HB3	1.66	0.60
1:C:40:ARG:HD2	1:C:43:LEU:HD12	1.82	0.60
1:C:540:ALA:HB1	1:C:541:PRO:CD	2.32	0.60
1:D:668:GLY:HA3	3:D:2064:HOH:O	2.02	0.59
1:C:153:ALA:CB	1:C:154:ARG:HA	2.12	0.58
1:C:93:HIS:ND1	1:D:395:ASN:HB2	2.18	0.58
1:D:154:ARG:HH12	1:D:504:GLU:HG3	1.69	0.58
1:B:569:LEU:HD13	1:B:598:LYS:H	1.68	0.58
1:C:702:LEU:HD12	1:C:705:PHE:HA	1.84	0.58
1:D:415:HIS:HB2	1:D:416:ASN:CA	2.23	0.57
1:C:57:THR:HG23	1:C:63:ILE:HG12	1.86	0.57
1:D:571:VAL:HG22	1:D:624:ALA:HB3	1.84	0.57
1:D:563:LEU:HB3	1:D:564:PRO:CA	2.34	0.57
1:D:183:GLN:HG2	1:D:475:PHE:HD2	1.69	0.57
1:C:284:LEU:HD13	1:C:620:THR:HB	1.87	0.57
1:C:177:ILE:HG12	1:C:229:TRP:HB3	1.87	0.56
1:D:415:HIS:CB	1:D:416:ASN:HA	2.22	0.56
1:D:646:PRO:HD2	1:D:649:ARG:HG3	1.87	0.56
1:D:489:LEU:HB3	1:D:493:GLU:HB3	1.88	0.55
1:D:431:ILE:HD13	1:D:432:HIS:N	2.14	0.54
1:A:177:ILE:HG12	1:A:229:TRP:HB3	1.89	0.54
1:D:385:ARG:HG2	1:D:389:TYR:CE1	2.43	0.54
1:C:483:ARG:HD2	1:C:525:SER:HB2	1.89	0.54
1:B:177:ILE:HG12	1:B:229:TRP:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:533:ALA:HB1	1:C:539:GLU:HA	1.90	0.54
1:D:177:ILE:HG12	1:D:229:TRP:HB3	1.90	0.54
1:D:483:ARG:HD2	1:D:525:SER:HB2	1.90	0.54
1:A:136:VAL:HG21	1:A:347:MET:HG3	1.90	0.53
1:B:136:VAL:HG21	1:B:347:MET:HG3	1.90	0.53
1:C:138:VAL:HG22	1:C:161:THR:HG22	1.89	0.53
1:D:180:PHE:CD2	1:D:381:LEU:HD21	2.43	0.53
1:D:165:THR:OG1	1:D:168:GLY:O	2.25	0.53
1:A:275:ALA:HB3	1:A:558:ILE:HD13	1.90	0.53
1:A:467:LEU:HD22	1:B:78:LEU:HD11	1.90	0.53
1:C:632:GLU:HG3	1:C:673:ALA:HB2	1.91	0.52
1:D:136:VAL:HG21	1:D:347:MET:HG3	1.92	0.52
1:D:97:PRO:HD2	1:D:396:ARG:HA	1.91	0.52
1:C:100:VAL:HA	1:D:95:ARG:HG3	1.90	0.52
1:C:39:ALA:CB	1:C:351:ARG:HG3	2.38	0.52
1:C:282:GLN:O	1:D:286:GLY:HA3	2.10	0.52
1:B:483:ARG:HD2	1:B:525:SER:HB2	1.92	0.52
1:C:90:HIS:H	1:C:93:HIS:HD2	1.58	0.52
1:B:660:TRP:HE3	1:B:662:LYS:HE3	1.75	0.51
1:C:635:PHE:CE1	1:C:674:LEU:HD12	2.45	0.51
1:D:185:ALA:HA	2:D:4000:HEM:HBB1	1.92	0.51
1:A:419:ARG:HG3	1:A:433:HIS:HD2	1.76	0.51
1:A:458:THR:HB	1:A:461:ARG:HG3	1.92	0.51
1:A:276:LEU:HA	1:A:706:LYS:HE3	1.92	0.51
1:D:660:TRP:HE3	1:D:662:LYS:HE3	1.76	0.50
1:B:138:VAL:HG22	1:B:161:THR:HG23	1.94	0.50
1:C:156:VAL:HG23	1:C:177:ILE:HD12	1.94	0.50
1:C:102:HIS:CE1	1:C:143:VAL:HG22	2.46	0.50
1:D:323:TYR:HD1	1:D:338:PHE:CD2	2.29	0.50
1:C:574:LEU:HD21	1:C:653:ILE:HG23	1.92	0.50
1:C:589:LYS:O	1:C:593:GLU:HB2	2.10	0.50
1:A:660:TRP:HE3	1:A:662:LYS:HE3	1.76	0.49
1:A:273:LYS:HB3	1:A:558:ILE:HG22	1.93	0.49
1:D:696:LYS:HA	1:D:699:GLU:HG2	1.93	0.49
1:D:278:TRP:O	1:D:282:GLN:HG2	2.12	0.49
1:B:234:ASN:ND2	1:B:558:ILE:HD11	2.27	0.49
1:A:78:LEU:HD11	1:B:467:LEU:HD22	1.94	0.49
1:A:42:ARG:HG2	1:A:43:LEU:HD22	1.95	0.49
1:B:568:THR:OG1	1:B:569:LEU:HA	2.13	0.49
1:C:136:VAL:HG21	1:C:347:MET:HG3	1.94	0.49
1:B:458:THR:HB	1:B:461:ARG:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PHE:HB2	1:C:332:LYS:HD3	1.94	0.48
1:D:699:GLU:HA	1:D:700:GLU:HA	1.65	0.48
1:D:418:HIS:CG	1:D:419:ARG:H	2.29	0.48
1:B:418:HIS:O	1:B:419:ARG:HD3	2.13	0.48
1:C:94:GLU:O	1:C:95:ARG:NH1	2.46	0.48
1:D:383:GLN:O	1:D:386:LEU:HG	2.13	0.48
1:C:566:ILE:HD13	1:C:699:GLU:HG2	1.95	0.48
