Full wwPDB X-ray Structure Validation Report ⓘ

PDB ID	:	2ZQX
Title	:	Cytochrome P450BSbeta cocrystallized with heptanoic acid
Authors	:	Shoji, O.; Fujishiro, T.; Nagano, S.; Hirose, T.; Shiro, Y.; Watanabe, Y.
Deposited on	:	2008-08-22
Resolution	:	2.37 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 (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.37 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	Percentile Ranks	Value
Rfree		0.231
Clashscore		17
Ramachandran outliers		0.3%
Sidechain outliers		6.1%
RSRZ outliers		3.1%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution
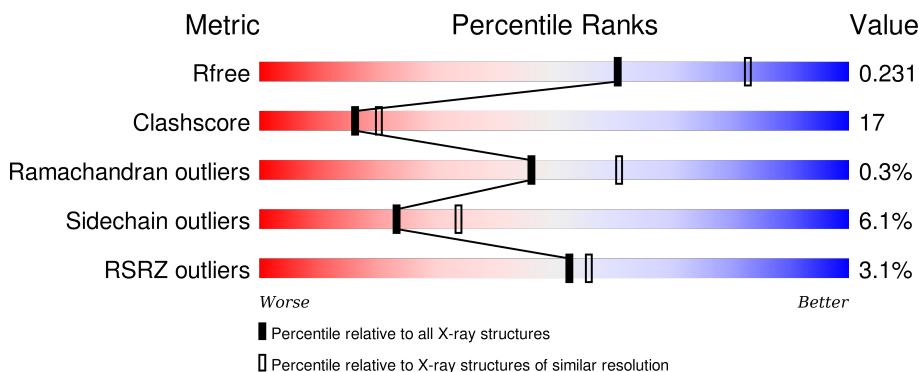
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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	417	% 71% 25% ··
1	B	417	% 66% 29% ··
1	C	417	7% 59% 36% ··
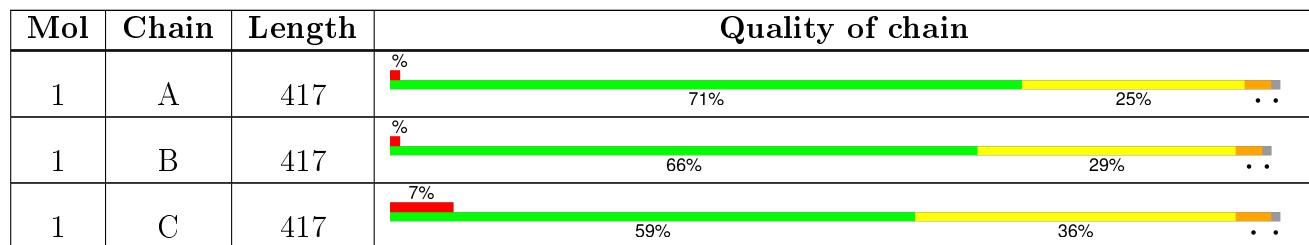
2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 10327 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 P450 152A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	B	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			
1	C	411	Total	C	N	O	S	0	0	0
			3339	2125	594	601	19			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
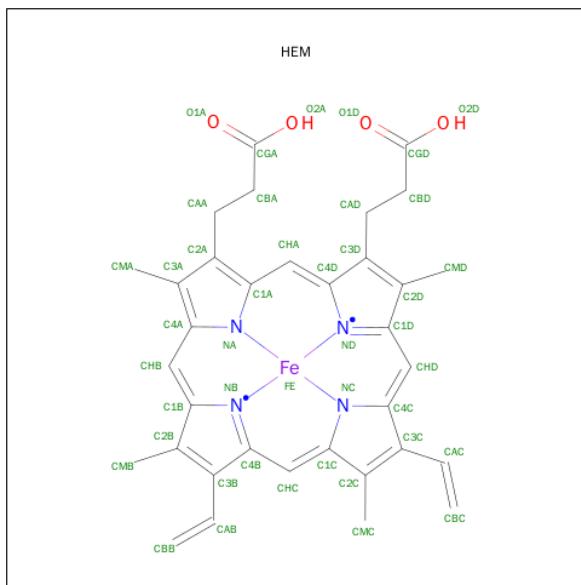
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

• Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	88	Total 88	O 88	0	0
3	B	67	Total 67	O 67	0	0
3	C	26	Total 26	O 26	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 P450 152A1

Chain A:

- Molecule 1: Cytochrome P450 152A1

Chain B:

