



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:50 PM GMT

PDB ID : 1CQE  
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEX WITH FLURBIPROFEN  
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Deposited on : 1999-06-15  
Resolution : 3.10 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

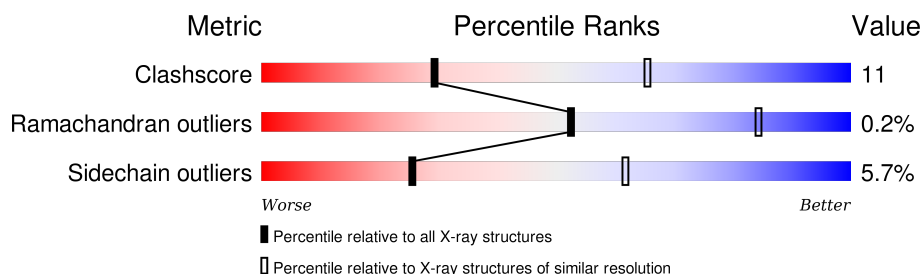
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	580	 68% 25% • 5%
1	B	580	 68% 24% • 5%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9413 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.

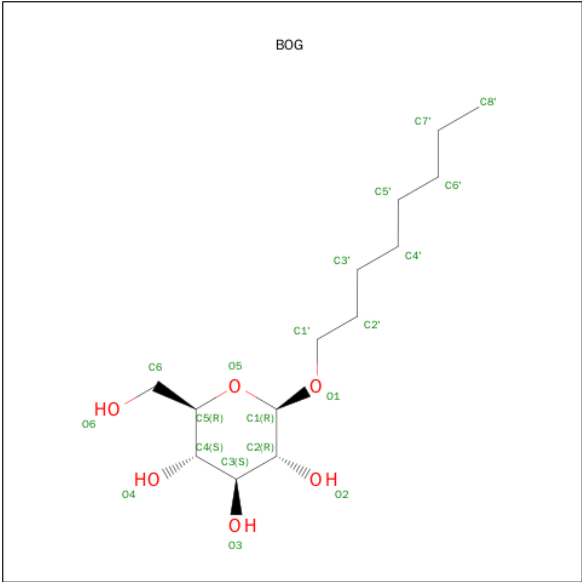
- Molecule 1 is a protein called PROTEIN (PROSTAGLANDIN H2 SYNTHASE-1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4458	2891	750	789	28			
1	B	553	Total	C	N	O	S	0	0	0
			4465	2896	751	790	28			

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-NAG).

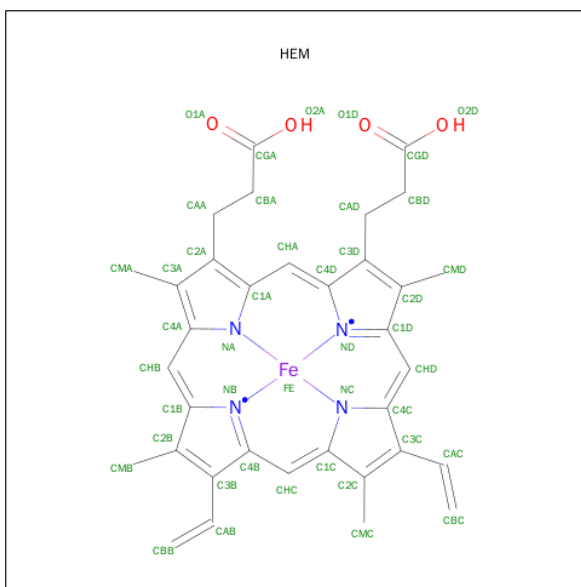
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

