Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 08:23 AM GMT

PDB ID	:	3EH5
Title	:	Structure of the reduced form of cytochrome ba3 oxidase from Thermus thermophilus
Authors	:	Liu,B; Chen,Y.; Doukov,T.; Soltis,S.M.; Stout,D.; Fee,J.A.
Deposited on	:	2008-09-11
Resolution	:	2.80 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:

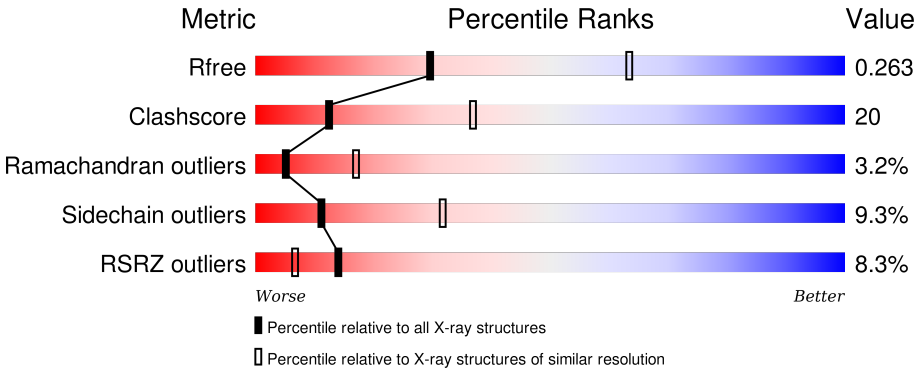
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	618	8% 55% 29% 5% • 10%
2	B	166	7% 68% 27% 5%
3	C	33	6% 73% 27%

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
8	BNG	A	807	-	-	-	X
8	BNG	C	804	-	-	-	X

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6244 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4409	2985	709	699	16	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-55	SER	-	EXPRESSION TAG	UNP Q5SJ79
A	-54	GLU	-	EXPRESSION TAG	UNP Q5SJ79
A	-53	ILE	-	EXPRESSION TAG	UNP Q5SJ79
A	-52	SER	-	EXPRESSION TAG	UNP Q5SJ79
A	-51	ARG	-	EXPRESSION TAG	UNP Q5SJ79
A	-50	VAL	-	EXPRESSION TAG	UNP Q5SJ79
A	-49	TYR	-	EXPRESSION TAG	UNP Q5SJ79
A	-48	GLU	-	EXPRESSION TAG	UNP Q5SJ79
A	-47	ALA	-	EXPRESSION TAG	UNP Q5SJ79
A	-46	TYR	-	EXPRESSION TAG	UNP Q5SJ79
A	-45	PRO	-	EXPRESSION TAG	UNP Q5SJ79
A	-44	GLU	-	EXPRESSION TAG	UNP Q5SJ79
A	-43	LYS	-	EXPRESSION TAG	UNP Q5SJ79
A	-42	LYS	-	EXPRESSION TAG	UNP Q5SJ79
A	-41	ALA	-	EXPRESSION TAG	UNP Q5SJ79
A	-40	THR	-	EXPRESSION TAG	UNP Q5SJ79
A	-39	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-38	TYR	-	EXPRESSION TAG	UNP Q5SJ79
A	-37	PHE	-	EXPRESSION TAG	UNP Q5SJ79
A	-36	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-35	VAL	-	EXPRESSION TAG	UNP Q5SJ79
A	-34	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-33	GLY	-	EXPRESSION TAG	UNP Q5SJ79
A	-32	PHE	-	EXPRESSION TAG	UNP Q5SJ79
A	-31	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-30	ALA	-	EXPRESSION TAG	UNP Q5SJ79
A	-29	LEU	-	EXPRESSION TAG	UNP Q5SJ79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ILE	-	EXPRESSION TAG	UNP Q5SJ79
A	-27	VAL	-	EXPRESSION TAG	UNP Q5SJ79
A	-26	GLY	-	EXPRESSION TAG	UNP Q5SJ79
A	-25	SER	-	EXPRESSION TAG	UNP Q5SJ79
A	-24	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-23	PHE	-	EXPRESSION TAG	UNP Q5SJ79
A	-22	GLY	-	EXPRESSION TAG	UNP Q5SJ79
A	-21	PRO	-	EXPRESSION TAG	UNP Q5SJ79
A	-20	PHE	-	EXPRESSION TAG	UNP Q5SJ79
A	-19	GLN	-	EXPRESSION TAG	UNP Q5SJ79
A	-18	ALA	-	EXPRESSION TAG	UNP Q5SJ79
A	-17	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-16	ASN	-	EXPRESSION TAG	UNP Q5SJ79
A	-15	TYR	-	EXPRESSION TAG	UNP Q5SJ79
A	-14	GLY	-	EXPRESSION TAG	UNP Q5SJ79
A	-13	ASN	-	EXPRESSION TAG	UNP Q5SJ79
A	-12	VAL	-	EXPRESSION TAG	UNP Q5SJ79
A	-11	ASP	-	EXPRESSION TAG	UNP Q5SJ79
A	-10	ALA	-	EXPRESSION TAG	UNP Q5SJ79
A	-9	TYR	-	EXPRESSION TAG	UNP Q5SJ79
A	-8	PRO	-	EXPRESSION TAG	UNP Q5SJ79
A	-7	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-6	LEU	-	EXPRESSION TAG	UNP Q5SJ79
A	-5	MET	-	EXPRESSION TAG	UNP Q5SJ79
A	-4	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-3	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-2	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	-1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	0	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	1	HIS	-	EXPRESSION TAG	UNP Q5SJ79
A	258	ARG	LYS	ENGINEERED	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	ENGINEERED	UNP Q5SJ80