- Molecule 1: Cytochrome P450 152A1

Chain C:
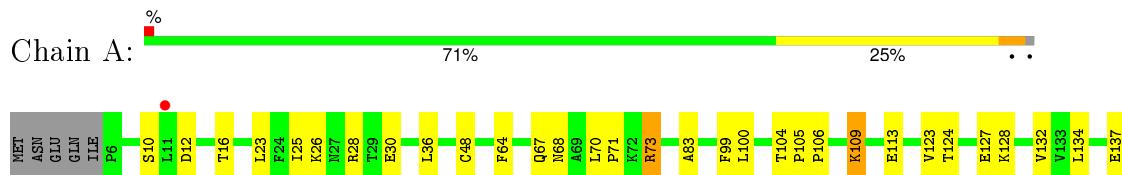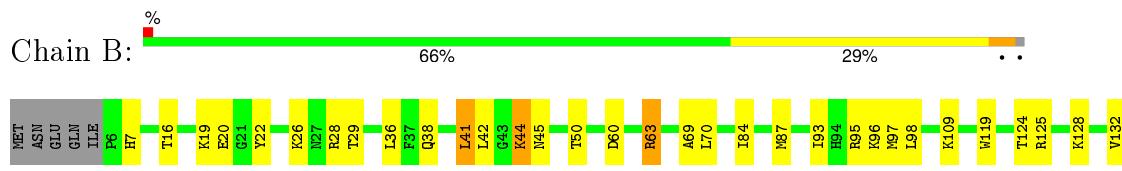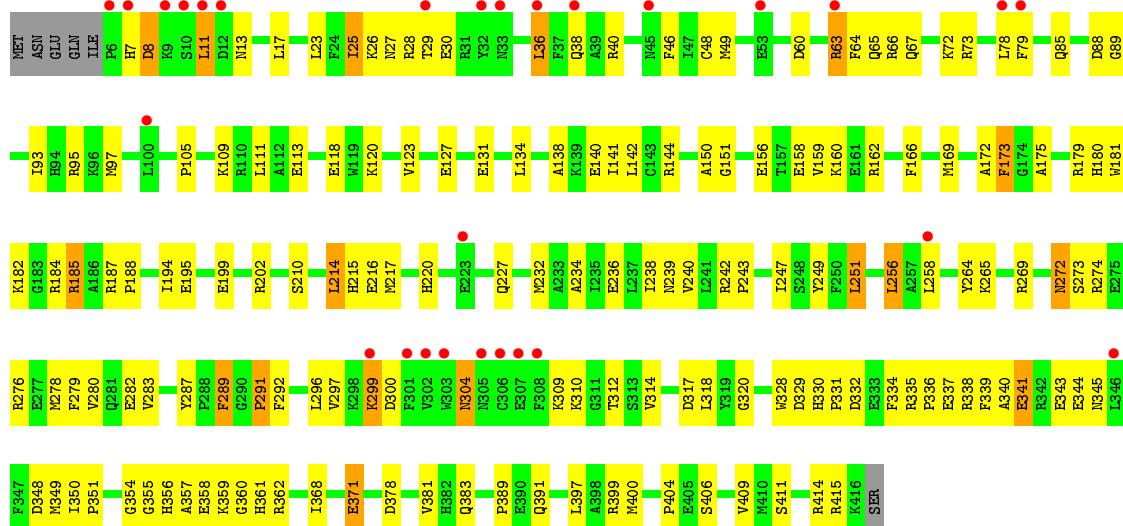
4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	172.23Å 172.23Å 277.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.57 – 2.37 44.57 – 2.35	Depositor EDS
% Data completeness (in resolution range)	93.6 (44.57-2.37) 93.5 (44.57-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.52 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.278 0.228 , 0.231	Depositor DCC
R_{free} test set	3061 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	35.3	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 44.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	Xtriage
Outliers	0 of 61621 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10327	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.84% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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	0.41	0/3422	0.59	0/4614
1	B	0.38	0/3422	0.58	0/4614
1	C	0.32	0/3422	0.53	0/4614
All	All	0.37	0/10266	0.56	0/13842

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3339	0	3290	91	0
1	B	3339	0	3290	111	0
1	C	3339	0	3290	135	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
3	A	88	0	0	2	0
3	B	67	0	0	5	0
3	C	26	0	0	2	0
All	All	10327	0	9960	338	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 17.