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



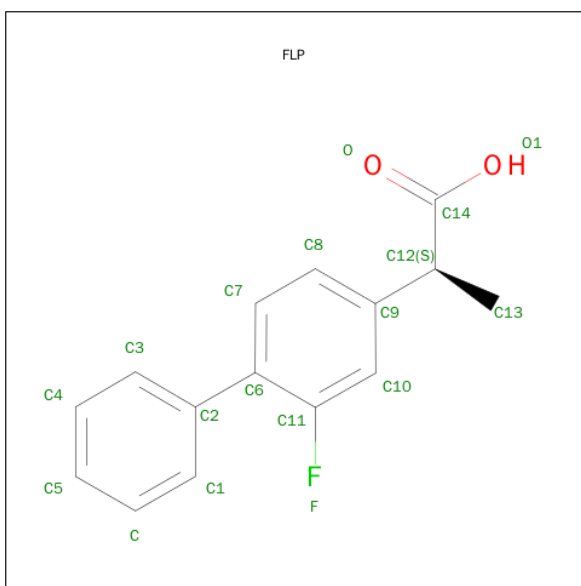
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C	O	0	0
			20	14	6		
3	B	1	Total	C	O	0	0
			10	9	1		
3	B	1	Total	C	O	0	0
			10	9	1		

- 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 FLURBIPROFEN (three-letter code: FLP) (formula:  $C_{15}H_{13}FO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			18	15	1	2		
5	B	1	Total	C	F	O	0	0
			18	15	1	2		

- Molecule 6 is water.

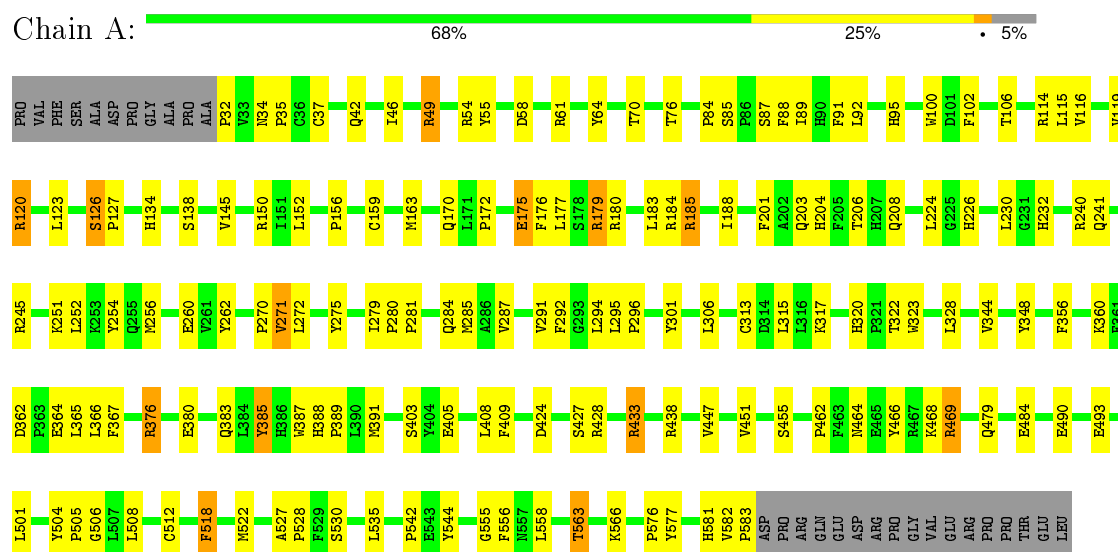
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	72	Total 72	O 72	0	0
6	B	58	Total 58	O 58	0	0