1:C:366:GLN:HG2	1:C:390:LEU:HD22	1.95	0.48
1:C:458:THR:HB	1:C:461:ARG:HG3	1.94	0.48
1:C:39:ALA:HB3	1:C:40:ARG:HB3	1.95	0.48
1:D:234:ASN:ND2	1:D:558:ILE:HD11	2.29	0.48
1:B:667:VAL:HG22	1:B:694:VAL:HG21	1.95	0.48
1:C:276:LEU:HA	1:C:706:LYS:HE3	1.96	0.47
1:C:606:LEU:HA	1:C:610:VAL:HB	1.97	0.47
1:D:122:THR:HB	1:D:253:LEU:HB3	1.95	0.47
1:C:153:ALA:HB2	1:C:235:GLY:O	2.14	0.47
1:D:652:GLN:NE2	1:D:656:ASP:OD2	2.46	0.47
1:C:39:ALA:HB2	1:C:351:ARG:HH11	1.79	0.47
1:D:260:SER:HB3	1:D:458:THR:CG2	2.45	0.47
1:C:518:LEU:HB3	1:C:540:ALA:HB2	1.96	0.47
1:A:566:ILE:HA	1:A:569:LEU:HD12	1.96	0.47
1:A:495:GLN:OE1	1:A:531:ARG:NH2	2.37	0.47
1:B:708:LEU:HD22	1:B:708:LEU:H	1.79	0.47
1:C:225:HIS:CE1	1:C:481:GLN:HB3	2.49	0.46
1:C:202:GLU:HB2	1:D:356:TYR:CG	2.50	0.46
1:C:144:ALA:HB3	1:C:155:ASP:OD2	2.15	0.46
1:D:323:TYR:HD1	1:D:338:PHE:HD2	1.61	0.46
1:C:637:GLY:O	1:C:641:MET:HB2	2.16	0.46
1:D:254:VAL:N	1:D:373:GLY:O	2.47	0.46
1:B:154:ARG:HG3	1:B:236:ILE:HG23	1.97	0.46
1:B:175:ASN:HB2	1:B:248:ILE:HD11	1.97	0.46
1:C:284:LEU:HD11	1:C:291:PHE:CD1	2.51	0.46
1:C:111:ILE:HD11	1:C:133:GLN:HG2	1.97	0.46
1:C:569:LEU:HB2	1:C:597:LEU:HD23	1.96	0.46
1:C:432:HIS:HB2	1:C:440:ASN:HB3	1.96	0.46
1:C:310:LEU:HD23	1:C:344:LEU:HB2	1.98	0.46
1:D:360:THR:O	1:D:363:ILE:HG22	2.16	0.46
1:C:540:ALA:HB1	1:C:541:PRO:HD3	1.98	0.45
1:D:188:PHE:CZ	1:D:192:ILE:HD11	2.51	0.45
1:C:623:ASP:HB3	1:C:702:LEU:HD11	1.98	0.45
1:A:175:ASN:HB2	1:A:248:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:LEU:CB	1:D:564:PRO:HA	2.46	0.45
1:D:106:ALA:HB2	1:D:293:ARG:HG2	1.98	0.45
1:C:143:VAL:HG23	1:C:156:VAL:O	2.17	0.45
1:D:623:ASP:O	1:D:662:LYS:HB3	2.16	0.45
1:C:218:SER:HB2	1:C:516:ASN:HB3	1.99	0.45
1:C:116:GLY:HA2	1:C:130:LYS:HG3	1.99	0.45
1:B:261:LYS:HB2	3:B:2013:HOH:O	2.16	0.45
1:C:467:LEU:HD22	1:D:78:LEU:HD11	1.98	0.45
1:B:440:ASN:HD22	1:B:442:GLY:H	1.65	0.45
1:A:138:VAL:HG23	1:A:349:LEU:HD21	1.99	0.45
1:D:490:THR:OG1	1:D:493:GLU:HB2	2.17	0.45
1:A:559:PHE:CD2	1:A:708:LEU:HD21	2.51	0.45
1:B:569:LEU:HD22	1:B:597:LEU:HA	1.99	0.44
1:D:314:LEU:HD23	1:D:314:LEU:H	1.82	0.44
1:D:418:HIS:HB3	1:D:430:ASN:HD22	1.82	0.44
1:B:650:PRO:HA	1:B:653:ILE:HD12	1.99	0.44
1:D:564:PRO:HD2	3:D:2026:HOH:O	2.16	0.44
1:A:571:VAL:HG13	1:A:599:VAL:HG13	1.99	0.44
1:C:93:HIS:HE1	1:D:394:LEU:HG	1.83	0.44
1:D:569:LEU:O	1:D:623:ASP:HB2	2.17	0.44
1:C:173:VAL:HB	1:C:385:ARG:HH22	1.83	0.44
1:A:559:PHE:HB3	1:A:708:LEU:HD11	2.00	0.44
1:D:181:PHE:HB2	1:D:191:LEU:HD11	2.00	0.43
1:B:363:ILE:HD12	1:B:407:ILE:HG13	2.00	0.43
1:D:218:SER:HB2	1:D:516:ASN:HB3	2.00	0.43
1:C:652:GLN:NE2	1:D:652:GLN:OE1	2.52	0.43
1:C:336:GLU:H	1:C:336:GLU:HG2	1.59	0.43
1:C:153:ALA:CB	1:C:236:ILE:HG23	2.49	0.43
1:C:635:PHE:CE2	1:C:673:ALA:HB1	2.54	0.43
1:A:173:VAL:HB	1:A:385:ARG:HH22	1.83	0.43
1:C:394:LEU:O	1:C:398:ARG:HA	2.18	0.43
1:D:541:PRO:HB2	1:D:542:GLN:H	1.64	0.43
1:B:493:GLU:OE1	1:B:557:SER:OG	2.35	0.43
1:D:364:SER:HB3	1:D:393:GLN:CD	2.39	0.43
1:A:434:TYR:CE2	1:A:437:SER:HB2	2.54	0.42
1:C:326:ASP:HB2	1:C:474:THR:HB	2.00	0.42
1:D:173:VAL:HB	1:D:367:PRO:HG3	2.01	0.42
1:B:594:LYS:HA	1:C:579:GLY:H	1.84	0.42