All (338) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:PRO:HB3	1:C:400:MET:HE1	1.47	0.96
1:C:25:ILE:H	1:C:25:ILE:HD12	1.28	0.95
1:C:391:GLN:HE22	1:C:409:VAL:H	0.97	0.95
1:B:391:GLN:HE22	1:B:409:VAL:H	1.05	0.93
1:A:391:GLN:HE22	1:A:409:VAL:H	1.10	0.91
1:A:100:LEU:HD13	1:A:358:GLU:HG2	1.54	0.89
1:C:127:GLU:HG2	1:C:414:ARG:HA	1.55	0.87
1:C:67:GLN:HG3	1:C:88:ASP:OD2	1.75	0.87
1:B:232:MET:HE2	1:B:236:GLU:HG2	1.58	0.85
1:A:265:LYS:HE2	1:A:269:ARG:HH22	1.43	0.83
1:A:160:LYS:HZ2	1:A:160:LYS:H	1.25	0.82
1:B:391:GLN:NE2	1:B:409:VAL:H	1.77	0.82
1:C:391:GLN:NE2	1:C:409:VAL:H	1.77	0.81
1:B:139:LYS:HE2	1:B:167:ILE:HD12	1.62	0.80
1:B:44:LYS:HE2	1:B:45:ASN:H	1.44	0.80
1:C:291:PRO:HB3	1:C:400:MET:CE	2.13	0.79
1:B:69:ALA:HA	1:B:296:LEU:HD13	1.67	0.77
1:C:181:TRP:HB3	1:C:185:ARG:NH1	2.01	0.76
1:B:391:GLN:HE22	1:B:409:VAL:N	1.82	0.74
1:A:391:GLN:NE2	1:A:409:VAL:H	1.86	0.74
1:C:109:LYS:O	1:C:113:GLU:HG3	1.87	0.73
1:C:234:ALA:O	1:C:238:ILE:HG12	1.89	0.73
1:A:309:LYS:O	1:A:312:THR:HG23	1.88	0.73
1:B:239:ASN:HD22	1:B:242:ARG:HH12	1.38	0.72
1:A:265:LYS:HE2	1:A:269:ARG:NH2	2.05	0.72
1:B:44:LYS:HE2	1:B:45:ASN:N	2.06	0.70
1:B:284:ARG:NE	1:B:370:ILE:HD11	2.07	0.69
1:B:265:LYS:HZ2	1:B:269:ARG:HH12	1.39	0.69
1:C:272:ASN:ND2	1:C:273:SER:H	1.89	0.69
1:B:256:LEU:HD22	1:B:260:GLU:HG3	1.74	0.68
1:B:293:LEU:HG	1:B:318:LEU:HD11	1.74	0.68
1:B:239:ASN:ND2	1:B:242:ARG:HH12	1.91	0.68
1:C:269:ARG:HB2	1:C:269:ARG:NH1	2.09	0.68
1:C:25:ILE:HG21	1:C:317:ASP:HB2	1.76	0.67
1:B:195:GLU:OE1	1:B:231:ARG:HD3	1.95	0.67
1:C:187:ARG:HB3	1:C:188:PRO:HD3	1.75	0.67
1:C:247:ILE:HA	2:C:501:HEM:HBB1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ASP:OD2	1:B:63:ARG:HD3	1.95	0.66
1:B:265:LYS:NZ	1:B:269:ARG:HH12	1.92	0.66
1:A:274:ARG:HE	1:A:278:MET:CE	2.07	0.66
1:B:232:MET:HE3	1:B:235:ILE:HB	1.77	0.66
1:C:166:PHE:HA	1:C:169:MET:HE3	1.76	0.66
1:C:236:GLU:HA	1:C:236:GLU:OE2	1.96	0.65
1:A:274:ARG:HE	1:A:278:MET:HE2	1.62	0.65
1:C:65:GLN:HG2	1:C:296:LEU:HB3	1.78	0.65
1:A:100:LEU:CD1	1:A:358:GLU:HG2	2.25	0.65
1:A:391:GLN:HE22	1:A:409:VAL:N	1.91	0.64
1:C:242:ARG:HB3	1:C:243:PRO:HD3	1.78	0.64
1:B:403:LEU:HG	1:B:404:PRO:HD2	1.78	0.64
1:A:152:VAL:HG13	1:A:197:MET:SD	2.38	0.64
1:C:355:GLY:O	1:C:362:ARG:HD2	1.98	0.64
1:C:156:GLU:HA	1:C:159:VAL:HG23	1.80	0.63
1:C:265:LYS:HE2	1:C:381:VAL:HG13	1.80	0.63
1:B:139:LYS:HG3	1:B:140:GLU:N	2.13	0.63
1:A:109:LYS:HE3	1:A:109:LYS:HA	1.81	0.63
1:B:394:HIS:O	1:B:405:GLU:HG3	1.98	0.63
1:B:242:ARG:HB3	1:B:243:PRO:HD3	1.79	0.63
1:B:96:LYS:HE3	1:B:364:PRO:HD3	1.81	0.63
1:C:23:LEU:HB3	1:C:27:ASN:ND2	2.14	0.63
1:C:131:GLU:HG2	1:C:411:SER:HB3	1.81	0.63
1:C:194:ILE:HG13	1:C:238:ILE:HD11	1.79	0.63
1:B:264:TYR:CZ	1:B:336:PRO:HD2	2.33	0.62
1:A:109:LYS:O	1:A:113:GLU:HG3	2.00	0.62
1:A:268:LEU:HD23	1:A:275:GLU:HB3	1.82	0.62
1:B:140:GLU:OE1	1:B:160:LYS:HE3	1.99	0.62
1:B:187:ARG:HB3	1:B:188:PRO:HD3	1.81	0.62
1:B:194:ILE:HG13	1:B:238:ILE:HD11	1.82	0.62
1:A:16:THR:HG21	1:A:28:ARG:NH2	2.15	0.62
1:A:236:GLU:HA	1:A:236:GLU:OE1	2.00	0.61
1:C:328:TRP:HB2	1:C:331:PRO:HB3	1.82	0.61
1:C:73:ARG:NH2	1:C:175:ALA:O	2.34	0.61
1:C:247:ILE:O	1:C:251:LEU:HD22	2.00	0.61
1:C:11:LEU:HD13	1:C:40:ARG:HG2	1.81	0.61
1:B:234:ALA:O	1:B:238:ILE:HG12	2.01	0.61
1:A:380:LEU:HA	1:A:384:ILE:HD11	1.82	0.61
1:B:292:PHE:HA	1:B:318:LEU:HD13	1.82	0.60
1:C:25:ILE:O	1:C:29:THR:HG23	2.01	0.60
1:A:185:ARG:O	1:A:188:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:328:TRP:O	1:C:331:PRO:HD3	2.01	0.59
1:C:150:ALA:O	1:C:214:LEU:HB2	2.03	0.59
1:C:339:PHE:O	1:C:341:GLU:N	2.35	0.59
1:B:370:ILE:O	1:B:374:LYS:HG3	2.03	0.59
1:A:124:THR:HG22	1:A:128:LYS:NZ	2.18	0.59