### 3 Residue-property plots

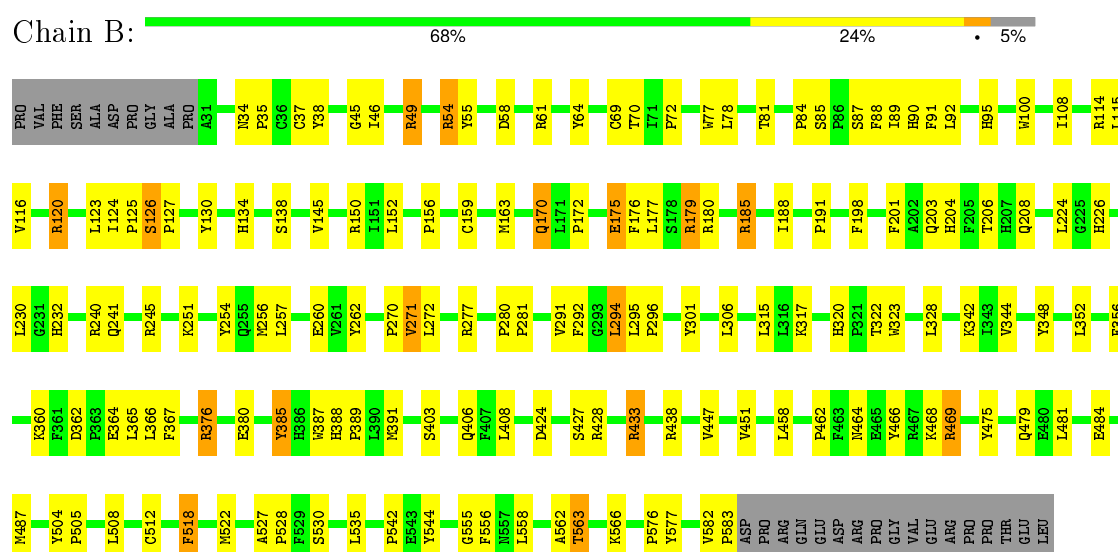
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

#### • Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-1)



#### • Molecule 1: PROTEIN (PROSTAGLANDIN H2 SYNTHASE-1)



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.40 Å   210.30 Å   233.10 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	94.3 (20.00-3.10)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.186 , 0.226	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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: FLP, NAG, HEM, 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	0.63	2/4596 (0.0%)	0.75	1/6245 (0.0%)
1	B	0.62	1/4604 (0.0%)	0.74	0/6257
All	All	0.63	3/9200 (0.0%)	0.74	1/12502 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	CYS	CB-SG	-6.43	1.71	1.82
1	B	512	CYS	CB-SG	-5.99	1.72	1.81
1	A	512	CYS	CB-SG	-5.33	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	32	PRO	N-CA-CB	5.68	110.12	103.30

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	4458	0	4330	98	0
1	B	4465	0	4340	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	84	0	75	1	0
2	B	84	0	75	3	0
3	A	50	0	73	3	0
3	B	20	0	34	1	0
4	A	43	0	30	5	0
4	B	43	0	30	4	0
5	A	18	0	12	1	0
5	B	18	0	12	0	0
6	A	72	0	0	5	0
6	B	58	0	0	3	0
All	All	9413	0	9011	206	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 11.

