



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HT8  
Title : THE 2.7 ANGSTROM RESOLUTION MODEL OF OVINE COX-1 COM-  
PLEXED WITH ALCLOFENAC  
Authors : Selinsky, B.S.; Gupta, K.; Sharkey, C.T.; Loll, P.J.  
Deposited on : 2000-12-29  
Resolution : 2.69 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](mailto: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.

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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

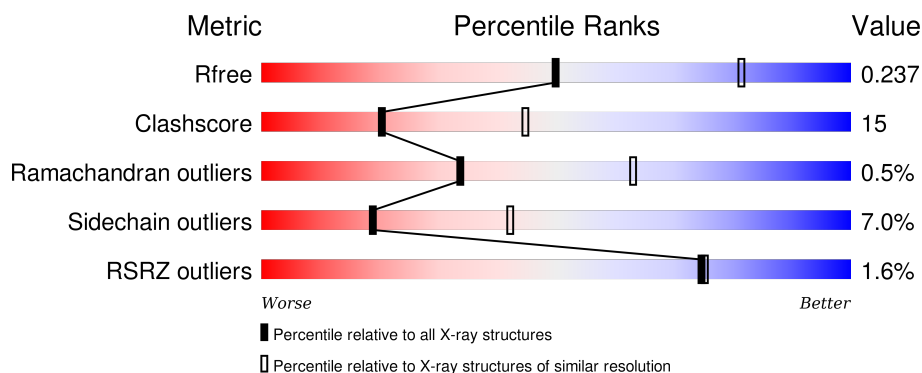
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.69 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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  $\geq 3$ , 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	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 25%, green 72%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>72%</span> <span>25%</span> <span>•</span> </div> </div>
1	B	551	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 2%, yellow 28%, green 69%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>69%</span> <span>28%</span> <span>•</span> </div> </div>

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
2	NAG	A	1661	-	-	-	X
2	NAG	A	1671	-	-	-	X
2	NAG	A	1681	-	-	-	X
2	NAG	B	2661	-	-	-	X
2	NAG	B	2671	-	-	-	X
2	NAG	B	2681	-	-	-	X
3	BOG	A	1801	-	-	-	X
3	BOG	A	1802	-	-	-	X
3	BOG	B	2802	-	-	-	X
5	34C	A	1701	-	-	-	X
5	34C	B	2701	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9477 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 PROTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			
1	B	551	Total	C	N	O	S	0	0	0
			4477	2903	758	788	28			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



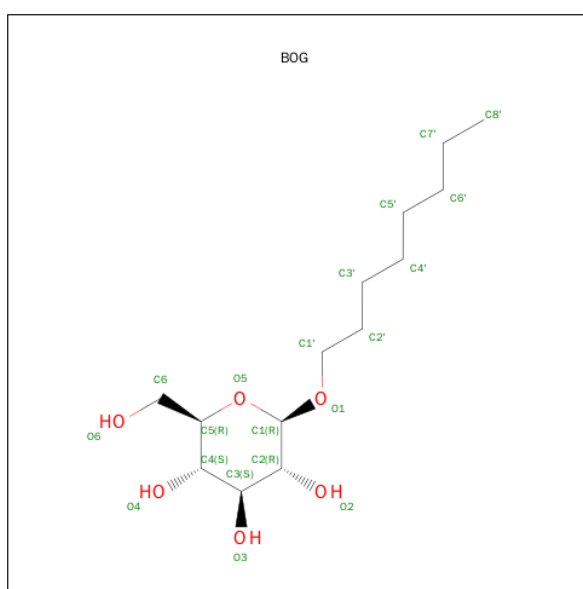
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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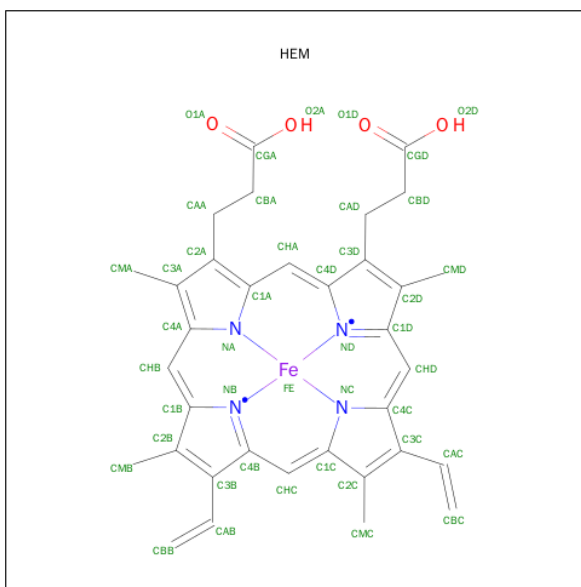
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



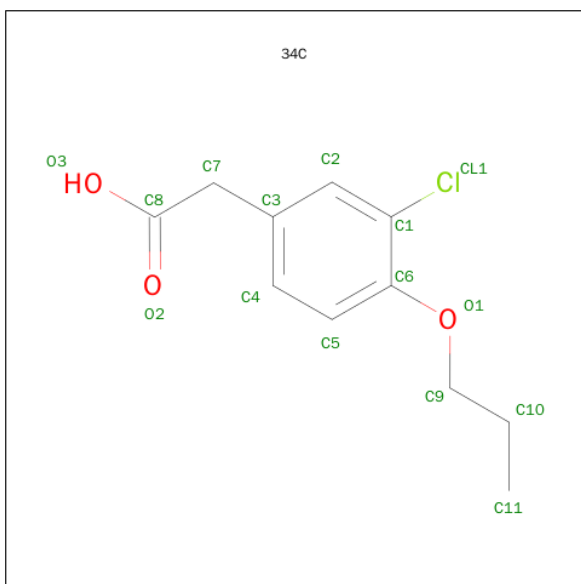
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>4</sub>).