1:A:70:LEU:HB3	1:A:71:PRO:HD2	1.84	0.59
1:A:109:LYS:CE	1:A:109:LYS:HA	2.32	0.58
1:C:120:LYS:HG2	1:C:383:GLN:HE21	1.68	0.58
1:C:345:ASN:HB3	1:C:348:ASP:OD1	2.02	0.58
1:B:152:VAL:HG13	1:B:197:MET:SD	2.44	0.58
1:B:276:ARG:HH11	1:B:276:ARG:CB	2.17	0.58
1:A:138:ALA:O	1:A:142:LEU:HD13	2.03	0.57
1:A:288:PRO:HG3	1:A:397:LEU:HD23	1.86	0.57
1:A:247:ILE:HG22	1:A:251:LEU:HD13	1.86	0.57
1:A:187:ARG:HB3	1:A:188:PRO:HD3	1.85	0.57
1:A:187:ARG:O	1:A:191:GLU:HG3	2.04	0.57
1:C:335:ARG:O	1:C:338:ARG:HG2	2.04	0.57
1:C:17:LEU:C	1:C:17:LEU:HD23	2.25	0.57
1:B:142:LEU:HG	1:B:244:ILE:O	2.05	0.57
1:C:354:GLY:HA2	1:C:362:ARG:NH1	2.20	0.57
1:B:22:TYR:CE1	1:B:400:MET:HG2	2.40	0.57
1:A:67:GLN:HG2	1:A:68:ASN:OD1	2.05	0.56
1:C:317:ASP:OD2	1:C:320:GLY:HA3	2.05	0.56
1:A:354:GLY:HA2	1:A:362:ARG:NH1	2.20	0.56
1:C:232:MET:HE3	1:C:232:MET:O	2.06	0.56
1:C:11:LEU:HD22	1:C:40:ARG:HG2	1.88	0.56
1:A:71:PRO:HB2	3:A:528:HOH:O	2.04	0.56
1:B:360:GLY:HA3	3:B:520:HOH:O	2.05	0.56
1:A:25:ILE:HG21	1:A:317:ASP:HB2	1.86	0.56
1:C:276:ARG:HH11	1:C:276:ARG:HG3	1.69	0.56
1:B:132:VAL:HG13	1:B:137:GLU:HG3	1.87	0.56
1:C:265:LYS:HE3	1:C:381:VAL:HA	1.88	0.56
1:A:328:TRP:O	1:A:331:PRO:HD3	2.06	0.56
1:A:335:ARG:O	1:A:338:ARG:HG2	2.07	0.55
1:B:69:ALA:HA	1:B:296:LEU:CD1	2.36	0.55
1:C:180:HIS:NE2	1:C:184:ARG:NH1	2.50	0.55
1:C:11:LEU:CD1	1:C:40:ARG:HG2	2.37	0.55
1:B:263:LYS:NZ	1:B:263:LYS:HB2	2.23	0.54
1:C:138:ALA:O	1:C:142:LEU:HD23	2.07	0.54
1:A:384:ILE:H	1:A:384:ILE:HD13	1.71	0.54
1:B:272:ASN:ND2	1:B:273:SER:H	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:298:LYS:O	1:B:310:LYS:HG3	2.07	0.54
1:B:284:ARG:CZ	1:B:370:ILE:HD11	2.38	0.54
1:C:391:GLN:HE22	1:C:409:VAL:N	1.82	0.53
1:A:279:PHE:O	1:A:283:VAL:HG23	2.08	0.53
1:C:158:GLU:HG2	1:C:162:ARG:HG2	1.90	0.53
1:A:288:PRO:HG3	1:A:397:LEU:CD2	2.38	0.53
1:B:16:THR:HA	1:B:19:LYS:HG2	1.89	0.53
1:A:36:LEU:O	1:A:36:LEU:HD12	2.08	0.53
1:A:282:GLU:HA	1:A:282:GLU:OE1	2.09	0.53
1:C:63:ARG:HD2	1:C:299:LYS:HE2	1.90	0.53
1:A:104:THR:OG1	1:A:106:PRO:HD2	2.09	0.53
1:B:93:ILE:O	1:B:97:MET:HG2	2.10	0.52
1:C:194:ILE:HG13	1:C:238:ILE:CD1	2.38	0.52
1:C:318:LEU:HD12	1:C:350:ILE:HD12	1.92	0.52
1:B:330:HIS:O	1:B:333:GLU:HB2	2.09	0.52
1:B:7:HIS:CD2	1:B:38:GLN:HG3	2.43	0.52
1:B:173:PHE:CD1	1:B:174:GLY:N	2.78	0.52
1:A:264:TYR:CZ	1:A:336:PRO:HD2	2.45	0.52
1:B:26:LYS:HG2	3:B:550:HOH:O	2.10	0.51
1:C:151:GLY:O	1:C:214:LEU:HD12	2.10	0.51
1:B:153:PRO:HD2	1:B:197:MET:SD	2.50	0.51
1:C:23:LEU:HB3	1:C:27:ASN:HD21	1.76	0.51
1:C:343:GLU:HG3	1:C:344:GLU:H	1.75	0.51
1:A:36:LEU:C	1:A:36:LEU:HD12	2.31	0.51
1:A:173:PHE:CE1	1:A:291:PRO:HG2	2.46	0.51
1:C:25:ILE:H	1:C:25:ILE:CD1	2.05	0.51
1:B:385:GLU:OE2	1:B:416:LYS:HD3	2.11	0.51
1:B:276:ARG:NH1	1:B:374:LYS:HB3	2.26	0.50
1:B:403:LEU:HG	1:B:404:PRO:CD	2.42	0.50
1:C:11:LEU:CD2	1:C:40:ARG:HG2	2.41	0.50
1:C:332:ASP:HB2	3:C:518:HOH:O	2.10	0.50
1:C:65:GLN:CG	1:C:296:LEU:HB3	2.41	0.50
1:C:335:ARG:HG3	1:C:335:ARG:HH11	1.77	0.50
1:A:10:SER:HB3	1:A:12:ASP:OD2	2.10	0.50
1:B:416:LYS:HB3	1:B:416:LYS:NZ	2.27	0.50
1:A:267:TRP:CH2	1:A:278:MET:HE3	2.47	0.50
1:A:73:ARG:NH1	1:A:73:ARG:HB2	2.27	0.50
1:A:349:MET:HG2	1:A:351:PRO:HD3	1.94	0.50
1:C:118:GLU:OE1	1:C:141:ILE:HG12	2.12	0.50
1:A:391:GLN:NE2	1:A:406:SER:OG	2.43	0.50
1:C:111:LEU:HD12	1:C:368:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:CE1	1:A:314:VAL:HG21	2.47	0.50
1:A:293:LEU:O	1:A:315:LEU:HA	2.12	0.50
1:A:83:ALA:HA	1:A:232:MET:HE1	1.94	0.50
1:A:173:PHE:HE1	1:A:291:PRO:HG2	1.77	0.49
1:C:256:LEU:HD12	1:C:404:PRO:HG3	1.94	0.49
1:B:307:GLU:OE1	1:B:309:LYS:HG3	2.12	0.49
1:C:67:GLN:NE2	1:C:88:ASP:HB2	2.27	0.49
1:C:23:LEU:HD11	1:C:397:LEU:HD13	1.95	0.49