All (206) 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:185:ARG:HH11	1:B:438:ARG:HH11	1.19	0.89
1:B:185:ARG:NH1	1:B:438:ARG:HH11	1.74	0.85
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.59	0.82
1:B:185:ARG:NH1	1:B:438:ARG:NH1	2.29	0.81
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.63	0.80
1:A:150:ARG:HD3	1:A:152:LEU:O	1.82	0.80
1:B:150:ARG:HD3	1:B:152:LEU:O	1.83	0.78
1:B:176:PHE:CZ	1:B:180:ARG:HD2	2.18	0.78
1:A:116:VAL:O	1:A:120:ARG:HB2	1.86	0.76
1:B:116:VAL:O	1:B:120:ARG:HB2	1.87	0.74
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.69	0.74
1:A:88:PHE:CE2	1:A:92:LEU:HD11	2.23	0.73
1:A:391:MET:HG3	4:A:601:HEM:HAB	1.72	0.72
1:B:88:PHE:CE2	1:B:92:LEU:HD11	2.27	0.70
1:B:277:ARG:HG2	1:B:277:ARG:HH11	1.57	0.70
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.28	0.69
1:B:563:THR:HG22	1:B:566:LYS:H	1.58	0.68
3:A:1702:BOG:C1	6:A:1124:HOH:O	2.40	0.68
1:A:563:THR:HG22	1:A:566:LYS:H	1.58	0.67
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.28	0.67
2:B:661:NAG:H3	2:B:662:NAG:HN2	1.60	0.66
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.36	0.65
1:A:123:LEU:O	1:A:469:ARG:NH2	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.34	0.63
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.30	0.62
1:B:208:GLN:NE2	1:B:230:LEU:H	1.97	0.62
1:A:175:GLU:O	1:A:179:ARG:HG3	1.99	0.62
1:A:208:GLN:NE2	1:A:230:LEU:H	1.96	0.62
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.35	0.61
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.35	0.61
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.36	0.61
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.83	0.61
1:B:366:LEU:HD12	1:B:535:LEU:HD12	1.83	0.60
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.41	0.60
1:A:49:ARG:NH1	6:A:842:HOH:O	2.34	0.60
1:A:294:LEU:HD22	1:A:409:PHE:CE1	2.36	0.60
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.84	0.59
1:A:88:PHE:CZ	1:A:92:LEU:HD21	2.37	0.59
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.84	0.59
1:B:294:LEU:O	1:B:294:LEU:HG	2.02	0.59
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.33	0.59
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.32	0.59
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.38	0.59
1:B:77:TRP:CE2	1:B:81:THR:HG21	2.38	0.58
1:B:123:LEU:O	1:B:469:ARG:NH2	2.37	0.58
1:B:91:PHE:CE2	1:B:95:HIS:CD2	2.93	0.57
1:B:91:PHE:CZ	1:B:95:HIS:HD2	2.23	0.57
1:B:185:ARG:NH1	1:B:438:ARG:HG2	2.19	0.57
1:B:241:GLN:HE21	1:B:245:ARG:HH11	1.54	0.56
1:B:175:GLU:O	1:B:179:ARG:HG3	2.05	0.56
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.88	0.55
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.89	0.55
1:B:315:LEU:HD12	1:B:558:LEU:HD11	1.87	0.54
1:A:360:LYS:HE2	1:A:362:ASP:HB2	1.89	0.54
1:A:366:LEU:HD12	1:A:535:LEU:HD12	1.88	0.54
1:A:241:GLN:HE21	1:A:245:ARG:HH11	1.55	0.54
1:B:91:PHE:CE2	1:B:95:HIS:HD2	2.26	0.54
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.89	0.54
1:A:102:PHE:O	1:A:106:THR:HG23	2.07	0.53
1:A:403:SER:OG	1:A:405:GLU:HG2	2.07	0.53
1:B:88:PHE:CZ	1:B:92:LEU:HD21	2.44	0.53
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.44	0.53
1:B:45:GLY:HA3	1:B:69:CYS:SG	2.49	0.53
1:A:287:VAL:HA	6:A:833:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HD3	6:A:884:HOH:O	2.09	0.52
1:A:315:LEU:HD12	1:A:558:LEU:HD11	1.90	0.52
1:A:91:PHE:CE2	1:A:95:HIS:CD2	2.97	0.52
1:A:279:ILE:O	1:A:284:GLN:NE2	2.43	0.52
1:B:388:HIS:N	1:B:389:PRO:HD2	2.24	0.52