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

- Molecule 5 is (3-CHLORO-4-PROPOXY-PHENYL)-ACETIC ACID (three-letter code: 34C) (formula:  $C_{11}H_{13}ClO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Cl	O	0	0
			15	11	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	Cl	O	0	0
			15	11	1	3		

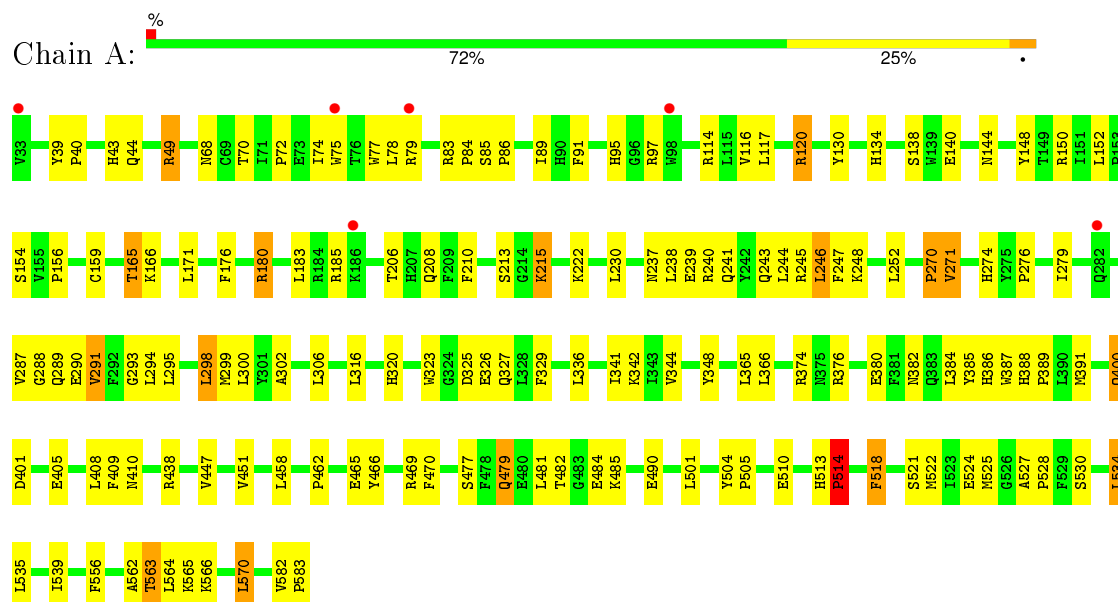
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	116	Total	O	0	0
			116	116		
6	B	119	Total	O	0	0
			119	119		

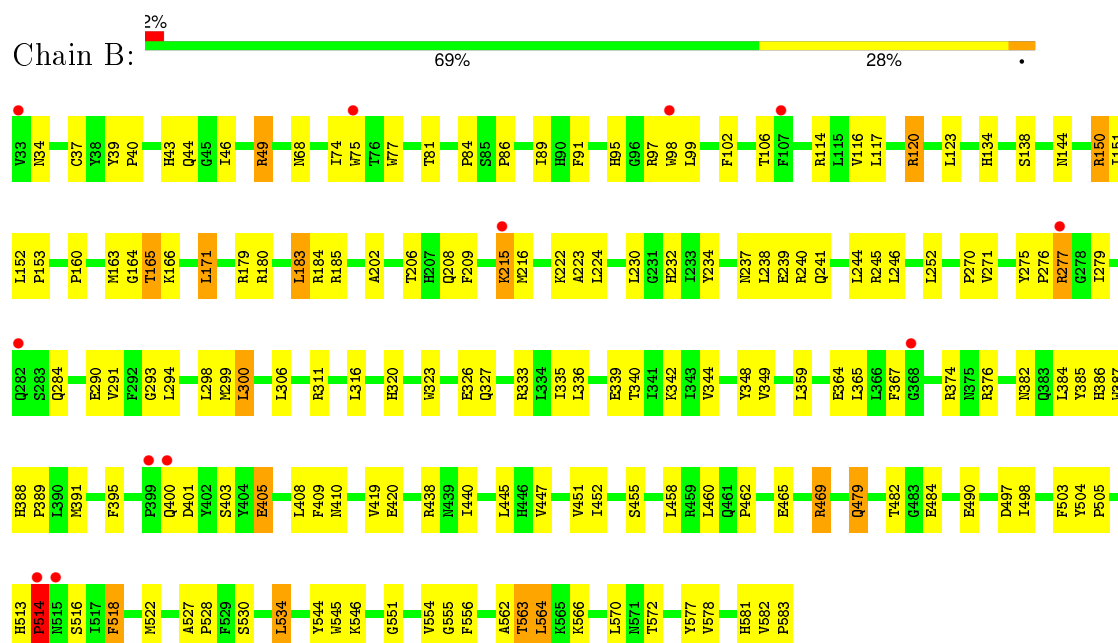
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.15Å 208.45Å 222.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.69 19.92 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.2 (19.92-2.69) 98.1 (19.92-2.69)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.62 (at 2.71Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.211 , 0.242 0.205 , 0.237	Depositor DCC
$R_{free}$ test set	4807 reflections (8.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.7	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 63346 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	9477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, 34C, NAG, BOG

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	0.40	0/4615	0.65	1/6264 (0.0%)
1	B	0.41	0/4615	0.64	0/6264
All	All	0.40	0/9230	0.64	1/12528 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-5.22	96.92	111.00

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	4477	0	4386	131	0
1	B	4477	0	4386	139	0
2	A	56	0	52	10	0
2	B	56	0	52	9	0
3	A	40	0	56	10	0
3	B	20	0	28	3	0
4	A	43	0	30	5	0
4	B	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	15	0	10	0	0
5	B	15	0	10	2	0
6	A	116	0	0	3	0
6	B	119	0	0	1	0
All	All	9477	0	9040	267	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 15.