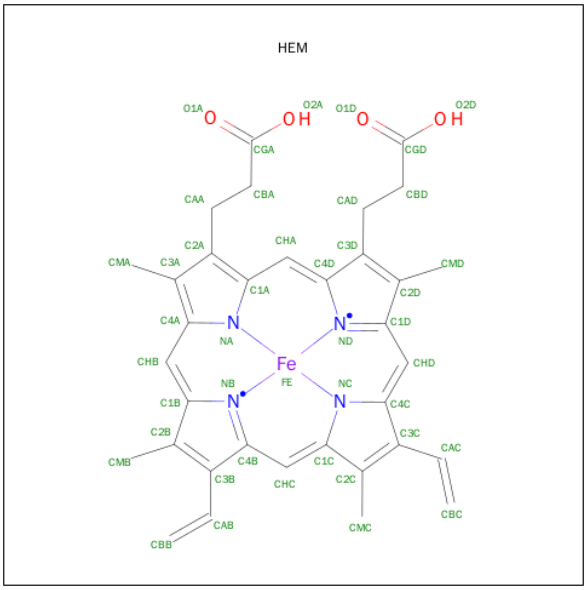
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

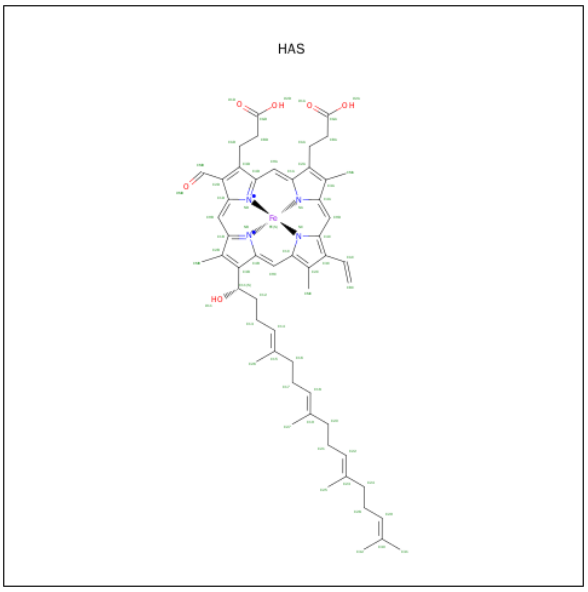
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



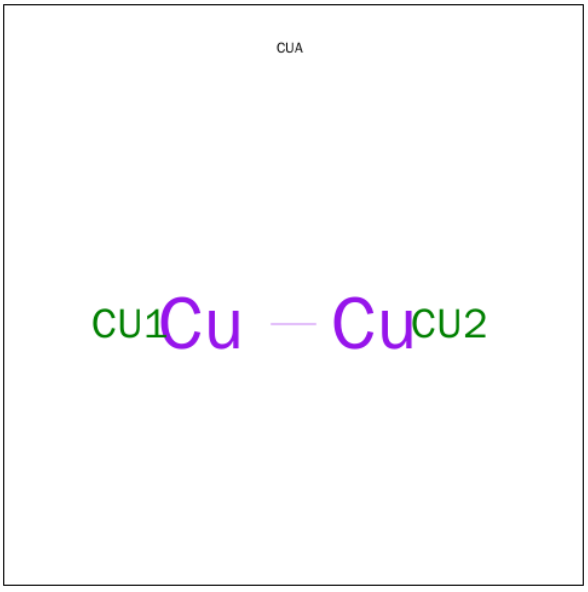
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is HEME-AS (three-letter code: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



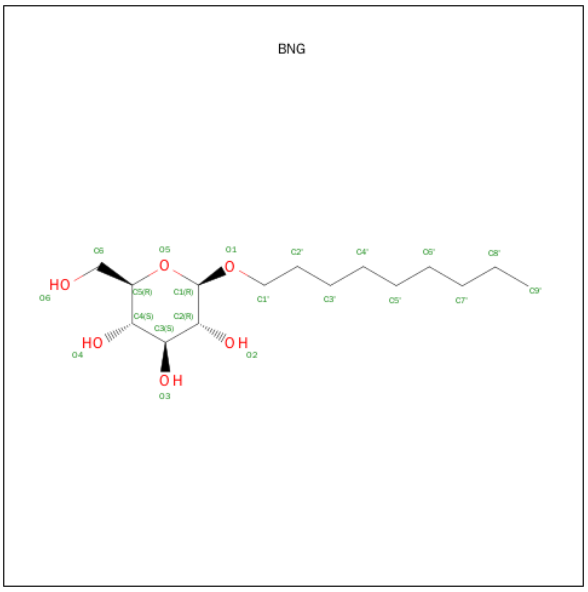
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Cu		0	0
			2	2			

- Molecule 8 is SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 21 15 6	0	0
8	A	1	Total C O 21 15 6	0	0
8	A	1	Total C O 21 15 6	0	0
8	A	1	Total C O 21 15 6	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	63	Total O 63 63	0	0
9	B	19	Total O 19 19	0	0
9	C	1	Total O 1 1	0	0

3 Residue-property plots (i)

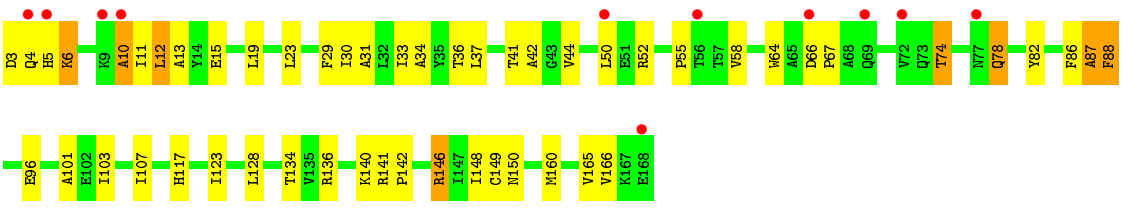
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Cytochrome c oxidase subunit 1

Chain A:

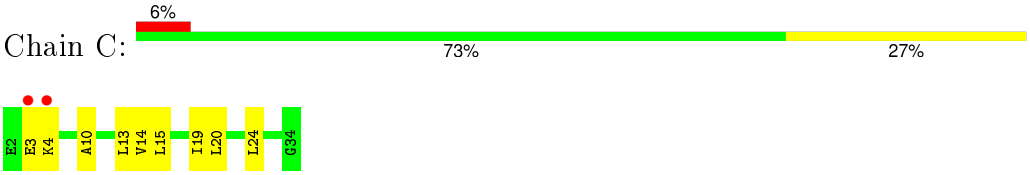
- Molecule 2: Cytochrome c oxidase subunit 2

Chain B:



• Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.63Å 115.63Å 149.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 19.99 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-2.80) 99.5 (19.99-2.55)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.40 (at 2.56Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.197 , 0.257 0.198 , 0.263	Depositor DCC
R_{free} test set	1274 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	79.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 103.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 33364 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6244	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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, HAS, BNG, CUA, CU1

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	0.87	1/4566 (0.0%)	0.94	7/6266 (0.1%)
2	B	0.91	0/1335	0.92	1/1822 (0.1%)
3	C	1.04	0/265	0.87	0/359
All	All	0.89	1/6166 (0.0%)	0.93	8/8447 (0.1%)

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	2
2	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	ARG	CG-CD	5.78	1.66	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	435	MET	CG-SD-CE	8.98	114.58	100.20
1	A	326	LEU	CA-CB-CG	6.54	130.34	115.30
2	B	146	ARG	CB-CG-CD	-5.74	96.67	111.60
1	A	432	MET	CG-SD-CE	5.31	108.70	100.20
1	A	450	ARG	NE-CZ-NH1	-5.11	117.74	120.30
1	A	326	LEU	CB-CG-CD1	5.06	119.60	111.00
1	A	54	LEU	CA-CB-CG	5.05	126.91	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	LEU	CB-CG-CD1	5.02	119.53	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	503	GLU	Peptide
1	A	8	ILE	Peptide
2	B	87	ALA	Peptide

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	4409	0	4516	204	1
2	B	1298	0	1282	43	0
3	C	259	0	279	5	0
4	A	1	0	0	0	0
5	A	43	0	30	6	0
6	A	65	0	61	8	0
7	B	2	0	0	0	0
8	A	63	0	90	2	0
8	C	21	0	30	0	0
9	A	63	0	0	47	1
9	B	19	0	0	7	0
9	C	1	0	0	0	0
All	All	6244	0	6288	243	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 20.