1:A:91:PHE:CZ	1:A:95:HIS:HD2	2.27	0.52
1:B:100:TRP:CD1	1:B:356:PHE:HB2	2.44	0.52
1:B:176:PHE:CE1	1:B:180:ARG:HD2	2.45	0.52
3:A:1702:BOG:C1	6:A:885:HOH:O	2.57	0.51
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.45	0.51
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.45	0.51
1:B:61:ARG:NH2	6:B:1005:HOH:O	2.43	0.51
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.93	0.50
1:B:360:LYS:HE2	1:B:362:ASP:HB2	1.92	0.50
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.92	0.50
1:B:464:ASN:O	1:B:468:LYS:HG3	2.11	0.50
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.47	0.50
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.93	0.50
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.52	0.50
1:B:163:MET:HB3	1:B:462:PRO:HG3	1.93	0.50
1:B:403:SER:OG	1:B:406:GLN:HG3	2.12	0.50
1:A:114:ARG:HD3	1:A:365:LEU:O	2.11	0.50
1:B:387:TRP:HB2	4:B:601:HEM:HAC	1.94	0.50
1:B:424:ASP:HB2	1:B:576:PRO:HB2	1.94	0.50
1:A:176:PHE:CZ	1:A:180:ARG:HG3	2.47	0.50
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.47	0.49
1:A:388:HIS:N	1:A:389:PRO:HD2	2.27	0.49
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.93	0.49
1:B:317:LYS:HD3	1:B:328:LEU:HD11	1.95	0.49
1:A:91:PHE:CE2	1:A:95:HIS:HD2	2.30	0.49
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.95	0.49
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.48	0.49
1:A:555:GLY:HA2	1:A:558:LEU:HD12	1.95	0.48
1:A:294:LEU:HD22	1:A:409:PHE:HE1	1.77	0.48
1:A:100:TRP:CD1	1:A:356:PHE:HB2	2.48	0.48
2:B:661:NAG:H61	2:B:662:NAG:C1	2.43	0.48
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.78	0.48
1:A:61:ARG:NH1	1:B:542:PRO:O	2.47	0.48
3:A:1701:BOG:O2	3:A:1701:BOG:H1'2	2.13	0.48
1:B:447:VAL:O	1:B:451:VAL:HG23	2.13	0.48
1:B:85:SER:O	1:B:89:ILE:HG12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.14	0.48
1:A:391:MET:CG	4:A:601:HEM:HAB	2.42	0.48
1:A:179:ARG:O	1:A:185:ARG:NH2	2.47	0.48
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.53	0.48
1:B:188:ILE:HD13	1:B:433:ARG:HH21	1.79	0.48
1:A:294:LEU:HD22	1:A:409:PHE:CD1	2.49	0.47
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.50	0.47
1:B:134:HIS:HD2	1:B:138:SER:OG	1.98	0.47
1:A:184:ARG:HA	1:A:438:ARG:O	2.14	0.47
1:A:387:TRP:HB2	4:A:601:HEM:HAC	1.97	0.47
1:A:542:PRO:O	1:B:61:ARG:NH1	2.47	0.47
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.97	0.47
1:B:49:ARG:NH1	6:B:942:HOH:O	2.46	0.47
1:A:134:HIS:HD2	1:A:138:SER:OG	1.96	0.47
1:A:256:MET:HA	1:A:260:GLU:O	2.15	0.47
1:A:464:ASN:O	1:A:468:LYS:HG3	2.14	0.46
1:A:262:TYR:HB3	1:A:285:MET:CE	2.45	0.46
1:B:77:TRP:CE3	1:B:78:LEU:HD23	2.50	0.46
1:A:317:LYS:HD3	1:A:328:LEU:HD11	1.96	0.46
1:A:85:SER:O	1:A:89:ILE:HG12	2.16	0.46
1:B:277:ARG:NH1	1:B:277:ARG:HG2	2.27	0.46
1:B:114:ARG:HD3	1:B:365:LEU:O	2.15	0.46
1:A:127:PRO:HG2	1:B:544:TYR:CE1	2.51	0.46
1:B:555:GLY:HA2	1:B:558:LEU:HD12	1.97	0.46
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.50	0.45
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.47	0.45
1:A:203:GLN:HA	4:A:601:HEM:HBC2	1.98	0.45
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.51	0.45
1:B:91:PHE:CZ	1:B:95:HIS:CD2	3.03	0.45
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.51	0.45
1:B:115:LEU:HD23	3:B:2802:BOG:H4'2	1.98	0.45
1:B:64:TYR:CE2	1:B:72:PRO:HB3	2.52	0.45
1:A:204:HIS:CD2	1:A:292:PHE:CE2	3.05	0.45
1:B:35:PRO:HB2	1:B:55:TYR:CD2	2.52	0.45
1:A:126:SER:HA	1:A:127:PRO:C	2.37	0.45
1:A:344:VAL:HA	1:A:348:TYR:HB3	1.99	0.45