All (267) 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:B:563:THR:HG22	1:B:566:LYS:H	1.11	1.11
1:A:144:ASN:HD21	2:A:1671:NAG:C1	1.65	1.10
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.34	1.06
1:A:563:THR:HG22	1:A:566:LYS:H	1.26	1.01
1:A:185:ARG:HH21	1:A:438:ARG:NH1	1.57	1.01
1:A:391:MET:HG3	4:A:601:HEM:HAB	1.42	1.00
1:B:185:ARG:HH21	1:B:438:ARG:NH1	1.62	0.96
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.04	0.93
1:A:68:ASN:HD21	2:A:1661:NAG:C1	1.83	0.92
1:A:144:ASN:ND2	2:A:1671:NAG:C1	2.36	0.88
1:B:68:ASN:HD21	2:B:2661:NAG:C1	1.87	0.86
1:B:276:PRO:HD2	1:B:279:ILE:HD12	1.59	0.84
1:A:116:VAL:O	1:A:120:ARG:HB2	1.78	0.84
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.13	0.83
1:B:86:PRO:HG3	3:B:2802:BOG:H61	1.64	0.80
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.50	0.77
1:A:410:ASN:HD21	2:A:1681:NAG:C1	1.96	0.77
1:A:240:ARG:NH1	1:A:271:VAL:HG13	1.99	0.77
1:B:144:ASN:ND2	2:B:2671:NAG:C1	2.49	0.76
1:A:208:GLN:NE2	1:A:230:LEU:H	1.83	0.76
1:B:563:THR:HG22	1:B:566:LYS:N	1.97	0.75
1:A:185:ARG:HH21	1:A:438:ARG:HH11	1.33	0.74
1:A:243:GLN:HG3	1:A:270:PRO:HD2	1.71	0.72
1:B:208:GLN:NE2	1:B:230:LEU:H	1.87	0.72
1:B:144:ASN:HD21	2:B:2671:NAG:C2	2.02	0.71
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.70	0.71
1:B:144:ASN:HD21	2:B:2671:NAG:C1	2.04	0.71
1:B:150:ARG:HD3	1:B:152:LEU:O	1.90	0.71
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TRP:HZ2	5:B:2701:34C:H111	1.57	0.70
1:B:114:ARG:HD3	1:B:365:LEU:O	1.92	0.69
1:B:208:GLN:HE21	1:B:230:LEU:H	1.40	0.69
1:B:410:ASN:HD21	2:B:2681:NAG:C1	2.05	0.69
1:B:185:ARG:HH21	1:B:438:ARG:HH11	1.39	0.68
1:A:150:ARG:HD3	1:A:152:LEU:O	1.94	0.68
1:A:116:VAL:HG22	3:A:1802:BOG:H2'1	1.75	0.68
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.75	0.68
1:A:185:ARG:HH21	1:A:438:ARG:HH12	1.43	0.67
1:B:241:GLN:HE21	1:B:245:ARG:HH11	1.41	0.67
1:B:237:ASN:ND2	1:B:239:GLU:HG2	2.10	0.67
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.77	0.67
1:A:49:ARG:O	1:B:320:HIS:HD2	1.77	0.67
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.77	0.66
1:B:185:ARG:HH21	1:B:438:ARG:HH12	1.42	0.65
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.80	0.64
1:B:447:VAL:O	1:B:451:VAL:HG23	1.98	0.64
1:B:150:ARG:HD2	1:B:153:PRO:HA	1.81	0.63
1:A:77:TRP:CZ2	3:A:1801:BOG:H7'2	2.32	0.63
1:A:213:SER:OG	1:A:215:LYS:HE3	1.99	0.62
1:B:180:ARG:O	1:B:438:ARG:NH1	2.32	0.62
1:B:180:ARG:HD3	1:B:490:GLU:OE2	1.99	0.62
1:B:68:ASN:ND2	2:B:2661:NAG:C1	2.61	0.62
1:A:294:LEU:O	1:A:408:LEU:O	2.16	0.62
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.30	0.62
1:A:410:ASN:ND2	2:A:1681:NAG:C1	2.63	0.62
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.00	0.62
1:A:86:PRO:HG3	3:A:1802:BOG:H61	1.81	0.61
2:B:2671:NAG:O4	2:B:2672:NAG:C1	2.49	0.61
1:B:293:GLY:HA2	1:B:299:MET:CE	2.31	0.60
1:A:144:ASN:HD21	2:A:1671:NAG:C2	2.15	0.60
1:A:77:TRP:NE1	3:A:1801:BOG:H5'2	2.16	0.60
1:B:116:VAL:HG22	3:B:2802:BOG:H2'1	1.82	0.60
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.37	0.60
1:B:563:THR:CG2	1:B:566:LYS:H	2.01	0.60
1:A:320:HIS:HD2	1:B:49:ARG:O	1.84	0.59
1:B:134:HIS:HD2	1:B:138:SER:OG	1.85	0.59
4:B:601:HEM:HMB1	4:B:601:HEM:HBB2	1.83	0.59
1:A:387:TRP:HB2	4:A:601:HEM:HAC	1.85	0.59
1:B:344:VAL:O	1:B:348:TYR:HB3	2.02	0.58
1:A:374:ARG:HB3	1:B:374:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:THR:HG22	1:B:166:LYS:HD3	1.86	0.58
1:A:185:ARG:NH2	1:A:438:ARG:HH11	2.00	0.57
1:A:208:GLN:HE21	1:A:230:LEU:H	1.51	0.57
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.86	0.57
2:A:1671:NAG:O4	2:A:1672:NAG:C1	2.52	0.57
1:B:215:LYS:HZ1	1:B:222:LYS:HD2	1.68	0.57
1:B:183:LEU:HD22	1:B:184:ARG:O	2.05	0.57
1:A:180:ARG:NH2	1:A:490:GLU:OE1	2.38	0.57
1:B:215:LYS:HG2	1:B:216:MET:N	2.19	0.57
1:A:114:ARG:HD3	1:A:365:LEU:O	2.05	0.56
1:B:276:PRO:HD2	1:B:279:ILE:CD1	2.32	0.56
1:B:216:MET:HE1	6:B:2812:HOH:O	2.05	0.56
1:A:185:ARG:NH2	1:A:438:ARG:NH1	2.41	0.56
1:A:563:THR:HG22	1:A:566:LYS:N	2.09	0.56
1:B:410:ASN:ND2	2:B:2681:NAG:C1	2.69	0.55
1:A:291:VAL:O	1:A:294:LEU:HG	2.06	0.55
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.40	0.55
1:B:179:ARG:HH11	1:B:179:ARG:HG2	1.71	0.55
1:B:91:PHE:O	1:B:95:HIS:HD2	1.89	0.55
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.89	0.55