All (243) 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:233:HIS:NE2	1:A:237:TYR:CE2	1.73	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:HIS:NE2	1:A:237:TYR:HE2	0.80	1.29
1:A:185:MET:CE	9:A:624:HOH:O	1.84	1.26
1:A:281:PHE:HD2	9:A:572:HOH:O	1.18	1.23
1:A:185:MET:HE3	9:A:624:HOH:O	1.38	1.23
1:A:273:LEU:HD12	9:A:607:HOH:O	1.46	1.15
1:A:506:LEU:HD23	1:A:506:LEU:H	1.14	1.13
1:A:93:PRO:HA	9:A:625:HOH:O	1.54	1.06
1:A:281:PHE:CD2	9:A:572:HOH:O	1.95	1.03
1:A:265:ALA:HB1	9:A:624:HOH:O	1.57	1.03
1:A:554:ASN:HD22	2:B:52:ARG:HG3	1.24	1.00
1:A:7:GLU:O	1:A:10:ARG:HG2	1.62	1.00
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.87	0.90
1:A:330:ARG:HG3	1:A:330:ARG:HH21	1.39	0.88
1:A:233:HIS:CD2	1:A:237:TYR:HE2	1.90	0.86
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.64	0.86
1:A:506:LEU:HD23	1:A:506:LEU:N	1.86	0.86
1:A:410:GLY:HA3	1:A:499:PRO:HG3	1.57	0.85
1:A:22:LEU:O	1:A:26:VAL:HG23	1.76	0.84
1:A:96:GLU:HG2	9:A:625:HOH:O	1.77	0.84
1:A:109:SER:CB	9:A:614:HOH:O	2.27	0.81
1:A:445:LEU:O	1:A:446:ASN:HB2	1.80	0.80
1:A:500:GLU:HG2	1:A:501:LEU:H	1.46	0.80
1:A:554:ASN:ND2	2:B:52:ARG:HG3	1.96	0.80
1:A:389:VAL:HG23	9:A:621:HOH:O	1.82	0.79
1:A:499:PRO:HB3	1:A:502:ALA:HB3	1.63	0.78
1:A:109:SER:HB3	9:A:614:HOH:O	1.81	0.78
1:A:233:HIS:CD2	1:A:237:TYR:CE2	2.70	0.77
1:A:520:LEU:HB2	9:A:617:HOH:O	1.84	0.76
2:B:101:ALA:O	2:B:103:ILE:HD12	1.84	0.76
1:A:86:GLN:HE22	1:A:155:SER:HB3	1.52	0.75
1:A:138:PRO:HB3	9:A:584:HOH:O	1.87	0.74
1:A:520:LEU:CB	9:A:617:HOH:O	2.34	0.74
1:A:505:PRO:HB3	9:A:594:HOH:O	1.88	0.73
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.02	0.73
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.70	0.73
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.72	0.72
2:B:3:ASP:N	2:B:6:LYS:HB3	2.05	0.72
1:A:7:GLU:O	1:A:10:ARG:CG	2.38	0.71
1:A:228:PHE:HB3	9:A:568:HOH:O	1.90	0.70
1:A:523:ALA:O	1:A:526:ARG:HB2	1.92	0.70
1:A:185:MET:HE1	9:A:624:HOH:O	1.63	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD22	1:A:61:PHE:HE1	1.56	0.69
1:A:167:TRP:HE3	9:A:616:HOH:O	1.77	0.67
1:A:192:MET:CB	9:A:607:HOH:O	2.42	0.67
1:A:273:LEU:HA	9:A:607:HOH:O	1.95	0.66
1:A:23:TYR:HB3	1:A:110:TRP:NE1	2.11	0.66
1:A:497:ARG:C	1:A:499:PRO:HD3	2.15	0.66
1:A:352:GLY:C	1:A:392:LEU:HD13	2.17	0.65
1:A:302:THR:O	1:A:305:VAL:HG12	1.97	0.65
2:B:148:ILE:HG22	9:B:181:HOH:O	1.96	0.65
1:A:217:GLU:O	9:A:587:HOH:O	2.15	0.64
1:A:500:GLU:HG2	1:A:501:LEU:N	2.12	0.64
1:A:125:LEU:HD22	9:A:578:HOH:O	1.96	0.64
1:A:264:MET:SD	2:B:15:GLU:HG2	2.37	0.64
1:A:220:ASP:HB3	1:A:223:VAL:HG22	1.81	0.63
1:A:52:TYR:N	1:A:53:PRO:HD2	2.13	0.62
1:A:97:LEU:HD21	1:A:180:PRO:HG2	1.80	0.62
2:B:134:THR:HG22	9:B:183:HOH:O	1.99	0.62
1:A:330:ARG:HH21	1:A:330:ARG:CG	2.11	0.62
1:A:410:GLY:HA3	1:A:499:PRO:CG	2.30	0.62
1:A:19:LYS:HG2	1:A:107:TRP:HZ2	1.64	0.62
1:A:449:ARG:HD2	1:A:450:ARG:HG3	1.82	0.61
2:B:86:PHE:O	2:B:88:PHE:N	2.32	0.61
1:A:498:LYS:N	1:A:499:PRO:HD3	2.15	0.61
2:B:142:PRO:HA	2:B:166:VAL:CG2	2.30	0.61
1:A:410:GLY:HA2	1:A:502:ALA:HB2	1.83	0.61
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.82	0.60
1:A:391:SER:HB3	9:A:577:HOH:O	2.00	0.60
1:A:120:ALA:O	1:A:123:PRO:HD2	2.00	0.60
1:A:402:TYR:CD2	1:A:402:TYR:N	2.69	0.60
1:A:506:LEU:H	1:A:506:LEU:CD2	1.84	0.60
1:A:262:ASP:HB3	1:A:263:PRO:HD3	1.83	0.60
3:C:15:LEU:O	3:C:19:ILE:HG13	2.02	0.59
1:A:404:LEU:HG	1:A:408:LEU:HD11	1.85	0.59
2:B:3:ASP:O	2:B:4:GLN:HB3	2.03	0.59
1:A:104:GLY:HA2	8:A:805:BNG:H4	1.85	0.58
1:A:237:TYR:O	1:A:241:LEU:HD13	2.02	0.58
1:A:182:VAL:HG21	1:A:508:PHE:CE2	2.38	0.58
2:B:74:THR:CG2	2:B:78:GLN:OE1	2.52	0.57
1:A:281:PHE:H	1:A:298:HIS:HD2	1.51	0.57