1:A:280:VAL:HG21	1:A:374:LYS:HG2	1.93	0.49
1:C:79:PHE:CD2	1:C:85:GLN:HG2	2.47	0.49
1:B:292:PHE:HA	1:B:318:LEU:CD1	2.43	0.49
1:B:210:SER:HA	1:B:215:HIS:CD2	2.47	0.49
1:B:330:HIS:HB3	1:B:333:GLU:HG3	1.93	0.49
1:A:175:ALA:HB2	1:A:179:ARG:CZ	2.43	0.49
1:A:384:ILE:HD13	1:A:384:ILE:N	2.27	0.49
1:B:125:ARG:HG3	3:B:542:HOH:O	2.13	0.49
1:C:343:GLU:HG3	1:C:344:GLU:N	2.28	0.49
1:C:274:ARG:CZ	1:C:278:MET:HE1	2.43	0.49
1:C:283:VAL:HG13	1:C:287:TYR:CD2	2.47	0.49
1:B:28:ARG:NH1	1:B:28:ARG:HG3	2.28	0.48
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.78	0.48
1:C:389:PRO:O	1:C:391:GLN:HG2	2.13	0.48
1:B:84:ILE:HA	1:B:87:MET:CE	2.43	0.48
1:B:135:PHE:CZ	1:B:167:ILE:HD13	2.48	0.48
1:C:36:LEU:HA	1:C:48:CYS:O	2.13	0.48
1:A:185:ARG:C	1:A:188:PRO:HD2	2.34	0.48
1:C:7:HIS:HB2	1:C:38:GLN:NE2	2.29	0.48
1:C:93:ILE:O	1:C:97:MET:HG2	2.14	0.48
1:A:160:LYS:HB2	1:A:160:LYS:HZ3	1.79	0.48
1:C:13:ASN:HB2	1:C:40:ARG:O	2.14	0.48
1:B:138:ALA:O	1:B:142:LEU:HB2	2.14	0.48
1:C:399:ARG:HG2	1:C:399:ARG:HH11	1.78	0.48
1:B:297:VAL:HG23	1:B:312:THR:O	2.13	0.48
1:C:309:LYS:HG2	1:C:310:LYS:N	2.27	0.48
1:C:140:GLU:OE1	1:C:160:LYS:HE3	2.13	0.48
1:C:28:ARG:HH11	1:C:28:ARG:HG3	1.79	0.47
1:B:385:GLU:HG2	1:B:416:LYS:HD3	1.95	0.47
1:B:354:GLY:HA2	1:B:362:ARG:NH1	2.28	0.47
1:B:236:GLU:OE1	1:B:236:GLU:HA	2.14	0.47
1:C:105:PRO:O	1:C:109:LYS:HD3	2.15	0.47
1:C:371:GLU:CA	1:C:371:GLU:OE2	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:HIS:ND1	1:C:8:ASP:O	2.47	0.47
1:A:242:ARG:HB3	1:A:243:PRO:HD3	1.96	0.47
1:B:139:LYS:HE2	1:B:167:ILE:CD1	2.37	0.47
1:B:187:ARG:O	1:B:191:GLU:HG3	2.14	0.47
1:C:297:VAL:HG23	1:C:312:THR:O	2.14	0.47
1:B:124:THR:HG22	1:B:128:LYS:NZ	2.29	0.47
1:B:276:ARG:HH11	1:B:276:ARG:HB3	1.78	0.47
1:C:11:LEU:HD13	1:C:11:LEU:O	2.15	0.47
1:C:356:HIS:C	1:C:358:GLU:N	2.67	0.47
1:A:300:ASP:OD1	1:A:310:LYS:N	2.42	0.47
1:C:7:HIS:HA	1:C:38:GLN:HB2	1.96	0.47
1:B:194:ILE:HG13	1:B:238:ILE:CD1	2.45	0.47
1:C:360:GLY:HA3	3:C:527:HOH:O	2.15	0.47
1:A:272:ASN:OD1	1:A:273:SER:N	2.43	0.46
1:C:391:GLN:NE2	1:C:406:SER:OG	2.48	0.46
1:B:330:HIS:HB3	1:B:333:GLU:CG	2.45	0.46
1:C:95:ARG:NH1	1:C:236:GLU:OE1	2.48	0.46
1:C:239:ASN:O	1:C:243:PRO:HG2	2.15	0.46
1:B:274:ARG:O	1:B:278:MET:HG3	2.16	0.46
1:A:240:VAL:O	1:A:243:PRO:HD2	2.16	0.46
1:A:281:GLN:HA	1:A:281:GLN:OE1	2.15	0.46
1:A:160:LYS:NZ	1:A:160:LYS:H	2.03	0.46
1:C:120:LYS:O	1:C:123:VAL:HG23	2.16	0.46
1:C:25:ILE:N	1:C:25:ILE:HD12	2.12	0.46
1:A:267:TRP:CZ2	1:A:275:GLU:HG3	2.51	0.46
1:A:232:MET:HE3	1:A:235:ILE:HB	1.98	0.46
1:A:247:ILE:HA	2:A:501:HEM:HBB1	1.96	0.46
1:C:172:ALA:HB1	1:C:180:HIS:HA	1.97	0.45
1:B:207:LYS:HA	3:B:535:HOH:O	2.16	0.45
1:B:247:ILE:HG22	1:B:251:LEU:HD13	1.98	0.45
1:B:87:MET:HB2	1:B:87:MET:HE2	1.75	0.45
1:A:123:VAL:O	1:A:127:GLU:HG3	2.16	0.45
1:B:302:VAL:HA	1:B:306:CYS:O	2.17	0.45
1:C:272:ASN:ND2	1:C:273:SER:N	2.63	0.45
1:C:329:ASP:CG	1:C:330:HIS:HD1	2.20	0.45
1:B:344:GLU:OE1	1:B:344:GLU:HA	2.16	0.45
1:B:318:LEU:HD12	1:B:318:LEU:N	2.31	0.45
1:B:264:TYR:CE1	1:B:336:PRO:HD2	2.51	0.45
1:C:330:HIS:N	1:C:331:PRO:CD	2.80	0.45
1:C:276:ARG:O	1:C:280:VAL:HG23	2.17	0.45
1:A:73:ARG:HH11	1:A:73:ARG:CB	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:HB1	1:A:208:THR:HG21	1.99	0.45
1:B:414:ARG:HG2	1:B:414:ARG:O	2.15	0.45
1:C:173:PHE:C	1:C:173:PHE:CD1	2.89	0.45
1:A:385:GLU:HG3	1:A:414:ARG:HH12	1.82	0.45
1:B:95:ARG:O	1:B:98:LEU:HB3	2.16	0.45
1:A:172:ALA:HB1	1:A:180:HIS:HA	1.99	0.44
1:C:240:VAL:O	1:C:243:PRO:HD2	2.17	0.44
1:A:355:GLY:O	1:A:362:ARG:HD2	2.17	0.44
1:C:63:ARG:HH11	1:C:63:ARG:HG2	1.81	0.44
1:C:279:PHE:O	1:C:283:VAL:HG23	2.17	0.44
1:C:79:PHE:CG	1:C:85:GLN:HG2	2.51	0.44
1:C:349:MET:HG2	1:C:351:PRO:CD	2.47	0.44