1:B:387:TRP:CZ2	5:B:2701:34C:H111	2.40	0.55
1:A:374:ARG:HD2	6:A:1900:HOH:O	2.06	0.55
1:B:497:ASP:OD2	1:B:498:ILE:N	2.41	0.54
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.88	0.54
1:B:323:TRP:CE3	1:B:327:GLN:HG2	2.43	0.54
1:B:98:TRP:CH2	1:B:99:LEU:HD13	2.43	0.54
1:B:294:LEU:O	1:B:408:LEU:O	2.26	0.54
1:B:241:GLN:NE2	1:B:245:ARG:HH11	2.05	0.53
1:A:237:ASN:ND2	1:A:239:GLU:HG2	2.22	0.53
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.43	0.53
1:A:274:HIS:O	1:A:294:LEU:HD21	2.09	0.53
1:A:68:ASN:ND2	2:A:1661:NAG:C1	2.63	0.53
1:B:364:GLU:HG2	1:B:367:PHE:CE1	2.44	0.53
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.73	0.53
1:B:116:VAL:O	1:B:120:ARG:HB2	2.09	0.53
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.43	0.53
1:B:84:PRO:HG2	1:B:89:ILE:CD1	2.24	0.53
1:B:382:ASN:OD1	1:B:386:HIS:HE1	1.92	0.52
1:A:462:PRO:HG2	1:A:465:GLU:CG	2.38	0.52
1:B:391:MET:HE1	1:B:395:PHE:HE2	1.74	0.52
1:B:388:HIS:N	1:B:389:PRO:CD	2.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.91	0.52
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.49	0.52
1:B:566:LYS:O	1:B:570:LEU:HB2	2.10	0.52
1:B:387:TRP:HB2	4:B:601:HEM:HAC	1.93	0.51
1:B:151:ILE:CG2	1:B:469:ARG:NH1	2.74	0.51
1:A:366:LEU:HD12	1:A:535:LEU:HD12	1.92	0.51
1:A:215:LYS:HZ1	1:A:222:LYS:HD2	1.76	0.51
1:A:91:PHE:O	1:A:95:HIS:HD2	1.94	0.51
1:A:291:VAL:HG22	1:A:294:LEU:HD12	1.93	0.51
1:A:49:ARG:HG3	6:A:1805:HOH:O	2.10	0.51
1:B:581:HIS:ND1	1:B:582:VAL:O	2.44	0.50
1:A:374:ARG:NH1	1:B:374:ARG:HB3	2.27	0.50
1:A:479:GLN:O	1:A:482:THR:O	2.29	0.50
1:A:287:VAL:HG11	1:A:302:ALA:HB1	1.92	0.50
1:B:163:MET:CE	1:B:171:LEU:HD21	2.42	0.50
1:A:295:LEU:HD21	4:A:601:HEM:HBB2	1.94	0.50
1:B:403:SER:OG	1:B:405:GLU:HG2	2.12	0.50
1:A:120:ARG:NH1	3:A:1802:BOG:H3	2.27	0.50
1:A:382:ASN:OD1	1:A:386:HIS:HE1	1.95	0.49
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.94	0.49
1:A:215:LYS:H	1:A:215:LYS:HE2	1.75	0.49
1:B:530:SER:O	1:B:534:LEU:HD22	2.12	0.49
1:B:581:HIS:HD1	1:B:582:VAL:N	2.10	0.49
1:B:183:LEU:HG	1:B:445:LEU:HD22	1.94	0.49
1:A:70:THR:O	1:A:72:PRO:HD3	2.13	0.49
1:B:240:ARG:HG3	1:B:271:VAL:HG22	1.94	0.49
1:B:563:THR:HB	1:B:566:LYS:HD3	1.93	0.49
1:A:215:LYS:H	1:A:215:LYS:CE	2.26	0.49
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.78	0.49
1:B:163:MET:HE2	1:B:171:LEU:HD21	1.94	0.49
1:B:144:ASN:CG	2:B:2671:NAG:C1	2.82	0.48
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.95	0.48
1:A:306:LEU:HD23	1:A:306:LEU:C	2.34	0.48
1:B:513:HIS:HB3	1:B:514:PRO:HD2	1.95	0.48
1:B:340:THR:O	1:B:344:VAL:HG23	2.13	0.48
1:B:185:ARG:NH2	1:B:438:ARG:NH1	2.46	0.48
1:A:563:THR:HG23	1:A:565:LYS:H	1.79	0.48
1:B:89:ILE:HD12	1:B:89:ILE:N	2.28	0.47
1:A:140:GLU:OE2	1:A:144:ASN:ND2	2.43	0.47
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.26	0.47
1:B:74:ILE:HG23	1:B:75:TRP:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:O	1:A:438:ARG:NH1	2.47	0.47
1:B:293:GLY:HA2	1:B:299:MET:HE2	1.97	0.47
1:B:179:ARG:HG2	1:B:179:ARG:NH1	2.28	0.47
1:B:185:ARG:NH2	1:B:438:ARG:HH11	2.11	0.47
1:B:290:GLU:CD	1:B:290:GLU:H	2.18	0.47
1:A:530:SER:O	1:A:534:LEU:HD22	2.15	0.47
1:B:320:HIS:CE1	1:B:551:GLY:O	2.68	0.47
1:A:388:HIS:N	1:A:389:PRO:CD	2.78	0.47
1:B:120:ARG:NH1	3:B:2802:BOG:H3	2.30	0.46
1:A:479:GLN:H	1:A:479:GLN:CD	2.18	0.46
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.44	0.46
1:A:144:ASN:CG	2:A:1671:NAG:C1	2.84	0.46
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.63	0.46
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.44	0.46
1:B:160:PRO:HD2	1:B:164:GLY:O	2.15	0.46
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.51	0.46
1:A:344:VAL:O	1:A:348:TYR:HB3	2.15	0.46
1:A:447:VAL:O	1:A:451:VAL:HG23	2.16	0.46
6:A:1817:HOH:O	1:B:546:LYS:HE3	2.16	0.46
1:A:176:PHE:CZ	1:A:180:ARG:HG3	2.51	0.46
1:B:77:TRP:CE2	1:B:81:THR:HG21	2.51	0.46
1:B:400:GLN:NE2	1:B:401:ASP:H	2.14	0.46
1:A:240:ARG:HE	1:A:288:GLY:HA2	1.81	0.45
1:B:384:LEU:C	1:B:384:LEU:HD23	2.37	0.45
1:A:566:LYS:O	1:A:570:LEU:HB2	2.17	0.45
1:A:210:PHE:HB3	4:A:601:HEM:HBD1	1.98	0.45
1:A:79:ARG:HH11	1:A:79:ARG:HG2	1.81	0.45
1:A:185:ARG:HG2	1:A:185:ARG:NH1	2.31	0.45
1:B:513:HIS:O	1:B:514:PRO:C	2.55	0.45
1:A:134:HIS:HD2	1:A:138:SER:OG	2.00	0.45
1:A:386:HIS:CE1	4:A:601:HEM:HAD2	2.52	0.45
1:A:83:ARG:HD3	3:A:1802:BOG:O6	2.17	0.45