1:A:59:LEU:HD22	1:A:61:PHE:CE1	2.39	0.57
1:A:267:LEU:HD13	9:A:618:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:HD23	9:A:618:HOH:O	2.03	0.57
1:A:345:ALA:HA	1:A:399:GLY:O	2.04	0.56
1:A:192:MET:HB2	9:A:607:HOH:O	2.04	0.56
1:A:477:LEU:CD1	5:A:800:HEM:HMB3	2.35	0.56
1:A:221:PRO:HB2	2:B:128:LEU:HD23	1.88	0.56
1:A:267:LEU:CD1	9:A:618:HOH:O	2.53	0.56
1:A:12:TYR:HB3	1:A:19:LYS:HD3	1.88	0.56
1:A:48:ASN:HD21	1:A:457:PRO:HA	1.71	0.56
1:A:207:PHE:HB3	1:A:219:VAL:HG13	1.87	0.56
1:A:499:PRO:HB3	1:A:502:ALA:CB	2.34	0.55
1:A:449:ARG:NH1	6:A:801:HAS:O2A	2.38	0.55
1:A:366:ASN:HB3	6:A:801:HAS:CMD	2.37	0.55
1:A:506:LEU:O	1:A:508:PHE:N	2.39	0.55
1:A:410:GLY:CA	1:A:502:ALA:HB2	2.35	0.55
1:A:389:VAL:CG2	9:A:621:HOH:O	2.50	0.55
1:A:47:GLY:HA3	1:A:471:VAL:HG23	1.89	0.54
1:A:366:ASN:HB3	6:A:801:HAS:HMD	1.89	0.54
3:C:10:ALA:O	3:C:14:VAL:HG23	2.08	0.54
2:B:4:GLN:HG3	2:B:4:GLN:O	2.08	0.53
1:A:106:MET:HA	1:A:162:ILE:HD11	1.91	0.53
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.43	0.53
1:A:364:ILE:HD12	3:C:19:ILE:HD13	1.91	0.53
1:A:280:GLY:HA3	1:A:542:TYR:OH	2.09	0.53
1:A:486:TYR:O	1:A:486:TYR:CG	2.62	0.52
1:A:515:PRO:HD3	2:B:5:HIS:NE2	2.24	0.52
1:A:465:VAL:HG13	9:A:604:HOH:O	2.08	0.52
1:A:518:ARG:HD2	9:A:605:HOH:O	2.09	0.52
2:B:150:ASN:HB3	9:B:181:HOH:O	2.10	0.52
1:A:160:ILE:CD1	1:A:194:PHE:HB2	2.40	0.52
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.44	0.52
2:B:74:THR:HG22	2:B:78:GLN:HB3	1.91	0.52
1:A:207:PHE:O	1:A:210:PRO:HD2	2.09	0.51
1:A:157:TRP:HA	1:A:160:ILE:HG13	1.93	0.51
1:A:477:LEU:HD12	5:A:800:HEM:HMB3	1.93	0.51
1:A:412:PRO:HG3	1:A:498:LYS:HB2	1.93	0.51
1:A:257:GLY:HA3	1:A:323:ALA:HB2	1.92	0.50
1:A:140:LYS:CD	9:A:588:HOH:O	2.59	0.50
1:A:272:PHE:O	1:A:276:SER:HB2	2.11	0.50
1:A:136:TYR:HE2	9:A:568:HOH:O	1.95	0.50
2:B:12:LEU:HD13	9:B:173:HOH:O	2.12	0.50
1:A:518:ARG:HH21	1:A:518:ARG:CG	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:THR:HA	9:A:582:HOH:O	2.12	0.50
1:A:89:MET:HB3	1:A:190:TRP:NE1	2.26	0.50
1:A:518:ARG:O	1:A:522:LEU:HB2	2.11	0.50
1:A:401:LEU:O	1:A:405:LEU:HB2	2.12	0.49
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.47	0.49
1:A:207:PHE:HB3	1:A:219:VAL:CG1	2.42	0.49
2:B:149:CYS:C	9:B:181:HOH:O	2.50	0.49
1:A:89:MET:HB3	1:A:190:TRP:HE1	1.77	0.49
1:A:362:GLY:HA3	9:A:575:HOH:O	2.12	0.49
1:A:156:THR:O	1:A:160:ILE:HG13	2.12	0.49
1:A:86:GLN:NE2	1:A:155:SER:HB3	2.24	0.49
1:A:17:GLU:OE1	1:A:100:ARG:HD3	2.12	0.49
1:A:90:VAL:O	1:A:93:PRO:HD2	2.13	0.49
2:B:50:LEU:HD22	2:B:52:ARG:NE	2.28	0.49
2:B:74:THR:HG23	2:B:78:GLN:OE1	2.12	0.48
2:B:29:PHE:HZ	3:C:20:LEU:HD23	1.77	0.48
2:B:55:PRO:O	2:B:58:VAL:HG12	2.13	0.48
1:A:9:SER:C	1:A:11:VAL:N	2.66	0.48
1:A:446:ASN:ND2	2:B:117:HIS:CE1	2.82	0.48
1:A:125:LEU:CB	9:A:578:HOH:O	2.61	0.48
1:A:106:MET:HA	1:A:162:ILE:CD1	2.44	0.48
1:A:239:TRP:HE3	6:A:801:HAS:HBC2	1.77	0.48
1:A:520:LEU:HB3	9:A:617:HOH:O	2.06	0.47
1:A:537:LEU:HA	1:A:537:LEU:HD23	1.70	0.47
1:A:20:ALA:HB3	1:A:106:MET:CE	2.45	0.47
1:A:458:ASP:HB2	9:A:590:HOH:O	2.13	0.47
2:B:33:ILE:O	2:B:36:THR:N	2.46	0.47
1:A:485:ILE:C	1:A:487:GLY:H	2.18	0.47
2:B:149:CYS:HB3	2:B:160:MET:HB3	1.96	0.47
1:A:402:TYR:HD2	1:A:402:TYR:N	2.13	0.47
1:A:527:ILE:HG22	1:A:528:GLY:N	2.29	0.47
1:A:389:VAL:CB	9:A:621:HOH:O	2.62	0.47
1:A:204:ALA:HA	1:A:208:LEU:HB2	1.98	0.46
1:A:104:GLY:CA	8:A:805:BNG:H4	2.45	0.46
1:A:192:MET:CA	9:A:607:HOH:O	2.63	0.46
1:A:192:MET:CG	9:A:607:HOH:O	2.63	0.46
1:A:8:ILE:C	1:A:10:ARG:N	2.67	0.46
1:A:174:ASN:O	1:A:177:LYS:HB2	2.16	0.46
1:A:125:LEU:HB3	9:A:578:HOH:O	2.16	0.46
1:A:330:ARG:HB2	1:A:334:GLY:HA3	1.98	0.45