1:C:112:PHE:HD1	1:C:347:MET:HB2	1.83	0.42
1:A:65:GLU:HB2	1:A:87:LYS:HD2	2.01	0.42
1:A:218:SER:HB2	1:A:516:ASN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:VAL:HG11	1:D:192:ILE:HD12	2.00	0.42
1:B:326:ASP:HB2	1:B:474:THR:HB	2.01	0.42
1:B:173:VAL:HB	1:B:385:ARG:HH22	1.84	0.42
1:B:255:THR:OG1	1:B:257:ASP:OD1	2.33	0.42
1:D:225:HIS:CE1	1:D:481:GLN:HB3	2.55	0.42
1:D:162:ARG:NH2	1:D:369:HIS:CE1	2.87	0.42
1:C:115:TYR:HD2	1:C:118:TRP:HZ2	1.67	0.42
1:D:326:ASP:HB2	1:D:474:THR:HB	2.02	0.41
1:B:225:HIS:CE1	1:B:481:GLN:HB3	2.55	0.41
1:D:136:VAL:HG12	1:D:163:PHE:HA	2.02	0.41
1:C:201:ASN:HB3	1:D:297:TRP:CE3	2.56	0.41
1:C:646:PRO:N	1:C:647:ALA:HA	2.35	0.41
1:A:566:ILE:HD12	1:A:597:LEU:HD11	2.01	0.41
1:A:326:ASP:HB2	1:A:474:THR:HB	2.01	0.41
1:C:185:ALA:HB3	1:C:384:GLY:HA3	2.02	0.41
1:D:163:PHE:HB2	1:D:170:PHE:O	2.20	0.41
1:C:252:ARG:NH1	1:C:461:ARG:HD3	2.35	0.41
1:D:389:TYR:HA	1:D:392:THR:HG22	2.01	0.41
1:C:260:SER:HB3	1:C:458:THR:CG2	2.51	0.41
1:D:234:ASN:HD21	1:D:558:ILE:HD11	1.86	0.41
1:D:499:ASN:HA	1:D:502:ARG:HD2	2.03	0.41
1:C:398:ARG:NH1	1:D:398:ARG:HG2	2.36	0.41
1:A:294:GLN:OE1	1:B:203:VAL:HG11	2.21	0.41
1:B:218:SER:HB2	1:B:516:ASN:HB3	2.02	0.41
1:C:139:ARG:HD3	2:C:4000:HEM:O2A	2.21	0.41
1:D:98:GLU:HA	1:D:396:ARG:HH21	1.85	0.41
1:A:667:VAL:HG22	1:A:694:VAL:HG21	2.02	0.41
1:C:363:ILE:HD12	1:C:407:ILE:HG13	2.03	0.41
1:B:701:GLY:HA2	1:B:707:PHE:HZ	1.86	0.41
1:D:657:GLY:HA2	1:D:662:LYS:HD2	2.03	0.40
1:A:225:HIS:CE1	1:A:481:GLN:HB3	2.57	0.40
2:C:4000:HEM:HBB2	2:C:4000:HEM:HMB1	2.02	0.40
1:A:112:PHE:HD1	1:A:347:MET:HB2	1.86	0.40
1:D:140:PHE:HE1	1:D:159:PHE:CZ	2.39	0.40
1:A:185:ALA:HB3	1:A:384:GLY:HA3	2.03	0.40
1:D:653:ILE:O	1:D:656:ASP:O	2.39	0.40
1:A:165:THR:C	1:A:167:GLU:H	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2016:HOH:O	3:D:2016:HOH:O[8_554]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	679/746 (91%)	640 (94%)	38 (6%)	1 (0%)	56	89
1	B	677/746 (91%)	628 (93%)	46 (7%)	3 (0%)	39	78
1	C	679/746 (91%)	619 (91%)	49 (7%)	11 (2%)	12	45
1	D	678/746 (91%)	585 (86%)	70 (10%)	23 (3%)	5	22
All	All	2713/2984 (91%)	2472 (91%)	203 (8%)	38 (1%)	14	49

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
1	D	259	LYS
1	D	411	VAL
1	D	415	HIS
1	D	428	HIS
1	D	541	PRO
1	B	570	ARG

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Mol	Chain	Res	Type
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%)	19	53
1	B	557/609 (92%)	511 (92%)	46 (8%)	14	43
1	C	559/609 (92%)	491 (88%)	68 (12%)	6	23
1	D	558/609 (92%)	472 (85%)	86 (15%)	3	14
All	All	2233/2436 (92%)	1994 (89%)	239 (11%)	8	29

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
1	A	700	GLU
1	A	706	LYS
1	B	41	GLN
1	B	42	ARG
1	B	45	GLU
1	B	65	GLU

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Mol	Chain	Res	Type
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
1	B	671	LYS
1	B	677	ILE
1	B	680	GLU
1	B	687	TYR
1	B	696	LYS
1	B	706	LYS

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Mol	Chain	Res	Type
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
1	C	422	GLN
1	C	424	GLN
1	C	441	LYS
1	C	450	THR