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.82	0.45
1:B:102:PHE:CE2	1:B:106:THR:HG21	2.52	0.44
1:A:400:GLN:HE21	1:A:401:ASP:N	2.16	0.44
1:B:479:GLN:O	1:B:482:THR:O	2.36	0.44
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.52	0.44
1:A:77:TRP:CZ3	1:A:78:LEU:HD23	2.53	0.44
1:A:485:LYS:HD3	1:A:485:LYS:HA	1.87	0.44
1:B:277:ARG:HA	1:B:277:ARG:HD2	1.73	0.44
1:A:240:ARG:CZ	1:A:271:VAL:HG13	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.52	0.44
1:A:77:TRP:CE2	3:A:1801:BOG:H5'2	2.53	0.44
1:A:293:GLY:HA2	1:A:299:MET:CE	2.48	0.44
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.83	0.43
1:B:344:VAL:HA	1:B:348:TYR:HB3	2.01	0.43
1:B:320:HIS:HE1	1:B:551:GLY:O	2.00	0.43
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.53	0.43
1:A:144:ASN:OD1	2:A:1671:NAG:C1	2.67	0.43
1:A:524:GLU:OE1	3:A:1802:BOG:H5	2.18	0.43
1:A:326:GLU:OE1	1:B:134:HIS:CE1	2.71	0.43
1:B:544:TYR:O	1:B:546:LYS:N	2.50	0.43
1:B:349:VAL:HG12	1:B:359:LEU:CD1	2.48	0.43
1:B:43:HIS:O	1:B:44:GLN:HB2	2.18	0.43
1:B:46:ILE:HD12	1:B:46:ILE:N	2.34	0.43
1:B:202:ALA:O	1:B:206:THR:HG23	2.18	0.43
1:B:40:PRO:O	1:B:68:ASN:HB3	2.18	0.43
1:A:246:LEU:O	1:A:247:PHE:HB2	2.18	0.43
1:B:564:LEU:HD13	1:B:578:VAL:HG22	2.00	0.43
1:B:554:VAL:HG13	1:B:555:GLY:N	2.34	0.43
1:B:275:TYR:CD2	1:B:284:GLN:HG2	2.54	0.43
1:B:39:TYR:N	1:B:40:PRO:CD	2.82	0.43
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.34	0.43
1:A:291:VAL:O	1:A:291:VAL:HG13	2.18	0.42
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.74	0.42
1:B:237:ASN:HD22	1:B:239:GLU:HG2	1.78	0.42
1:B:420:GLU:HG3	1:B:572:THR:HB	2.01	0.42
1:A:85:SER:O	1:A:89:ILE:HD12	2.18	0.42
1:A:582:VAL:HG22	1:A:583:PRO:HD2	2.00	0.42
1:A:43:HIS:O	1:A:44:GLN:HB2	2.19	0.42
1:A:477:SER:OG	1:A:479:GLN:HG2	2.19	0.42
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.83	0.42
1:B:223:ALA:C	1:B:224:LEU:O	2.55	0.42
1:A:470:PHE:CD2	1:A:525:MET:HG2	2.54	0.42
1:B:98:TRP:CG	1:B:99:LEU:N	2.88	0.42
1:A:130:TYR:HB2	1:A:150:ARG:HG3	2.01	0.42
1:A:341:ILE:HD12	1:A:539:ILE:HD11	2.01	0.42
1:B:513:HIS:HB2	1:B:516:SER:OG	2.20	0.42
1:A:241:GLN:NE2	1:A:245:ARG:HH11	2.17	0.42
1:A:180:ARG:HH21	1:A:490:GLU:CD	2.23	0.42
1:A:290:GLU:CD	1:A:290:GLU:H	2.22	0.42
4:B:601:HEM:CMB	4:B:601:HEM:HBB2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:LEU:HD21	1:B:419:VAL:HG13	2.02	0.42
1:A:326:GLU:OE1	1:B:134:HIS:HE1	2.03	0.41
1:A:120:ARG:NH1	3:A:1802:BOG:H1	2.34	0.41
1:A:384:LEU:HG	1:A:522:MET:SD	2.61	0.41
1:B:306:LEU:HD23	1:B:306:LEU:C	2.40	0.41
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.20	0.41
1:B:180:ARG:NH2	1:B:490:GLU:OE1	2.53	0.41
1:A:230:LEU:HD21	1:A:336:LEU:HB3	2.02	0.41
1:A:513:HIS:O	1:A:514:PRO:C	2.59	0.41
1:A:206:THR:HB	1:A:210:PHE:CD2	2.55	0.41
1:A:510:GLU:OE2	1:A:521:SER:HB2	2.20	0.41
1:A:243:GLN:CG	1:A:270:PRO:HD2	2.45	0.41
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.60	0.41
1:B:582:VAL:HG22	1:B:583:PRO:CD	2.49	0.41
1:A:295:LEU:HD12	1:A:298:LEU:HD22	2.03	0.41
1:A:39:TYR:N	1:A:40:PRO:CD	2.84	0.41
1:A:40:PRO:O	1:A:68:ASN:HB3	2.20	0.41
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.55	0.41
1:A:74:ILE:HG23	1:A:75:TRP:N	2.36	0.41
1:B:335:ILE:O	1:B:339:GLU:HG3	2.20	0.41
1:A:165:THR:HG22	1:A:166:LYS:HD3	2.03	0.41
1:B:311:ARG:NH2	1:B:570:LEU:HD23	2.36	0.40
1:B:230:LEU:HD21	1:B:336:LEU:HB3	2.02	0.40
1:A:150:ARG:NH1	1:A:154:SER:HA	2.35	0.40
1:A:134:HIS:CE1	1:B:326:GLU:OE1	2.74	0.40
1:B:452:ILE:O	1:B:455:SER:HB3	2.21	0.40
1:A:237:ASN:ND2	1:A:240:ARG:H	2.20	0.40
1:A:77:TRP:CE2	3:A:1801:BOG:H7'2	2.56	0.40
1:B:180:ARG:HH21	1:B:490:GLU:CD	2.25	0.40
1:A:342:LYS:HG2	1:A:562:ALA:HB3	2.04	0.40
1:A:481:LEU:HD22	1:A:501:LEU:HD22	2.04	0.40
1:B:206:THR:HA	1:B:209:PHE:CZ	2.56	0.40
1:A:246:LEU:HD13	1:A:248:LYS:HB3	2.03	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	549/551 (100%)	518 (94%)	29 (5%)	2 (0%)	39	69
1	B	549/551 (100%)	516 (94%)	29 (5%)	4 (1%)	26	55
All	All	1098/1102 (100%)	1034 (94%)	58 (5%)	6 (0%)	34	63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	B	270	PRO
1	B	503	PHE
1	B	545	TRP
1	A	270	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	486/486 (100%)	452 (93%)	34 (7%)	19	42
1	B	486/486 (100%)	452 (93%)	34 (7%)	19	42
All	All	972/972 (100%)	904 (93%)	68 (7%)	19	42