1:A:282:HIS:HA	1:A:285:PHE:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:ARG:HA	1:A:495:ARG:HD3	1.54	0.45
1:A:134:THR:HG22	1:A:228:PHE:CE2	2.51	0.45
2:B:41:THR:O	2:B:44:VAL:HG22	2.17	0.45
1:A:241:LEU:HA	1:A:244:TYR:HB2	1.98	0.45
1:A:134:THR:HG22	1:A:228:PHE:CZ	2.52	0.45
1:A:61:PHE:CE2	1:A:62:VAL:HG23	2.51	0.45
1:A:71:LEU:O	1:A:75:LEU:HB2	2.17	0.45
1:A:459:ALA:O	2:B:146:ARG:NH1	2.42	0.45
1:A:72:HIS:O	1:A:76:ASN:HB2	2.16	0.45
1:A:8:ILE:HA	1:A:10:ARG:HG3	1.98	0.45
2:B:37:LEU:HA	2:B:42:ALA:HB2	1.98	0.45
2:B:66:ASP:HA	2:B:67:PRO:HD2	1.69	0.44
1:A:20:ALA:HB3	1:A:106:MET:HE2	1.99	0.44
1:A:85:ALA:O	1:A:89:MET:HB2	2.18	0.44
1:A:101:PRO:HB3	1:A:166:LEU:HD11	1.99	0.44
1:A:455:GLN:C	1:A:457:PRO:HD3	2.37	0.44
1:A:189:PHE:CE1	1:A:241:LEU:HB2	2.53	0.44
2:B:12:LEU:HG	2:B:12:LEU:O	2.18	0.44
2:B:37:LEU:HD12	2:B:37:LEU:N	2.33	0.44
1:A:366:ASN:CB	6:A:801:HAS:CMD	2.96	0.44
1:A:386:HIS:CE1	5:A:800:HEM:C1A	3.06	0.44
1:A:262:ASP:OD2	1:A:266:ARG:NE	2.50	0.44
1:A:386:HIS:HE1	5:A:800:HEM:C1A	2.36	0.43
1:A:515:PRO:O	1:A:517:ASP:N	2.51	0.43
1:A:192:MET:HA	9:A:607:HOH:O	2.18	0.43
1:A:332:LEU:HG	1:A:332:LEU:O	2.18	0.43
2:B:10:ALA:O	2:B:13:ALA:N	2.41	0.43
1:A:330:ARG:HG3	1:A:330:ARG:NH2	2.17	0.43
1:A:498:LYS:HB3	1:A:498:LYS:HE2	1.65	0.43
2:B:103:ILE:O	2:B:136:ARG:HA	2.18	0.43
2:B:64:TRP:CE2	2:B:82:TYR:HD2	2.35	0.43
2:B:44:VAL:CG2	9:B:176:HOH:O	2.66	0.43
1:A:140:LYS:NZ	9:A:593:HOH:O	2.36	0.43
1:A:56:LYS:HE2	1:A:60:PRO:O	2.19	0.43
1:A:8:ILE:C	1:A:10:ARG:H	2.22	0.43
1:A:477:LEU:HD13	5:A:800:HEM:HMB3	2.01	0.42
1:A:282:HIS:CD2	1:A:283:HIS:CD2	3.07	0.42
1:A:411:LYS:HE2	1:A:494:SER:O	2.19	0.42
1:A:7:GLU:HB3	1:A:13:GLU:HG2	2.01	0.42
1:A:35:GLY:HA3	1:A:76:ASN:ND2	2.34	0.42
1:A:307:VAL:HA	1:A:310:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:96:GLU:HA	2:B:165:VAL:O	2.19	0.42
1:A:339:LEU:HB3	1:A:346:PHE:CZ	2.54	0.42
2:B:44:VAL:HG21	9:B:176:HOH:O	2.18	0.42
2:B:58:VAL:HG22	2:B:64:TRP:HB2	2.00	0.42
1:A:56:LYS:HD3	1:A:56:LYS:O	2.20	0.42
1:A:23:TYR:HB3	1:A:110:TRP:CD1	2.55	0.42
1:A:282:HIS:HA	1:A:285:PHE:CE1	2.55	0.42
1:A:342:ASP:OD1	1:A:342:ASP:N	2.44	0.42
1:A:12:TYR:CG	1:A:19:LYS:HB2	2.55	0.42
1:A:259:LEU:HD11	9:A:565:HOH:O	2.20	0.42
6:A:801:HAS:HBC2	9:A:621:HOH:O	2.20	0.42
1:A:506:LEU:N	1:A:506:LEU:CD2	2.57	0.42
1:A:225:ARG:HD3	1:A:287:ASP:OD1	2.19	0.41
1:A:182:VAL:O	1:A:185:MET:HB2	2.20	0.41
1:A:343:ASN:HA	1:A:344:PRO:HD2	1.95	0.41
1:A:281:PHE:N	9:A:572:HOH:O	2.53	0.41
1:A:410:GLY:HA3	1:A:499:PRO:CB	2.51	0.41
2:B:117:HIS:HD2	2:B:123:ILE:O	2.03	0.41
1:A:228:PHE:CG	9:A:568:HOH:O	2.72	0.41
2:B:146:ARG:HD3	2:B:148:ILE:HD11	2.02	0.41
1:A:401:LEU:HA	1:A:401:LEU:HD12	1.88	0.41
1:A:102:ASN:OD1	1:A:105:LEU:N	2.44	0.41
1:A:392:LEU:HA	1:A:392:LEU:HD12	1.64	0.41
1:A:274:LEU:CD1	1:A:274:LEU:N	2.83	0.41
1:A:386:HIS:HE1	5:A:800:HEM:C4D	2.38	0.41
1:A:225:ARG:NH2	1:A:287:ASP:OD2	2.54	0.41
1:A:281:PHE:H	1:A:298:HIS:CD2	2.36	0.41
1:A:152:PHE:O	1:A:155:SER:HB2	2.21	0.41
1:A:344:PRO:HG2	1:A:402:TYR:CD1	2.56	0.41
1:A:196:ALA:HB1	1:A:234:PRO:HG2	2.02	0.41
2:B:31:ALA:O	2:B:34:ALA:HB3	2.21	0.41
1:A:343:ASN:O	1:A:347:VAL:HG23	2.21	0.40
1:A:92:LEU:HB3	1:A:182:VAL:HG11	2.03	0.40
1:A:262:ASP:HB3	1:A:263:PRO:CD	2.51	0.40
1:A:250:ILE:HD12	1:A:403:TRP:CH2	2.56	0.40
3:C:3:GLU:HG3	3:C:4:LYS:N	2.36	0.40
1:A:499:PRO:CB	1:A:502:ALA:HB3	2.43	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)
1:A:330:ARG:CD	9:A:590:HOH:O[4_444]	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	555/618 (90%)	464 (84%)	71 (13%)	20 (4%)	4 14
2	B	164/166 (99%)	146 (89%)	14 (8%)	4 (2%)	7 25
3	C	31/33 (94%)	29 (94%)	2 (6%)	0	100 100
All	All	750/817 (92%)	639 (85%)	87 (12%)	24 (3%)	5 17