1:B:180:ARG:HH11	1:B:180:ARG:HB3	1.82	0.45
1:A:208:GLN:HE21	1:A:230:LEU:H	1.65	0.45
1:B:203:GLN:HA	4:B:601:HEM:HBC2	1.99	0.44
1:A:42:GLN:HG3	1:A:70:THR:HG22	1.99	0.44
1:A:254:TYR:HB3	1:A:306:LEU:HD21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:MET:HA	1:B:260:GLU:O	2.17	0.44
1:B:391:MET:CG	4:B:601:HEM:HAB	2.41	0.44
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.52	0.44
1:B:198:PHE:HZ	1:B:352:LEU:HD13	1.82	0.44
1:A:447:VAL:O	1:A:451:VAL:HG23	2.18	0.44
1:B:179:ARG:HH11	1:B:179:ARG:HB3	1.83	0.44
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.52	0.44
1:B:38:TYR:CZ	2:B:662:NAG:H61	2.52	0.43
1:A:391:MET:SD	4:A:601:HEM:HAB	2.58	0.43
1:B:150:ARG:NH2	1:B:458:LEU:O	2.48	0.43
1:A:183:LEU:HD12	1:A:184:ARG:H	1.84	0.43
1:B:208:GLN:HE21	1:B:230:LEU:H	1.64	0.43
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.54	0.43
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.78	0.43
1:A:581:HIS:ND1	1:A:582:VAL:O	2.49	0.43
1:A:295:LEU:CD2	1:A:408:LEU:HD23	2.49	0.43
1:B:344:VAL:HA	1:B:348:TYR:HB3	2.00	0.43
1:A:88:PHE:O	1:A:92:LEU:HG	2.18	0.42
1:A:35:PRO:HB2	1:A:55:TYR:CD2	2.55	0.42
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.87	0.42
1:A:252:LEU:HA	1:A:252:LEU:HD12	1.91	0.42
1:A:544:TYR:CE1	1:B:127:PRO:HG2	2.54	0.42
1:B:180:ARG:HB3	1:B:180:ARG:NH1	2.34	0.42
1:B:126:SER:HA	1:B:127:PRO:C	2.39	0.42
1:B:204:HIS:CD2	1:B:292:PHE:CE2	3.08	0.42
1:A:46:ILE:HB	1:A:58:ASP:HB3	2.01	0.42
1:B:90:HIS:CE1	6:B:1207:HOH:O	2.72	0.42
1:B:46:ILE:HB	1:B:58:ASP:HB3	2.02	0.42
1:B:54:ARG:HB2	1:B:54:ARG:HH11	1.85	0.42
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.55	0.42
2:A:661:NAG:H61	2:A:662:NAG:H2	2.01	0.42
1:A:501:LEU:HD21	1:A:506:GLY:HA2	2.02	0.42
1:B:254:TYR:HB3	1:B:306:LEU:HD21	2.01	0.42
1:A:240:ARG:HG3	1:A:271:VAL:HG22	2.02	0.41
1:A:115:LEU:O	1:A:119:VAL:HB	2.20	0.41
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.55	0.41
1:B:124:ILE:HA	1:B:125:PRO:HD2	1.96	0.41
1:A:91:PHE:CZ	1:A:95:HIS:CD2	3.08	0.41
1:A:183:LEU:HD12	1:A:184:ARG:N	2.36	0.41
1:A:424:ASP:O	1:A:428:ARG:HG3	2.20	0.41
1:B:201:PHE:HD2	1:B:301:TYR:CE1	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:LEU:HB2	1:B:262:TYR:CD2	2.56	0.41
1:B:240:ARG:HG3	1:B:271:VAL:HG22	2.02	0.41
1:B:295:LEU:HD21	1:B:408:LEU:CD2	2.51	0.41
1:A:188:ILE:HD13	1:A:433:ARG:HH21	1.86	0.41
1:B:240:ARG:HG3	1:B:271:VAL:HG21	2.02	0.41
1:A:385:TYR:OH	5:A:1650:FLP:H	2.21	0.41
1:A:262:TYR:HB3	1:A:285:MET:HE1	2.03	0.41
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.56	0.40
1:A:201:PHE:HD2	1:A:301:TYR:CE1	2.39	0.40
1:B:108:ILE:HG22	1:B:108:ILE:O	2.21	0.40
1:A:383:GLN:OE1	1:A:455:SER:HB2	2.21	0.40
1:B:198:PHE:CD1	1:B:198:PHE:C	2.94	0.40
1:B:130:TYR:HB2	1:B:150:ARG:HG3	2.03	0.40
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.36	0.40
1:B:342:LYS:HD3	1:B:562:ALA:HB3	2.02	0.40
1:B:424:ASP:O	1:B:428:ARG:HG3	2.21	0.40
1:B:191:PRO:HD2	1:B:433:ARG:HG3	2.04	0.40
1:B:438:ARG:HH21	1:B:487:MET:HG3	1.85	0.40
1:B:170:GLN:HE21	1:B:170:GLN:HB2	1.75	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	550/580 (95%)	523 (95%)	26 (5%)	1 (0%)	52	84
1	B	551/580 (95%)	524 (95%)	26 (5%)	1 (0%)	52	84
All	All	1101/1160 (95%)	1047 (95%)	52 (5%)	2 (0%)	52	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	PRO
1	B	270	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	481/510 (94%)	454 (94%)	27 (6%)	26	62
1	B	482/510 (94%)	454 (94%)	28 (6%)	25	61
All	All	963/1020 (94%)	908 (94%)	55 (6%)	25	62