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	97	ARG
1	A	117	LEU
1	A	120	ARG
1	A	165	THR
1	A	171	LEU
1	A	180	ARG
1	A	183	LEU
1	A	215	LYS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	291	VAL
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	376	ARG
1	A	385	TYR
1	A	400	GLN
1	A	405	GLU
1	A	458	LEU
1	A	469	ARG
1	A	479	GLN
1	A	484	GLU
1	A	514	PRO
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	A	570	LEU
1	B	49	ARG
1	B	97	ARG
1	B	117	LEU
1	B	120	ARG
1	B	123	LEU
1	B	150	ARG
1	B	165	THR
1	B	171	LEU
1	B	183	LEU

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Mol	Chain	Res	Type
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	277	ARG
1	B	291	VAL
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	376	ARG
1	B	385	TYR
1	B	405	GLU
1	B	458	LEU
1	B	460	LEU
1	B	469	ARG
1	B	479	GLN
1	B	484	GLU
1	B	514	PRO
1	B	518	PHE
1	B	534	LEU
1	B	556	PHE
1	B	563	THR
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	68	ASN
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	274	HIS
1	A	320	HIS
1	A	375	ASN
1	A	386	HIS
1	A	400	GLN

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Mol	Chain	Res	Type
1	A	443	HIS
1	B	42	GLN
1	B	56	GLN
1	B	68	ASN
1	B	95	HIS
1	B	134	HIS
1	B	144	ASN
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	274	HIS
1	B	320	HIS
1	B	358	GLN
1	B	375	ASN
1	B	386	HIS
1	B	400	GLN
1	B	443	HIS