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	57	ARG
1	A	58	LEU
1	A	330	ARG
1	A	501	LEU
1	A	517	ASP
1	A	518	ARG
2	B	10	ALA
2	B	11	ILE
2	B	87	ALA
2	B	88	PHE
1	A	11	VAL
1	A	87	ALA
1	A	88	ILE
1	A	102	ASN
1	A	127	ASN
1	A	452	TYR
1	A	486	TYR
1	A	516	GLU

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Mol	Chain	Res	Type
1	A	98	ASN
1	A	280	GLY
1	A	68	GLY
1	A	526	ARG
1	A	515	PRO

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	453/503 (90%)	407 (90%)	46 (10%)	9 26
2	B	136/136 (100%)	127 (93%)	9 (7%)	21 51
3	C	26/26 (100%)	24 (92%)	2 (8%)	16 41
All	All	615/665 (92%)	558 (91%)	57 (9%)	11 32

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	17	GLU
1	A	25	LEU
1	A	48	ASN
1	A	54	LEU
1	A	89	MET
1	A	95	ARG
1	A	96	GLU
1	A	122	LEU
1	A	133	TYR
1	A	155	SER
1	A	168	ARG
1	A	178	VAL
1	A	219	VAL
1	A	230	TRP
1	A	235	ILE
1	A	250	ILE

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Mol	Chain	Res	Type
1	A	274	LEU
1	A	276	SER
1	A	282	HIS
1	A	309	SER
1	A	315	THR
1	A	326	LEU
1	A	330	ARG
1	A	337	ARG
1	A	339	LEU
1	A	354	LEU
1	A	369	PHE
1	A	370	THR
1	A	371	LEU
1	A	391	SER
1	A	401	LEU
1	A	430	LEU
1	A	435	MET
1	A	439	LEU
1	A	452	TYR
1	A	465	VAL
1	A	472	LEU
1	A	478	LEU
1	A	490	SER
1	A	495	ARG
1	A	506	LEU
1	A	518	ARG
1	A	520	LEU
1	A	526	ARG
1	A	527	ILE
2	B	6	LYS
2	B	12	LEU
2	B	19	LEU
2	B	23	LEU
2	B	74	THR
2	B	78	GLN
2	B	107	ILE
2	B	140	LYS
2	B	141	ARG
3	C	13	LEU
3	C	24	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	48	ASN
1	A	76	ASN
1	A	82	GLN
1	A	86	GLN
1	A	127	ASN
1	A	254	GLN
1	A	284	GLN
1	A	298	HIS
1	A	388	GLN
1	A	446	ASN
1	A	554	ASN
2	B	117	HIS
2	B	122	ASN

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

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 for Mogul analysis.

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	$\#\|Z\| > 2$
5	HEM	A	800	1	30,50,50	2.44	9 (30%)	24,82,82	2.99	11 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	HAS	A	801	1	45,72,72	1.83	9 (20%)	47,109,109	3.87	17 (36%)
8	BNG	A	805	-	21,21,21	0.80	1 (4%)	26,26,26	1.08	1 (3%)
8	BNG	A	806	-	21,21,21	1.00	1 (4%)	26,26,26	1.23	4 (15%)
8	BNG	A	807	-	21,21,21	0.66	1 (4%)	26,26,26	1.23	4 (15%)
7	CUA	B	802	2	0,1,1	0.00	-	0,0,0	0.00	-
8	BNG	C	804	-	21,21,21	0.80	1 (4%)	26,26,26	1.43	5 (19%)

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
5	HEM	A	800	1	-	0/10/54/54	0/0/8/8
6	HAS	A	801	1	-	0/30/82/82	0/0/8/8
8	BNG	A	805	-	-	0/12/32/32	0/1/1/1
8	BNG	A	806	-	-	0/12/32/32	0/1/1/1
8	BNG	A	807	-	-	0/12/32/32	0/1/1/1
7	CUA	B	802	2	-	0/0/0/0	0/0/0/0
8	BNG	C	804	-	-	0/12/32/32	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C3B-C4B	-6.67	1.45	1.51
5	A	800	HEM	C3D-C4D	-6.12	1.43	1.51
6	A	801	HAS	C3C-CAC	-5.39	1.36	1.47
5	A	800	HEM	C2C-C1C	-3.30	1.46	1.52
6	A	801	HAS	C14-C15	2.02	1.36	1.33
8	A	807	BNG	O1-C1	2.12	1.44	1.40
8	A	805	BNG	O1-C1	2.24	1.44	1.40
5	A	800	HEM	C3B-CAB	2.39	1.55	1.51
8	C	804	BNG	O1-C1	2.47	1.44	1.40
6	A	801	HAS	C4A-CHD	2.48	1.46	1.39
8	A	806	BNG	O1-C1	2.83	1.45	1.40
6	A	801	HAS	C1A-CHA	2.99	1.48	1.39
5	A	800	HEM	FE-NB	3.03	2.13	1.97
5	A	800	HEM	CAA-C2A	3.06	1.57	1.52
5	A	800	HEM	CMB-C2B	3.16	1.60	1.53
5	A	800	HEM	C1C-NC	3.25	1.40	1.36
6	A	801	HAS	C1D-CHB	3.31	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C3C-C2C	3.36	1.44	1.40
6	A	801	HAS	C2A-C3A	3.37	1.47	1.37
6	A	801	HAS	C1C-CHC	3.45	1.49	1.39
5	A	800	HEM	C4C-NC	4.45	1.41	1.36
6	A	801	HAS	C2D-C3D	5.55	1.47	1.40