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	54	ARG
1	A	87	SER
1	A	120	ARG
1	A	126	SER
1	A	170	GLN
1	A	175	GLU
1	A	179	ARG
1	A	185	ARG
1	A	232	HIS
1	A	251	LYS
1	A	271	VAL
1	A	272	LEU
1	A	291	VAL
1	A	296	PRO
1	A	322	THR
1	A	376	ARG
1	A	385	TYR
1	A	433	ARG
1	A	469	ARG
1	A	479	GLN
1	A	484	GLU

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Mol	Chain	Res	Type
1	A	493	GLU
1	A	518	PHE
1	A	530	SER
1	A	556	PHE
1	A	563	THR
1	B	49	ARG
1	B	54	ARG
1	B	70	THR
1	B	87	SER
1	B	120	ARG
1	B	126	SER
1	B	170	GLN
1	B	175	GLU
1	B	179	ARG
1	B	185	ARG
1	B	232	HIS
1	B	251	LYS
1	B	271	VAL
1	B	272	LEU
1	B	291	VAL
1	B	294	LEU
1	B	296	PRO
1	B	322	THR
1	B	376	ARG
1	B	385	TYR
1	B	433	ARG
1	B	469	ARG
1	B	479	GLN
1	B	484	GLU
1	B	518	PHE
1	B	530	SER
1	B	556	PHE
1	B	563	THR