### 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](#)

15 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	NAG	A	1661	-	14,14,15	1.43	2 (14%)	15,19,21	1.12	1 (6%)
2	NAG	A	1671	-	14,14,15	0.85	1 (7%)	15,19,21	0.85	0
2	NAG	A	1672	-	14,14,15	1.27	2 (14%)	15,19,21	1.16	2 (13%)
2	NAG	A	1681	-	14,14,15	1.44	3 (21%)	15,19,21	1.32	2 (13%)
5	34C	A	1701	-	12,15,15	1.37	2 (16%)	16,19,19	0.89	1 (6%)
3	BOG	A	1801	-	20,20,20	1.61	5 (25%)	25,25,25	1.15	2 (8%)
3	BOG	A	1802	-	20,20,20	1.42	4 (20%)	25,25,25	0.94	2 (8%)
4	HEM	A	601	1	30,50,50	2.31	10 (33%)	24,82,82	2.88	10 (41%)
2	NAG	B	2661	-	14,14,15	1.36	2 (14%)	15,19,21	1.11	1 (6%)
2	NAG	B	2671	-	14,14,15	1.01	1 (7%)	15,19,21	0.92	0
2	NAG	B	2672	-	14,14,15	1.15	2 (14%)	15,19,21	1.06	1 (6%)
2	NAG	B	2681	-	14,14,15	1.36	2 (14%)	15,19,21	1.15	1 (6%)
5	34C	B	2701	-	12,15,15	1.31	2 (16%)	16,19,19	0.75	0
3	BOG	B	2802	-	20,20,20	1.43	4 (20%)	25,25,25	0.93	2 (8%)
4	HEM	B	601	1	30,50,50	2.42	9 (30%)	24,82,82	2.71	10 (41%)

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	NAG	A	1661	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1671	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1672	-	-	0/6/23/26	0/1/1/1
2	NAG	A	1681	-	-	0/6/23/26	0/1/1/1
5	34C	A	1701	-	-	0/6/8/8	0/1/1/1
3	BOG	A	1801	-	-	0/11/31/31	0/1/1/1
3	BOG	A	1802	-	-	0/11/31/31	0/1/1/1
4	HEM	A	601	1	-	0/10/54/54	0/0/8/8
2	NAG	B	2661	-	-	0/6/23/26	0/1/1/1
2	NAG	B	2671	-	-	0/6/23/26	0/1/1/1
2	NAG	B	2672	-	-	0/6/23/26	0/1/1/1
2	NAG	B	2681	-	-	0/6/23/26	0/1/1/1
5	34C	B	2701	-	-	0/6/8/8	0/1/1/1
3	BOG	B	2802	-	-	0/11/31/31	0/1/1/1
4	HEM	B	601	1	-	0/10/54/54	0/0/8/8

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3D-C4D	-5.93	1.44	1.51
4	B	601	HEM	C2D-C3D	-5.75	1.37	1.54
4	A	601	HEM	C2D-C3D	-5.68	1.37	1.54
4	B	601	HEM	C3B-C4B	-4.87	1.47	1.51
4	A	601	HEM	C3D-C4D	-4.82	1.45	1.51
4	A	601	HEM	C3B-C4B	-4.81	1.47	1.51
4	B	601	HEM	C2C-C1C	-3.20	1.46	1.52
3	B	2802	BOG	C4-C5	-2.68	1.47	1.53
3	A	1802	BOG	C4-C5	-2.62	1.47	1.53
4	A	601	HEM	C2C-C1C	-2.61	1.47	1.52
3	A	1801	BOG	C3'-C2'	-2.58	1.36	1.51
3	A	1802	BOG	C3'-C2'	-2.41	1.37	1.51
3	A	1801	BOG	C4-C5	-2.34	1.48	1.53
4	A	601	HEM	C2B-C1B	-2.29	1.44	1.51
3	B	2802	BOG	C3'-C2'	-2.28	1.38	1.51
5	B	2701	34C	C11-C10	-2.21	1.30	1.49
4	B	601	HEM	C2B-C1B	-2.18	1.44	1.51
5	A	1701	34C	C11-C10	-2.17	1.31	1.49
4	A	601	HEM	C3B-CAB	2.01	1.55	1.51
2	B	2672	NAG	C3-C2	2.03	1.57	1.52
2	A	1681	NAG	C4-C3	2.04	1.57	1.52
2	B	2681	NAG	O5-C5	2.10	1.48	1.43
2	A	1672	NAG	C4-C3	2.14	1.58	1.52
4	A	601	HEM	C1C-NC	2.17	1.38	1.36
5	B	2701	34C	C6-C1	2.19	1.43	1.39
2	A	1672	NAG	C3-C2	2.31	1.57	1.52
3	A	1801	BOG	C4-C3	2.42	1.58	1.52
2	A	1671	NAG	C4-C5	2.43	1.58	1.53
2	A	1681	NAG	O5-C1	2.44	1.47	1.43
3	A	1802	BOG	O5-C5	2.46	1.50	1.44
2	B	2672	NAG	C4-C5	2.47	1.58	1.53
3	A	1801	BOG	O5-C5	2.49	1.50	1.44
2	B	2661	NAG	C4-C5	2.50	1.58	1.53
2	A	1661	NAG	C4-C5	2.55	1.58	1.53
2	A	1681	NAG	C3-C2	2.56	1.58	1.52
4	A	601	HEM	C4C-NC	2.58	1.39	1.36
4	B	601	HEM	C3B-CAB	2.59	1.56	1.51
3	B	2802	BOG	O5-C5	2.59	1.50	1.44
2	B	2681	NAG	C3-C2	2.70	1.58	1.52
2	B	2671	NAG	C4-C5	2.72	1.58	1.53
2	A	1661	NAG	C3-C2	2.89	1.59	1.52
3	A	1802	BOG	O5-C1	2.93	1.49	1.41
3	B	2802	BOG	O5-C1	2.95	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C1C-NC	2.98	1.39	1.36
5	A	1701	34C	C6-C1	2.99	1.45	1.39
2	B	2661	NAG	C3-C2	3.07	1.59	1.52
3	A	1801	BOG	O5-C1	3.38	1.50	1.41
4	B	601	HEM	CBC-CAC	3.89	1.51	1.29
4	A	601	HEM	CBC-CAC	4.05	1.52	1.29
4	A	601	HEM	CBB-CAB	4.06	1.52	1.29
4	B	601	HEM	CBB-CAB	4.16	1.53	1.29