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CMA-C3A-C4A	-6.20	118.10	128.36
6	A	801	HAS	CAA-CBA-CGA	-5.80	102.12	112.75
6	A	801	HAS	CAD-CBD-CGD	-5.23	103.16	112.75
5	A	800	HEM	CAA-C2A-C1A	-4.93	121.65	127.01
6	A	801	HAS	C4D-C3D-C2D	-4.89	102.18	107.07
6	A	801	HAS	O11-C11-C3B	-2.93	103.16	111.82
5	A	800	HEM	C1D-CHD-C4C	-2.87	121.03	125.82
6	A	801	HAS	C24-C28-C29	-2.78	104.40	111.69
6	A	801	HAS	C12-C11-C3B	-2.55	107.32	112.59
8	A	807	BNG	O6-C6-C5	-2.43	103.30	111.33
5	A	800	HEM	C4B-CHC-C1C	-2.31	121.96	125.82
5	A	800	HEM	C3B-CAB-CBB	-2.28	120.96	124.46
8	C	804	BNG	O5-C1-C2	-2.28	105.60	110.28
8	A	806	BNG	O2-C2-C1	-2.20	105.20	110.02
8	C	804	BNG	C6-C5-C4	-2.18	107.63	113.02
8	A	807	BNG	C6-C5-C4	-2.12	107.78	113.02
6	A	801	HAS	C31-C30-C29	-2.11	115.81	122.61
6	A	801	HAS	CBD-CAD-C3D	-2.07	108.83	112.53
8	A	806	BNG	O4-C4-C3	2.02	114.88	110.34
8	A	807	BNG	C4-C3-C2	2.18	114.86	110.79
6	A	801	HAS	CMA-C3A-C2A	2.19	129.82	125.24
8	C	804	BNG	O5-C5-C4	2.26	113.92	109.68
6	A	801	HAS	C4B-C3B-C11	2.46	129.67	127.01
8	A	806	BNG	O3-C3-C4	2.52	116.00	110.34
8	A	805	BNG	O1-C1-C2	2.55	111.25	108.04
8	C	804	BNG	C4-C3-C2	2.57	115.58	110.79
6	A	801	HAS	C26-C15-C16	2.77	119.63	115.41
5	A	800	HEM	CMD-C2D-C3D	2.81	126.76	114.35
6	A	801	HAS	CAD-C3D-C4D	2.87	130.13	127.01
5	A	800	HEM	CAD-C3D-C4D	3.03	123.17	112.47
8	A	807	BNG	O5-C5-C4	3.04	115.38	109.68
8	C	804	BNG	C3-C4-C5	3.32	115.98	110.20
6	A	801	HAS	C2D-C1D-ND	3.38	113.58	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	801	HAS	O11-C11-C12	3.48	118.22	109.73
6	A	801	HAS	C32-C30-C31	3.55	123.37	114.64
8	A	806	BNG	C1-C2-C3	3.62	117.10	109.97
5	A	800	HEM	CMA-C3A-C2A	3.86	133.30	125.24
5	A	800	HEM	CMB-C2B-C3B	3.93	126.33	116.53
6	A	801	HAS	CMC-C2C-C1C	4.55	135.89	128.36
5	A	800	HEM	CMC-C2C-C3C	5.26	129.66	116.53
5	A	800	HEM	CAD-C3D-C2D	6.64	132.29	113.22
6	A	801	HAS	C3C-CAC-CBC	21.85	171.03	126.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	6	0
6	A	801	HAS	8	0
8	A	805	BNG	2	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	557/618 (90%)	0.14	50 (8%) 12 6	63, 85, 124, 190	0
2	B	166/166 (100%)	0.03	11 (6%) 22 13	66, 85, 118, 160	0
3	C	33/33 (100%)	-0.46	2 (6%) 25 15	67, 77, 125, 144	0
All	All	756/817 (92%)	0.09	63 (8%) 14 7	63, 85, 126, 190	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	ILE	10.3
1	A	495	ARG	8.4
1	A	494	SER	8.1
1	A	6	SER	8.1
2	B	69	GLN	8.1
1	A	515	PRO	7.6
1	A	493	LEU	6.6
1	A	7	GLU	6.4
1	A	514	GLY	5.9
1	A	12	TYR	4.9
1	A	177	LYS	4.8
1	A	498	LYS	4.8
1	A	9	SER	4.7
2	B	9	LYS	4.2
2	B	77	ASN	4.1
1	A	416	ALA	4.1
1	A	56	LYS	4.0
1	A	178	VAL	4.0
2	B	66	ASP	3.7
1	A	213	PHE	3.6
1	A	57	ARG	3.6
1	A	497	ARG	3.4
1	A	217	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	496	GLU	3.3
1	A	528	GLY	3.2
2	B	10	ALA	3.2
1	A	215	LEU	3.1
1	A	15	TYR	3.1
1	A	111	TRP	2.9
1	A	368	SER	2.8
1	A	499	PRO	2.8
1	A	172	ALA	2.7
1	A	330	ARG	2.7
1	A	218	GLY	2.6
2	B	168	GLU	2.6
1	A	61	PHE	2.6
1	A	214	GLY	2.6
1	A	168	ARG	2.5
1	A	60	PRO	2.4
2	B	4	GLN	2.4
1	A	175	PRO	2.4
1	A	161	TYR	2.4
1	A	513	SER	2.4
1	A	542	TYR	2.3
1	A	519	ARG	2.3
2	B	50	LEU	2.3
1	A	176	GLY	2.2
1	A	532	ALA	2.2
1	A	170	TRP	2.2
3	C	3	GLU	2.2
1	A	13	GLU	2.1
2	B	56	THR	2.1
1	A	331	GLY	2.1
3	C	4	LYS	2.1
1	A	553	LEU	2.1
1	A	293	THR	2.1
1	A	415	ASP	2.1
1	A	294	TRP	2.1
2	B	5	HIS	2.0
1	A	53	PRO	2.0
1	A	11	VAL	2.0
2	B	72	VAL	2.0
1	A	16	PRO	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
8	BNG	A	807	21/21	0.49	0.37	3.10	120,150,158,159	0
8	BNG	C	804	21/21	0.65	0.39	2.35	89,134,146,146	0
6	HAS	A	801	65/65	0.97	0.12	-0.84	58,66,77,83	0
5	HEM	A	800	43/43	0.98	0.10	-1.20	56,62,74,79	0
7	CUA	B	802	2/2	0.98	0.05	-2.35	80,80,80,80	0
8	BNG	A	805	21/21	0.64	0.35	-	146,158,162,163	0
8	BNG	A	806	21/21	0.61	0.40	-	134,141,143,144	0
4	CU1	A	803	1/1	0.99	0.08	-	80,80,80,80	0

6.5 Other polymers (i)

There are no such residues in this entry.