1:C:357:ALA:HA	1:C:362:ARG:HB3	1.99	0.44
1:C:127:GLU:CG	1:C:414:ARG:HA	2.36	0.44
1:A:264:TYR:O	1:A:267:TRP:HB3	2.18	0.44
1:A:274:ARG:HH11	1:A:274:ARG:HG3	1.82	0.44
1:A:240:VAL:C	1:A:243:PRO:HD2	2.38	0.44
1:B:29:THR:HG21	1:B:50:THR:CG2	2.47	0.44
1:C:269:ARG:HB2	1:C:269:ARG:CZ	2.48	0.44
1:B:119:TRP:HB3	1:B:379:PHE:CE1	2.53	0.44
1:B:185:ARG:NH1	1:B:185:ARG:HB2	2.33	0.44
1:A:26:LYS:O	1:A:30:GLU:HG3	2.17	0.44
1:C:276:ARG:HG3	1:C:276:ARG:NH1	2.32	0.44
1:B:140:GLU:CD	1:B:160:LYS:HE3	2.38	0.43
1:C:232:MET:CE	1:C:236:GLU:HG2	2.48	0.43
1:B:132:VAL:CG1	1:B:137:GLU:HG3	2.49	0.43
1:B:272:ASN:ND2	1:B:273:SER:N	2.66	0.43
1:C:26:LYS:O	1:C:30:GLU:HG3	2.17	0.43
1:B:155:LYS:HB2	1:B:158:GLU:HG2	2.01	0.43
1:B:264:TYR:HH	1:B:337:GLU:CD	2.22	0.43
1:B:264:TYR:O	1:B:267:TRP:HB3	2.18	0.43
1:C:276:ARG:NH2	1:C:378:ASP:OD2	2.47	0.43
1:A:277:GLU:HG2	1:A:374:LYS:HD3	2.00	0.43
1:B:368:ILE:HD12	2:B:501:HEM:HBC2	2.00	0.43
1:C:249:TYR:HB2	1:C:289:PHE:CE2	2.53	0.43
1:A:305:ASN:HD22	1:A:305:ASN:HA	1.60	0.43
1:B:119:TRP:HB3	1:B:379:PHE:CD1	2.53	0.43
1:C:127:GLU:CD	1:C:415:ARG:H	2.21	0.43
1:A:357:ALA:HA	1:A:362:ARG:HB3	2.00	0.43
1:C:338:ARG:HB2	1:C:338:ARG:HH11	1.82	0.43
1:A:363:CYS:HB2	2:A:501:HEM:NA	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:THR:HB	1:A:105:PRO:HD2	2.01	0.43
1:C:66:ARG:HG3	1:C:361:HIS:CD2	2.54	0.43
1:C:210:SER:HA	1:C:215:HIS:CD2	2.54	0.43
1:C:258:LEU:HD11	1:C:265:LYS:CD	2.49	0.42
1:A:99:PHE:CZ	1:A:236:GLU:HG3	2.54	0.42
1:A:109:LYS:HE3	1:A:109:LYS:CA	2.48	0.42
1:B:363:CYS:HB2	2:B:501:HEM:NA	2.33	0.42
1:B:150:ALA:HB1	1:B:213:ALA:HB3	2.01	0.42
1:C:195:GLU:O	1:C:199:GLU:HG3	2.19	0.42
1:C:216:GLU:O	1:C:220:HIS:HB2	2.18	0.42
1:C:338:ARG:HG3	1:C:339:PHE:CD1	2.54	0.42
1:C:78:LEU:HG	1:C:79:PHE:CD1	2.53	0.42
1:C:179:ARG:HA	1:C:182:LYS:HE2	2.01	0.42
1:B:302:VAL:HG13	1:B:306:CYS:O	2.20	0.42
1:B:379:PHE:O	1:B:383:GLN:HB2	2.18	0.42
1:B:176:VAL:HG12	1:B:177:GLY:N	2.35	0.42
1:C:335:ARG:HG3	1:C:335:ARG:NH1	2.34	0.42
1:C:158:GLU:HG2	1:C:162:ARG:CG	2.49	0.42
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.20	0.42
1:A:265:LYS:CE	1:A:269:ARG:NH2	2.81	0.42
1:B:140:GLU:OE2	1:B:160:LYS:HG3	2.20	0.42
1:B:316:LEU:O	1:B:318:LEU:HD12	2.20	0.42
1:B:41:LEU:HD22	1:B:42:LEU:HD22	2.02	0.42
1:C:264:TYR:CZ	1:C:336:PRO:HD2	2.54	0.42
1:A:264:TYR:CE1	1:A:336:PRO:HD2	2.54	0.41
1:B:247:ILE:HA	2:B:501:HEM:HBB1	2.02	0.41
1:C:60:ASP:OD2	1:C:63:ARG:HB2	2.20	0.41
1:B:158:GLU:O	1:B:162:ARG:HG2	2.20	0.41
1:C:304:ASN:HD22	1:C:304:ASN:HA	1.52	0.41
1:A:36:LEU:HA	1:A:48:CYS:O	2.20	0.41
1:A:160:LYS:NZ	1:A:160:LYS:HB2	2.36	0.41
1:C:64:PHE:CE1	1:C:314:VAL:HG21	2.56	0.41
1:A:182:LYS:HG2	3:A:525:HOH:O	2.20	0.41
1:C:175:ALA:O	1:C:180:HIS:HB2	2.20	0.41
1:B:155:LYS:O	1:B:158:GLU:HG2	2.21	0.41
1:A:151:GLY:O	1:A:214:LEU:HD12	2.20	0.41
1:B:50:THR:HG21	3:B:503:HOH:O	2.20	0.41
1:C:335:ARG:HB3	1:C:337:GLU:OE1	2.21	0.41
1:C:166:PHE:O	1:C:169:MET:HB2	2.21	0.41
1:C:60:ASP:OD2	1:C:63:ARG:HD3	2.20	0.41
1:A:379:PHE:CD1	1:A:383:GLN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:VAL:HG13	1:A:137:GLU:CG	2.51	0.41
1:B:16:THR:HG22	1:B:20:GLU:HG3	2.01	0.41
1:C:282:GLU:HG3	1:C:334:PHE:CD1	2.55	0.40
1:C:202:ARG:HD3	1:C:227:GLN:HE22	1.86	0.40
2:C:501:HEM:HBC2	2:C:501:HEM:HMC2	2.02	0.40
1:B:152:VAL:HA	1:B:153:PRO:HD3	1.98	0.40
1:C:28:ARG:HG3	1:C:28:ARG:NH1	2.36	0.40
1:B:70:LEU:HD21	1:B:294:GLY:HA3	2.02	0.40
1:C:89:GLY:O	1:C:93:ILE:HG12	2.22	0.40
1:C:144:ARG:HG3	1:C:144:ARG:HH11	1.86	0.40
1:C:356:HIS:C	1:C:358:GLU:H	2.24	0.40
1:A:298:LYS:O	1:A:310:LYS:HB2	2.22	0.40
1:B:345:ASN:HB3	1:B:348:ASP:OD1	2.20	0.40
1:B:265:LYS:CE	1:B:269:ARG:HH12	2.34	0.40