1	C	471	LEU
1	C	474	THR

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Mol	Chain	Res	Type
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
1	D	120	ASN
1	D	126	PHE
1	D	127	LEU
1	D	131	ASP
1	D	146	SER
1	D	155	ASP

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Mol	Chain	Res	Type
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
1	D	469	ARG
1	D	470	GLU
1	D	476	ASP
1	D	478	HIS
1	D	502	ARG
1	D	528	VAL

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Mol	Chain	Res	Type
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. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	ASN
1	A	468	ASN
1	A	516	ASN
1	A	591	GLN
1	A	652	GLN
1	B	234	ASN
1	B	440	ASN
1	B	516	ASN
1	B	522	ASN
1	B	526	ASN

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Mol	Chain	Res	Type
1	B	652	GLN
1	C	176	ASN
1	C	516	ASN
1	C	652	GLN
1	C	691	GLN
1	D	86	GLN
1	D	234	ASN
1	D	304	ASN
1	D	417	ASN
1	D	432	HIS
1	D	468	ASN
1	D	516	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	30,50,50	2.38	5 (16%)	24,82,82	2.71	13 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	4000	1	30,50,50	2.35	6 (20%)	24,82,82	2.68	13 (54%)
2	HEM	C	4000	1	30,50,50	2.26	8 (26%)	24,82,82	2.63	13 (54%)
2	HEM	D	4000	-	30,50,50	2.08	4 (13%)	24,82,82	2.42	11 (45%)

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	-	0/10/54/54	0/0/8/8
2	HEM	B	4000	1	-	0/10/54/54	0/0/8/8
2	HEM	C	4000	1	-	0/10/54/54	0/0/8/8
2	HEM	D	4000	-	-	0/10/54/54	0/0/8/8

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4000	HEM	C2D-C3D	-8.05	1.30	1.54
2	A	4000	HEM	C2D-C3D	-8.03	1.30	1.54
2	C	4000	HEM	C2D-C3D	-7.58	1.31	1.54
2	A	4000	HEM	C2C-C1C	-7.17	1.39	1.52
2	D	4000	HEM	C2D-C3D	-7.08	1.33	1.54
2	B	4000	HEM	C2C-C1C	-6.08	1.41	1.52
2	C	4000	HEM	C2C-C1C	-6.03	1.41	1.52
2	D	4000	HEM	C2C-C1C	-5.81	1.41	1.52
2	B	4000	HEM	C3B-C4B	-4.50	1.47	1.51
2	A	4000	HEM	C3D-C4D	-3.96	1.46	1.51
2	C	4000	HEM	C3B-C4B	-3.12	1.49	1.51
2	D	4000	HEM	C3C-CAC	-2.80	1.46	1.51
2	A	4000	HEM	C2B-C1B	-2.80	1.42	1.51
2	C	4000	HEM	C2B-C1B	-2.74	1.42	1.51
2	C	4000	HEM	CAA-C2A	-2.70	1.47	1.52
2	B	4000	HEM	C2B-C1B	-2.61	1.43	1.51
2	C	4000	HEM	C3D-C4D	-2.61	1.48	1.51
2	B	4000	HEM	CAD-C3D	-2.57	1.49	1.54
2	A	4000	HEM	C3B-C4B	-2.37	1.49	1.51
2	C	4000	HEM	CAD-C3D	-2.23	1.49	1.54
2	C	4000	HEM	C4C-NC	2.08	1.38	1.36
2	B	4000	HEM	C4C-NC	2.34	1.38	1.36
2	D	4000	HEM	C4C-NC	3.49	1.40	1.36

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	HEM	CAA-C2A-C1A	-3.70	122.99	127.01
2	B	4000	HEM	CAA-C2A-C1A	-3.65	123.05	127.01
2	D	4000	HEM	CAA-C2A-C1A	-3.49	123.22	127.01
2	D	4000	HEM	CMA-C3A-C4A	-3.47	122.62	128.36
2	C	4000	HEM	CAA-C2A-C1A	-3.34	123.38	127.01
2	A	4000	HEM	CMA-C3A-C4A	-3.02	123.36	128.36
2	B	4000	HEM	CBD-CAD-C3D	-2.93	105.02	113.55
2	B	4000	HEM	C1D-CHD-C4C	-2.90	120.97	125.82
2	D	4000	HEM	CAD-CBD-CGD	-2.85	101.39	113.02
2	C	4000	HEM	CBD-CAD-C3D	-2.81	105.37	113.55
2	D	4000	HEM	C1D-CHD-C4C	-2.72	121.28	125.82
2	B	4000	HEM	CMA-C3A-C4A	-2.71	123.88	128.36
2	A	4000	HEM	CBD-CAD-C3D	-2.70	105.70	113.55
2	B	4000	HEM	C3C-CAC-CBC	-2.66	120.38	124.46
2	C	4000	HEM	CMA-C3A-C4A	-2.62	124.03	128.36