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	CBA-CAA-C2A	-5.48	102.70	112.53
4	A	601	HEM	C3B-CAB-CBB	-4.45	117.63	124.46
4	B	601	HEM	CBA-CAA-C2A	-4.44	104.57	112.53
4	B	601	HEM	C3C-CAC-CBC	-3.92	118.45	124.46
4	A	601	HEM	C3C-CAC-CBC	-3.37	119.29	124.46
4	B	601	HEM	C3B-CAB-CBB	-3.13	119.66	124.46
2	A	1661	NAG	O7-C7-C8	-2.28	117.87	122.06
2	A	1672	NAG	O7-C7-C8	-2.26	117.91	122.06
2	A	1681	NAG	O7-C7-C8	-2.22	117.99	122.06
2	B	2672	NAG	O7-C7-C8	-2.21	118.01	122.06
2	A	1672	NAG	C4-C3-C2	-2.14	107.91	111.23
2	B	2661	NAG	O7-C7-C8	-2.09	118.22	122.06
5	A	1701	34C	C11-C10-C9	2.23	126.88	112.32
2	B	2681	NAG	C1-O5-C5	2.27	115.14	112.25
3	B	2802	BOG	C1'-O1-C1	2.56	118.42	113.94
3	A	1802	BOG	C1'-O1-C1	2.69	118.65	113.94
3	A	1801	BOG	O1-C1-C2	2.75	111.51	108.04
3	A	1802	BOG	O1-C1-C2	2.82	111.60	108.04
2	A	1681	NAG	C2-N2-C7	2.84	126.69	123.04
4	B	601	HEM	CAA-CBA-CGA	2.86	117.98	112.75
3	B	2802	BOG	O1-C1-C2	3.02	111.85	108.04
4	B	601	HEM	CMD-C2D-C3D	3.19	128.44	114.35
4	A	601	HEM	CMD-C2D-C3D	3.23	128.63	114.35
4	A	601	HEM	C2D-C3D-C4D	3.41	107.29	101.50
4	B	601	HEM	C2D-C3D-C4D	3.45	107.35	101.50
4	B	601	HEM	CAD-C3D-C4D	3.51	124.83	112.47
4	A	601	HEM	CAD-C3D-C4D	3.59	125.15	112.47
3	A	1801	BOG	C1'-O1-C1	4.25	121.37	113.94
4	A	601	HEM	CAA-CBA-CGA	4.29	120.61	112.75
4	A	601	HEM	CMC-C2C-C3C	4.64	128.10	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	HEM	CMC-C2C-C3C	4.72	128.30	116.53
4	A	601	HEM	CAD-C3D-C2D	4.99	127.56	113.22
4	B	601	HEM	CAD-C3D-C2D	5.07	127.81	113.22
4	A	601	HEM	CMB-C2B-C3B	5.48	130.22	116.53
4	B	601	HEM	CMB-C2B-C3B	5.78	130.97	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1661	NAG	2	0
2	A	1671	NAG	6	0
2	A	1672	NAG	1	0
2	A	1681	NAG	2	0
3	A	1801	BOG	4	0
3	A	1802	BOG	6	0
4	A	601	HEM	5	0
2	B	2661	NAG	2	0
2	B	2671	NAG	5	0
2	B	2672	NAG	1	0
2	B	2681	NAG	2	0
5	B	2701	34C	2	0
3	B	2802	BOG	3	0
4	B	601	HEM	4	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/551 (100%)	-0.53	6 (1%) 82 83	10, 23, 39, 53	0
1	B	551/551 (100%)	-0.52	12 (2%) 65 66	9, 23, 38, 52	0
All	All	1102/1102 (100%)	-0.52	18 (1%) 74 75	9, 23, 39, 53	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	GLN	3.9
1	B	215	LYS	2.8
1	A	33	VAL	2.6
1	B	514	PRO	2.6
1	A	75	TRP	2.4
1	B	400	GLN	2.4
1	B	98	TRP	2.4
1	B	33	VAL	2.4
1	A	79	ARG	2.3
1	B	368	GLY	2.3
1	B	107	PHE	2.3
1	B	75	TRP	2.2
1	B	399	PRO	2.1
1	A	98	TRP	2.1
1	B	277	ARG	2.1
1	A	186	LYS	2.1
1	B	282	GLN	2.1
1	B	515	ASN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	BOG	A	1801	20/20	0.44	1.02	11.21	38,63,68,69	0
5	34C	B	2701	15/15	0.86	0.22	7.03	35,37,43,44	0
2	NAG	B	2661	14/15	0.77	0.29	6.06	40,42,44,45	0
5	34C	A	1701	15/15	0.81	0.21	5.07	36,37,44,46	0
2	NAG	A	1661	14/15	0.78	0.29	4.69	40,44,45,45	0
2	NAG	B	2681	14/15	0.68	0.33	4.01	45,48,51,51	0
2	NAG	A	1671	14/15	0.93	0.15	3.42	6,15,18,21	0
2	NAG	A	1681	14/15	0.73	0.35	2.72	45,47,49,52	0
3	BOG	A	1802	20/20	0.74	0.30	2.70	37,54,65,68	0
3	BOG	B	2802	20/20	0.82	0.28	2.59	37,54,65,68	0
2	NAG	B	2671	14/15	0.94	0.15	2.39	9,17,19,23	0
4	HEM	B	601	43/43	0.94	0.16	0.98	22,24,33,39	0
4	HEM	A	601	43/43	0.94	0.14	0.46	23,25,32,38	0
2	NAG	A	1672	14/15	0.83	0.27	-	26,28,31,31	0
2	NAG	B	2672	14/15	0.82	0.25	-	26,28,30,31	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.