There are no symmetry-related clashes.

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	409/417 (98%)	395 (97%)	13 (3%)	1 (0%)	52	68
1	B	409/417 (98%)	393 (96%)	15 (4%)	1 (0%)	52	68
1	C	409/417 (98%)	385 (94%)	22 (5%)	2 (0%)	34	46
All	All	1227/1251 (98%)	1173 (96%)	50 (4%)	4 (0%)	46	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	340	ALA
1	A	291	PRO
1	B	291	PRO

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Mol	Chain	Res	Type
1	C	291	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	352/358 (98%)	333 (95%)	19 (5%)	27	40
1	B	352/358 (98%)	331 (94%)	21 (6%)	24	35
1	C	352/358 (98%)	328 (93%)	24 (7%)	20	28
All	All	1056/1074 (98%)	992 (94%)	64 (6%)	23	34

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	73	ARG
1	A	109	LYS
1	A	134	LEU
1	A	160	LYS
1	A	182	LYS
1	A	192	GLU
1	A	214	LEU
1	A	217	MET
1	A	236	GLU
1	A	237	LEU
1	A	274	ARG
1	A	277	GLU
1	A	289	PHE
1	A	292	PHE
1	A	304	ASN
1	A	305	ASN
1	A	312	THR
1	A	384	ILE
1	B	36	LEU
1	B	41	LEU

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Mol	Chain	Res	Type
1	B	44	LYS
1	B	63	ARG
1	B	109	LYS
1	B	134	LEU
1	B	142	LEU
1	B	214	LEU
1	B	217	MET
1	B	237	LEU
1	B	256	LEU
1	B	263	LYS
1	B	272	ASN
1	B	276	ARG
1	B	289	PHE
1	B	292	PHE
1	B	305	ASN
1	B	307	GLU
1	B	403	LEU
1	B	414	ARG
1	B	416	LYS
1	C	8	ASP
1	C	11	LEU
1	C	25	ILE
1	C	36	LEU
1	C	46	PHE
1	C	49	MET
1	C	63	ARG
1	C	72	LYS
1	C	134	LEU
1	C	173	PHE
1	C	185	ARG
1	C	214	LEU
1	C	217	MET
1	C	251	LEU
1	C	256	LEU
1	C	272	ASN
1	C	289	PHE
1	C	292	PHE
1	C	299	LYS
1	C	300	ASP
1	C	304	ASN
1	C	341	GLU
1	C	359	LYS

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Mol	Chain	Res	Type
1	C	371	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	304	ASN
1	A	305	ASN
1	A	356	HIS
1	A	391	GLN
1	B	227	GLN
1	B	239	ASN
1	B	272	ASN
1	B	305	ASN
1	B	391	GLN
1	C	13	ASN
1	C	27	ASN
1	C	67	GLN
1	C	215	HIS
1	C	227	GLN
1	C	272	ASN
1	C	304	ASN
1	C	382	HIS
1	C	383	GLN
1	C	391	GLN

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)