2	A	4000	HEM	C3C-CAC-CBC	-2.44	120.71	124.46
2	C	4000	HEM	C1D-CHD-C4C	-2.41	121.80	125.82
2	B	4000	HEM	CAA-CBA-CGA	-2.25	108.61	112.75
2	C	4000	HEM	C3C-CAC-CBC	-2.23	121.03	124.46
2	A	4000	HEM	C1D-CHD-C4C	-2.10	122.32	125.82
2	A	4000	HEM	CAA-CBA-CGA	-2.07	108.95	112.75
2	C	4000	HEM	CAA-CBA-CGA	-2.05	108.99	112.75
2	D	4000	HEM	CMB-C2B-C3B	2.52	122.83	116.53
2	B	4000	HEM	CMA-C3A-C2A	2.63	130.74	125.24
2	C	4000	HEM	CMA-C3A-C2A	2.70	130.89	125.24
2	D	4000	HEM	C2D-C3D-C4D	2.71	106.10	101.50
2	A	4000	HEM	CMA-C3A-C2A	2.75	131.00	125.24
2	D	4000	HEM	CMA-C3A-C2A	2.77	131.02	125.24
2	D	4000	HEM	CMD-C2D-C3D	2.94	127.36	114.35
2	B	4000	HEM	CMD-C2D-C3D	3.14	128.25	114.35
2	A	4000	HEM	C2D-C3D-C4D	3.20	106.92	101.50
2	A	4000	HEM	CMD-C2D-C3D	3.20	128.51	114.35
2	B	4000	HEM	C2D-C3D-C4D	3.24	107.00	101.50
2	C	4000	HEM	CAD-C3D-C4D	3.33	124.22	112.47
2	C	4000	HEM	CMD-C2D-C3D	3.36	129.23	114.35
2	C	4000	HEM	C2D-C3D-C4D	3.51	107.45	101.50
2	B	4000	HEM	CAD-C3D-C4D	3.56	125.04	112.47
2	A	4000	HEM	CAD-C3D-C4D	3.59	125.15	112.47
2	D	4000	HEM	CAD-C3D-C4D	3.73	125.61	112.47
2	C	4000	HEM	CMC-C2C-C3C	4.57	127.93	116.53
2	D	4000	HEM	CMC-C2C-C3C	4.57	127.94	116.53
2	B	4000	HEM	CMC-C2C-C3C	4.58	127.97	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	4000	HEM	CMC-C2C-C3C	4.88	128.71	116.53
2	A	4000	HEM	CMB-C2B-C3B	5.00	129.00	116.53
2	A	4000	HEM	CAD-C3D-C2D	5.01	127.63	113.22
2	B	4000	HEM	CAD-C3D-C2D	5.04	127.70	113.22
2	C	4000	HEM	CMB-C2B-C3B	5.05	129.14	116.53
2	B	4000	HEM	CMB-C2B-C3B	5.10	129.25	116.53
2	C	4000	HEM	CAD-C3D-C2D	5.16	128.06	113.22
2	D	4000	HEM	CAD-C3D-C2D	5.24	128.28	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4000	HEM	1	0
2	B	4000	HEM	1	0
2	C	4000	HEM	3	0
2	D	4000	HEM	1	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, 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%)	-0.02	19 (2%) 56 36	15, 51, 103, 141	0
1	B	679/746 (91%)	0.28	48 (7%) 19 10	19, 63, 154, 227	0
1	C	681/746 (91%)	1.37	182 (26%) 1 0	32, 79, 138, 169	0
1	D	680/746 (91%)	2.21	321 (47%) 0 0	32, 94, 149, 188	0
All	All	2721/2984 (91%)	0.96	570 (20%) 1 1	15, 75, 140, 227	0

All (570) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	579	GLY	10.7
1	D	443	TYR	10.2
1	D	446	GLN	9.9
1	D	444	PRO	9.8
1	C	708	LEU	9.2
1	D	445	ALA	8.7
1	C	605	TYR	8.4
1	D	466	VAL	8.1
1	D	127	LEU	8.1
1	C	60	GLY	7.7
1	B	687	TYR	7.4
1	D	455	PHE	7.2
1	D	321	GLN	7.2
1	C	651	SER	7.1
1	D	315	ILE	7.0
1	D	322	ALA	7.0
1	D	215	ASP	7.0
1	C	66	GLN	6.9
1	D	120	ASN	6.8
1	D	126	PHE	6.8
1	C	428	HIS	6.8

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Mol	Chain	Res	Type	RSRZ
1	D	128	GLY	6.8
1	D	314	LEU	6.7
1	D	388	SER	6.6
1	D	468	ASN	6.6
1	D	447	ALA	6.6
1	B	633	ARG	6.5
1	D	473	ALA	6.4
1	D	715	GLY	6.2
1	D	678	GLY	6.2
1	B	568	THR	6.2
1	D	311	ALA	6.0
1	D	416	ASN	5.9
1	D	442	GLY	5.9
1	D	559	PHE	5.8
1	B	688	ALA	5.8
1	C	84	PHE	5.7
1	D	37	VAL	5.7
1	D	690	ALA	5.6
1	D	417	ASN	5.5
1	D	434	TYR	5.5
1	D	491	PRO	5.4
1	B	691	GLN	5.4
1	D	552	VAL	5.4
1	D	687	TYR	5.3
1	C	609	GLY	5.3
1	D	441	LYS	5.2
1	D	121	ILE	5.2
1	D	418	HIS	5.2
1	C	345	GLY	5.2
1	D	450	THR	5.2
1	C	83	ILE	5.2
1	C	75	GLY	5.1
1	D	433	HIS	5.1
1	D	38	ASP	5.1
1	D	412	SER	5.0
1	C	623	ASP	5.0
1	C	637	GLY	5.0
1	C	635	PHE	5.0
1	D	641	MET	4.9
1	D	400	PRO	4.9
1	C	691	GLN	4.9
1	D	566	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	645	PHE	4.9
1	C	56	THR	4.9
1	C	687	TYR	4.9
1	C	59	PHE	4.8
1	D	456	PHE	4.8
1	D	464	SER	4.8
1	D	150	ALA	4.8
1	D	545	PRO	4.8
1	C	573	VAL	4.8
1	D	219	SER	4.7
1	C	360	THR	4.7
1	B	545	PRO	4.7
1	D	688	ALA	4.7
1	D	675	GLN	4.7
1	D	677	ILE	4.7
1	B	686	VAL	4.6
1	C	625	VAL	4.6
1	B	685	GLY	4.6
1	C	572	GLY	4.6
1	C	676	SER	4.6
1	D	684	ALA	4.6
1	C	659	ARG	4.6
1	D	377	THR	4.6
1	D	53	GLN	4.6
1	C	607	ALA	4.5
1	D	414	VAL	4.5
1	C	49	ASP	4.5
1	C	643	PRO	4.5
1	C	624	ALA	4.5
1	D	449	GLN	4.4
1	D	370	ILE	4.4
1	C	608	SER	4.4
1	D	115	TYR	4.4
1	D	324	GLY	4.4
1	C	73	GLY	4.3
1	D	116	GLY	4.3
1	C	642	SER	4.3
1	C	427	ILE	4.3
1	D	223	ALA	4.3
1	D	190	ASP	4.3
1	D	153	ALA	4.3
1	C	636	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	69	LEU	4.2
1	D	482	PRO	4.2
1	D	689	GLY	4.2
1	C	412	SER	4.2
1	D	623	ASP	4.2
1	D	353	PRO	4.2
1	D	352	ASN	4.2
1	C	63	ILE	4.2
1	D	304	ASN	4.2
1	D	207	ALA	4.2
1	C	672	LYS	4.1
1	D	285	ALA	4.1
1	D	454	GLY	4.1
1	C	580	GLY	4.1
1	D	155	ASP	4.1
1	C	47	GLU	4.1
1	D	435	SER	4.1
1	C	88	LEU	4.1
1	D	472	SER	4.1
1	D	110	GLY	4.0
1	D	432	HIS	4.0
1	B	637	GLY	4.0
1	D	565	THR	4.0
1	D	214	TRP	4.0
1	C	50	ASP	4.0
1	C	62	ASN	4.0
1	D	665	ALA	4.0
1	D	283	VAL	4.0
1	C	610	VAL	3.9
1	B	638	LYS	3.9
1	C	90	HIS	3.9
1	C	116	GLY	3.9
1	C	67	PHE	3.9
1	D	436	PRO	3.9
1	D	238	ARG	3.9
1	C	627	VAL	3.9
1	C	696	LYS	3.8
1	C	68	SER	3.8
1	D	575	SER	3.8
1	D	595	ASP	3.8
1	D	465	GLY	3.8
1	D	325	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	122	THR	3.8
1	D	539	GLU	3.8
1	D	378	GLU	3.8
1	D	183	GLN	3.8
1	D	206	ALA	3.8
1	D	242	HIS	3.8
1	B	695	ILE	3.8
1	D	49	ASP	3.8
1	D	380	PRO	3.8
1	D	439	LEU	3.7
1	D	519	GLU	3.7
1	D	338	PHE	3.7
1	C	699	GLU	3.7
1	D	541	PRO	3.7
1	C	79	LEU	3.7
1	D	225	HIS	3.7
1	B	639	GLY	3.7
1	D	431	ILE	3.7
1	D	525	SER	3.7
1	D	131	ASP	3.7
1	B	696	LYS	3.7
1	A	682	LYS	3.7
1	B	715	GLY	3.7
1	D	193	HIS	3.7
1	D	664	VAL	3.7
1	D	313	GLN	3.7
1	C	443	TYR	3.6
1	C	96	ILE	3.6
1	D	297	TRP	3.6
1	C	65	GLU	3.6
1	D	476	ASP	3.6
1	D	260	SER	3.6
1	C	638	LYS	3.6
1	D	676	SER	3.6
1	B	38	ASP	3.6
1	D	374	VAL	3.6
1	B	578	LYS	3.6
1	D	438	TYR	3.6
1	C	239	SER	3.6
1	C	490	THR	3.5
1	D	335	PRO	3.5
1	D	413	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	538	LEU	3.5
1	D	389	TYR	3.5
1	C	288	ASN	3.5
1	C	655	THR	3.5
1	C	52	GLY	3.5
1	C	338	PHE	3.5
1	D	550	ASN	3.5
1	D	458	THR	3.5
1	C	712	ALA	3.5
1	D	587	ALA	3.5
1	C	713	VAL	3.5
1	C	81	ASP	3.5
1	B	579	GLY	3.5
1	D	246	PHE	3.5
1	D	176	ASN	3.5
1	A	637	GLY	3.5
1	A	36	GLU	3.4
1	D	633	ARG	3.4
1	C	707	PHE	3.4
1	C	80	GLU	3.4
1	C	581	SER	3.4
1	A	538	LEU	3.4
1	D	625	VAL	3.4
1	D	119	SER	3.4
1	C	118	TRP	3.4
1	D	713	VAL	3.4
1	D	281	ALA	3.4
1	D	109	HIS	3.4
1	C	596	GLY	3.3
1	B	39	ALA	3.3
1	D	39	ALA	3.3
1	B	689	GLY	3.3
1	D	512	GLN	3.3
1	D	376	PHE	3.3
1	D	259	LYS	3.3
1	C	61	GLY	3.3
1	D	451	VAL	3.3
1	D	282	GLN	3.3
1	D	709	GLU	3.3
1	D	224	LEU	3.3
1	C	58	ASP	3.3