3 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	501	1	30,50,50	3.75	10 (33%)	24,82,82	2.84	11 (45%)
2	HEM	B	501	1	30,50,50	4.01	12 (40%)	24,82,82	2.89	8 (33%)
2	HEM	C	501	1	30,50,50	4.29	9 (30%)	24,82,82	2.73	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	501	1	-	0/10/54/54	0/0/8/8
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	HEM	C3C-CAC	-7.24	1.37	1.51
2	C	501	HEM	C3C-CAC	-6.88	1.38	1.51
2	B	501	HEM	C3D-C4D	-6.48	1.43	1.51
2	B	501	HEM	C3B-CAB	-6.10	1.39	1.51
2	B	501	HEM	C2D-C3D	-5.95	1.36	1.54
2	A	501	HEM	C3C-CAC	-5.88	1.40	1.51
2	C	501	HEM	C2D-C3D	-5.82	1.37	1.54
2	C	501	HEM	C3B-CAB	-5.69	1.40	1.51
2	C	501	HEM	C3B-C4B	-5.64	1.46	1.51
2	A	501	HEM	C2D-C3D	-5.26	1.38	1.54
2	A	501	HEM	C3B-CAB	-5.10	1.41	1.51
2	B	501	HEM	C2C-C1C	-4.87	1.43	1.52
2	A	501	HEM	C3B-C4B	-4.83	1.47	1.51
2	C	501	HEM	C3D-C4D	-4.76	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	HEM	C2C-C1C	-4.73	1.43	1.52
2	A	501	HEM	C2C-C1C	-4.62	1.43	1.52
2	A	501	HEM	C3D-C4D	-3.94	1.46	1.51
2	B	501	HEM	C3B-C4B	-2.58	1.49	1.51
2	B	501	HEM	C2B-C1B	-2.27	1.44	1.51
2	B	501	HEM	CHC-C4B	2.15	1.44	1.38
2	B	501	HEM	CHC-C1C	2.15	1.41	1.36
2	C	501	HEM	CHD-C1D	2.20	1.45	1.38
2	A	501	HEM	CAA-C2A	2.56	1.56	1.52
2	C	501	HEM	CHD-C4C	2.84	1.43	1.36
2	B	501	HEM	CHD-C1D	2.93	1.47	1.38
2	A	501	HEM	CHD-C4C	3.11	1.43	1.36
2	A	501	HEM	CHC-C1C	4.06	1.45	1.36
2	B	501	HEM	CHD-C4C	4.11	1.46	1.36
2	A	501	HEM	FE-NC	14.79	2.53	1.95
2	B	501	HEM	FE-NC	15.42	2.56	1.95
2	C	501	HEM	FE-NC	18.01	2.66	1.95

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C2C-C1C-NC	-2.74	105.59	110.21
2	C	501	HEM	CMA-C3A-C4A	-2.36	124.46	128.36
2	A	501	HEM	CMA-C3A-C4A	-2.24	124.66	128.36
2	C	501	HEM	CHD-C1D-ND	2.14	129.68	124.52
2	A	501	HEM	C3B-CAB-CBB	2.18	127.80	124.46
2	C	501	HEM	CMD-C2D-C3D	2.28	124.42	114.35
2	A	501	HEM	C2D-C3D-C4D	2.28	105.37	101.50
2	C	501	HEM	C2D-C3D-C4D	2.82	106.29	101.50
2	B	501	HEM	CAD-C3D-C4D	3.02	123.13	112.47
2	A	501	HEM	C1D-CHD-C4C	3.08	130.97	125.82
2	B	501	HEM	C4B-CHC-C1C	3.21	131.19	125.82
2	B	501	HEM	C2D-C3D-C4D	3.36	107.19	101.50
2	C	501	HEM	C1D-CHD-C4C	3.36	131.45	125.82
2	A	501	HEM	CAD-C3D-C4D	3.63	125.28	112.47
2	C	501	HEM	CMB-C2B-C3B	3.70	125.77	116.53
2	C	501	HEM	C4B-CHC-C1C	3.71	132.02	125.82
2	B	501	HEM	C1D-CHD-C4C	3.71	132.03	125.82
2	C	501	HEM	CAD-C3D-C4D	3.82	125.96	112.47
2	A	501	HEM	CMB-C2B-C3B	3.85	126.15	116.53
2	A	501	HEM	C4B-CHC-C1C	4.41	133.20	125.82
2	B	501	HEM	CMB-C2B-C3B	4.42	127.57	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	HEM	CAD-C3D-C2D	5.03	127.69	113.22
2	B	501	HEM	C2C-C1C-CHC	5.14	131.51	123.68
2	C	501	HEM	C2C-C1C-CHC	5.23	131.64	123.68
2	A	501	HEM	CAD-C3D-C2D	5.47	128.96	113.22
2	A	501	HEM	C2C-C1C-CHC	5.54	132.12	123.68
2	B	501	HEM	CAD-C3D-C2D	5.70	129.62	113.22
2	A	501	HEM	CMC-C2C-C3C	6.01	131.52	116.53
2	C	501	HEM	CMC-C2C-C3C	6.20	132.01	116.53
2	B	501	HEM	CMC-C2C-C3C	6.75	133.38	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HEM	2	0
2	B	501	HEM	3	0
2	C	501	HEM	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	411/417 (98%)	0.03	4 (0%)	84　86	17, 30, 49, 63	0
1	B	411/417 (98%)	0.15	6 (1%)	76　78	18, 33, 52, 70	0
1	C	411/417 (98%)	0.58	28 (6%)	20　23	34, 52, 69, 78	0
All	All	1233/1251 (98%)	0.25	38 (3%)	52　56	17, 38, 63, 78	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	11	LEU	6.5
1	C	305	ASN	5.5
1	C	306	CYS	4.8
1	C	9	LYS	4.7
1	B	343	GLU	4.2
1	C	308	PHE	4.2
1	C	10	SER	3.8
1	C	36	LEU	3.8
1	B	341	GLU	3.5
1	C	302	VAL	3.5
1	A	11	LEU	3.4
1	C	346	LEU	3.4
1	C	7	HIS	3.2
1	B	272	ASN	3.0
1	C	6	PRO	3.0
1	C	29	THR	3.0
1	C	53	GLU	2.8
1	C	223	GLU	2.7
1	C	299	LYS	2.6
1	A	343	GLU	2.6
1	C	63	ARG	2.5
1	C	79	PHE	2.5
1	C	303	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	266	GLU	2.5
1	C	301	PHE	2.4
1	B	270	SER	2.4
1	A	266	GLU	2.4
1	C	307	GLU	2.3
1	C	33	ASN	2.3
1	C	32	TYR	2.3
1	C	45	ASN	2.3
1	A	305	ASN	2.2
1	C	12	ASP	2.2
1	C	38	GLN	2.2
1	C	258	LEU	2.2
1	B	414	ARG	2.1
1	C	78	LEU	2.1
1	C	100	LEU	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	A	501	43/43	0.97	0.15	0.54	12,17,22,26	0
2	HEM	B	501	43/43	0.98	0.14	-0.08	17,19,22,26	0
2	HEM	C	501	43/43	0.95	0.14	-0.22	29,35,43,48	0

6.5 Other polymers (i)

There are no such residues in this entry.