1	D	691	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	453	ARG	3.3
1	C	539	GLU	3.3
1	D	426	TRP	3.3
1	D	129	ALA	3.2
1	C	491	PRO	3.2
1	D	701	GLY	3.2
1	C	590	GLU	3.2
1	D	333	PHE	3.2
1	D	597	LEU	3.2
1	D	600	THR	3.2
1	D	459	PRO	3.2
1	C	158	GLY	3.2
1	D	358	ALA	3.2
1	A	681	GLU	3.2
1	D	437	SER	3.2
1	D	422	GLN	3.2
1	D	118	TRP	3.2
1	D	198	SER	3.2
1	C	51	ASN	3.2
1	B	643	PRO	3.2
1	D	47	GLU	3.2
1	D	208	THR	3.2
1	D	194	SER	3.2
1	C	682	LYS	3.1
1	D	406	PRO	3.1
1	D	463	ALA	3.1
1	D	210	HIS	3.1
1	C	72	GLY	3.1
1	B	636	SER	3.1
1	D	50	ASP	3.1
1	D	560	ASN	3.1
1	D	440	ASN	3.1
1	D	680	GLU	3.1
1	C	426	TRP	3.1
1	C	86	GLN	3.1
1	C	675	GLN	3.1
1	C	71	ALA	3.1
1	D	343	VAL	3.1
1	D	236	ILE	3.1
1	C	703	LYS	3.1
1	C	669	SER	3.1
1	C	354	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	249	HIS	3.1
1	B	567	ALA	3.0
1	C	160	ALA	3.0
1	C	695	ILE	3.0
1	C	115	TYR	3.0
1	A	638	LYS	3.0
1	D	423	GLY	3.0
1	D	114	SER	3.0
1	C	570	ARG	3.0
1	D	460	GLY	3.0
1	D	45	GLU	3.0
1	D	518	LEU	3.0
1	C	694	VAL	3.0
1	D	562	SER	3.0
1	D	230	ALA	2.9
1	D	577	THR	2.9
1	B	684	ALA	2.9
1	A	691	GLN	2.9
1	C	716	ASP	2.9
1	D	514	LYS	2.9
1	D	117	ASP	2.9
1	C	425	ALA	2.9
1	B	577	THR	2.9
1	C	157	HIS	2.9
1	C	107	GLY	2.9
1	C	583	ASP	2.9
1	C	700	GLU	2.9
1	D	596	GLY	2.9
1	B	665	ALA	2.9
1	D	558	ILE	2.9
1	C	680	GLU	2.9
1	D	702	LEU	2.9
1	D	244	ASP	2.8
1	D	381	LEU	2.8
1	C	650	PRO	2.8
1	C	626	VAL	2.8
1	D	240	TYR	2.8
1	D	477	ASP	2.8
1	D	471	LEU	2.8
1	B	302	SER	2.8
1	D	542	GLN	2.8
1	D	348	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	638	LYS	2.8
1	B	716	ASP	2.8
1	D	130	LYS	2.8
1	D	310	LEU	2.8
1	A	688	ALA	2.8
1	C	120	ASN	2.8
1	D	233	GLY	2.8
1	C	48	VAL	2.8
1	B	131	ASP	2.8
1	D	228	PHE	2.8
1	D	292	HIS	2.8
1	D	299	ALA	2.8
1	D	564	PRO	2.8
1	B	693	GLU	2.7
1	B	595	ASP	2.7
1	D	549	HIS	2.7
1	A	550	ASN	2.7
1	D	461	ARG	2.7
1	D	334	LEU	2.7
1	B	690	ALA	2.7
1	A	698	VAL	2.7
1	D	312	VAL	2.7
1	C	578	LYS	2.7
1	D	448	ASN	2.7
1	C	701	GLY	2.7
1	C	78	LEU	2.7
1	D	397	HIS	2.7
1	A	675	GLN	2.7
1	C	161	THR	2.7
1	D	182	ILE	2.7
1	D	485	PHE	2.7
1	D	501	ILE	2.7
1	D	714	ASP	2.7
1	D	302	SER	2.7
1	B	683	GLU	2.6
1	C	709	GLU	2.6
1	D	142	THR	2.6
1	D	658	TYR	2.6
1	C	419	ARG	2.6
1	B	634	VAL	2.6
1	C	82	PHE	2.6
1	D	716	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	93	HIS	2.6
1	C	622	PHE	2.6
1	C	715	GLY	2.6
1	D	673	ALA	2.6
1	C	36	GLU	2.6
1	D	48	VAL	2.6
1	D	457	THR	2.6
1	D	350	ASN	2.6
1	D	204	PRO	2.6
1	C	571	VAL	2.6
1	D	371	VAL	2.6
1	D	698	VAL	2.6
1	C	204	PRO	2.6
1	D	387	TYR	2.6
1	D	671	LYS	2.6
1	D	396	ARG	2.6
1	D	695	ILE	2.6
1	B	542	GLN	2.6
1	D	527	ASP	2.6
1	D	543	PRO	2.6
1	D	209	ALA	2.6
1	D	712	ALA	2.6
1	B	539	GLU	2.5
1	C	64	GLU	2.5
1	C	404	GLN	2.5
1	C	652	GLN	2.5
1	D	556	VAL	2.5
1	D	627	VAL	2.5
1	A	640	ALA	2.5
1	D	351	ARG	2.5
1	C	44	LYS	2.5
1	A	542	GLN	2.5
1	D	385	ARG	2.5
1	D	424	GLN	2.5
1	C	57	THR	2.5
1	C	671	LYS	2.5
1	D	261	LYS	2.5
1	D	135	PRO	2.5
1	D	411	VAL	2.5
1	D	43	LEU	2.5
1	B	41	GLN	2.5
1	C	271	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	292	HIS	2.5
1	D	428	HIS	2.5
1	D	140	PHE	2.5
1	D	502	ARG	2.5
1	D	567	ALA	2.5
1	D	318	ASP	2.5
1	D	692	ASP	2.5
1	C	348	THR	2.5
1	C	620	THR	2.5
1	D	146	SER	2.5
1	D	367	PRO	2.5
1	D	670	ALA	2.5
1	B	632	GLU	2.5
1	D	375	ASP	2.5
1	D	217	PHE	2.5
1	D	624	ALA	2.4
1	C	647	ALA	2.4
1	D	262	LEU	2.4
1	C	302	SER	2.4
1	D	540	ALA	2.4
1	B	681	GLU	2.4
1	D	336	GLU	2.4
1	B	640	ALA	2.4
1	C	77	THR	2.4
1	D	395	ASN	2.4
1	D	452	GLY	2.4
1	D	470	GLU	2.4
1	C	692	ASP	2.4
1	D	179	VAL	2.4
1	D	184	ASP	2.4
1	D	467	LEU	2.4
1	D	265	TRP	2.4
1	D	614	TYR	2.4
1	D	383	GLN	2.4
1	A	593	GLU	2.4
1	D	711	PHE	2.4
1	D	263	VAL	2.4
1	C	409	ARG	2.4
1	B	598	LYS	2.4
1	C	433	HIS	2.4
1	D	553	THR	2.4
1	D	693	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	537	GLY	2.3
1	D	530	LYS	2.3
1	D	349	LEU	2.3
1	D	180	PHE	2.3
1	C	356	TYR	2.3
1	C	574	LEU	2.3
1	D	154	ARG	2.3
1	A	337	GLU	2.3
1	C	205	GLN	2.3
1	C	678	GLY	2.3
1	D	188	PHE	2.3
1	D	710	ARG	2.3
1	C	597	LEU	2.3
1	D	222	SER	2.3
1	D	546	THR	2.3
1	D	576	THR	2.3
1	D	379	ASP	2.3
1	C	408	ASN	2.3
1	C	670	ALA	2.3
1	D	515	LYS	2.3
1	B	694	VAL	2.3
1	D	46	VAL	2.3
1	D	175	ASN	2.3
1	D	252	ARG	2.3
1	D	216	PHE	2.3
1	D	475	PHE	2.3
1	C	202	GLU	2.3
1	C	43	LEU	2.3
1	D	40	ARG	2.3
1	D	245	GLY	2.3
1	C	547	TYR	2.3
1	C	300	ILE	2.3
1	C	272	GLY	2.3
1	C	322	ALA	2.3
1	C	587	ALA	2.3
1	D	108	ALA	2.3
1	D	487	ASN	2.3
1	D	598	LYS	2.3
1	C	111	ILE	2.2
1	D	356	TYR	2.2
1	D	308	TRP	2.2
1	D	574	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	153	ALA	2.2
1	C	197	PRO	2.2
1	C	85	ARG	2.2
1	D	143	VAL	2.2
1	A	38	ASP	2.2
1	B	45	GLU	2.2
1	D	255	THR	2.2
1	D	192	ILE	2.2
1	C	359	GLU	2.2
1	D	327	LEU	2.2
1	C	339	ALA	2.2
1	D	320	ALA	2.2
1	D	42	ARG	2.2
1	B	697	GLY	2.2
1	B	540	ALA	2.2
1	D	419	ARG	2.2
1	D	632	GLU	2.2
1	D	703	LYS	2.2
1	D	497	VAL	2.2
1	C	91	PHE	2.2
1	C	142	THR	2.2
1	C	55	MET	2.2
1	C	203	VAL	2.2
1	B	666	ALA	2.2
1	D	96	ILE	2.2
1	D	301	GLU	2.2
1	C	165	THR	2.2
1	C	601	VAL	2.2
1	C	445	ALA	2.2
1	D	218	SER	2.1
1	D	642	SER	2.1
1	C	54	PHE	2.1
1	A	665	ALA	2.1
1	C	417	ASN	2.1
1	D	124	ALA	2.1
1	C	697	GLY	2.1
1	D	254	VAL	2.1
1	D	481	GLN	2.1
1	A	587	ALA	2.1
1	D	617	ALA	2.1
1	D	170	PHE	2.1
1	D	229	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	594	LYS	2.1
1	D	589	LYS	2.1
1	D	626	VAL	2.1
1	C	600	THR	2.1
1	C	279	GLU	2.1
1	D	258	GLY	2.1
1	D	651	SER	2.1
1	D	330	PRO	2.1
1	D	347	MET	2.1
1	D	706	LYS	2.1
1	D	620	THR	2.1
1	D	235	GLY	2.1
1	B	133	GLN	2.1
1	C	297	TRP	2.1
1	C	308	TRP	2.1
1	D	405	LEU	2.1
1	B	116	GLY	2.1
1	C	303	GLY	2.1
1	D	637	GLY	2.1
1	C	154	ARG	2.1
1	C	238	ARG	2.1
1	C	89	GLN	2.1
1	D	44	LYS	2.1
1	D	178	PRO	2.1
1	C	150	ALA	2.1
1	D	425	ALA	2.1
1	C	677	ILE	2.1
1	C	137	PHE	2.0
1	C	307	SER	2.0
1	D	506	SER	2.0
1	C	646	PRO	2.0
1	D	474	THR	2.0
1	C	246	PHE	2.0
1	D	197	PRO	2.0
1	D	685	GLY	2.0
1	A	350	ASN	2.0
1	C	350	ASN	2.0
1	C	654	LEU	2.0
1	D	141	SER	2.0
1	C	420	ASP	2.0
1	C	304	ASN	2.0
1	C	690	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	640	ALA	2.0
1	C	365	PHE	2.0
1	D	622	PHE	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	HEM	D	4000	43/43	0.78	0.35	-0.09	92,93,97,101	0
2	HEM	A	4000	43/43	0.96	0.14	-0.14	31,34,38,40	0
2	HEM	B	4000	43/43	0.95	0.15	-0.15	43,46,50,59	0
2	HEM	C	4000	43/43	0.93	0.19	-0.77	60,62,68,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.