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	56	GLN
1	A	95	HIS
1	A	134	HIS
1	A	170	GLN
1	A	208	GLN

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Mol	Chain	Res	Type
1	A	241	GLN
1	A	358	GLN
1	A	375	ASN
1	A	513	HIS
1	A	557	ASN
1	B	56	GLN
1	B	95	HIS
1	B	134	HIS
1	B	170	GLN
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	282	GLN
1	B	375	ASN
1	B	557	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 ⓘ

12 carbohydrates 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	661	1,2	14,14,15	0.79	0	15,19,21	1.55	2 (13%)
2	NAG	A	662	2	14,14,15	0.88	1 (7%)	15,19,21	0.97	1 (6%)
2	NAG	A	671	1,2	14,14,15	0.47	0	15,19,21	1.02	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	A	672	2	14,14,15	0.59	0	15,19,21	0.78	0
2	NAG	A	681	1,2	14,14,15	0.63	0	15,19,21	1.01	2 (13%)
2	NAG	A	682	2	14,14,15	0.69	0	15,19,21	0.74	0
2	NAG	B	661	1,2	14,14,15	0.73	0	15,19,21	1.21	1 (6%)
2	NAG	B	662	2	14,14,15	0.96	1 (7%)	15,19,21	1.34	3 (20%)
2	NAG	B	671	1,2	14,14,15	0.60	0	15,19,21	1.18	2 (13%)
2	NAG	B	672	2	14,14,15	0.75	0	15,19,21	0.88	1 (6%)
2	NAG	B	681	1,2	14,14,15	0.57	0	15,19,21	0.69	0
2	NAG	B	682	2	14,14,15	0.45	0	15,19,21	0.77	1 (6%)

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	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	662	2	-	0/6/23/26	0/1/1/1
2	NAG	A	671	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	672	2	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	682	2	-	0/6/23/26	0/1/1/1
2	NAG	B	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	662	2	-	0/6/23/26	0/1/1/1
2	NAG	B	671	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	672	2	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	682	2	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	662	NAG	C3-C2	2.20	1.57	1.52
2	A	662	NAG	C1-C2	2.31	1.55	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	661	NAG	C2-N2-C7	-3.84	118.10	123.04
2	A	661	NAG	O4-C4-C3	-3.37	102.75	110.34
2	B	671	NAG	C2-N2-C7	-2.85	119.37	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	671	NAG	C4-C3-C2	-2.41	107.48	111.23
2	A	681	NAG	C2-N2-C7	-2.23	120.17	123.04
2	B	672	NAG	C2-N2-C7	-2.23	120.18	123.04
2	A	671	NAG	C2-N2-C7	-2.22	120.19	123.04
2	B	671	NAG	C4-C3-C2	-2.12	107.93	111.23
2	A	681	NAG	C4-C3-C2	-2.11	107.95	111.23
2	B	682	NAG	C2-N2-C7	-2.04	120.42	123.04
2	A	662	NAG	C4-C3-C2	2.05	114.41	111.23
2	B	662	NAG	C2-N2-C7	2.21	125.87	123.04
2	B	662	NAG	C4-C3-C2	2.43	115.00	111.23
2	B	662	NAG	C3-C4-C5	2.91	115.28	110.20
2	A	661	NAG	C4-C3-C2	3.44	116.58	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
2	A	662	NAG	1	0
2	B	661	NAG	2	0
2	B	662	NAG	3	0

## 5.6 Ligand geometry ⓘ

9 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
5	FLP	A	1650	-	16,19,19	1.75	2 (12%)	21,26,26	1.29	2 (9%)
3	BOG	A	1701	-	20,20,20	0.52	0	25,25,25	1.00	2 (8%)
3	BOG	A	1702	-	9,9,20	1.16	2 (22%)	8,8,25	0.88	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BOG	A	1703	-	20,20,20	0.49	0	25,25,25	0.91	1 (4%)
4	HEM	A	601	1	30,50,50	3.00	8 (26%)	24,82,82	2.67	11 (45%)
5	FLP	B	2650	-	16,19,19	2.08	3 (18%)	21,26,26	1.07	2 (9%)
3	BOG	B	2802	-	9,9,20	1.34	2 (22%)	8,8,25	0.74	0
3	BOG	B	2803	-	9,9,20	0.88	1 (11%)	8,8,25	0.71	0
4	HEM	B	601	1	30,50,50	3.07	12 (40%)	24,82,82	2.65	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
5	FLP	A	1650	-	-	0/8/12/12	0/2/2/2
3	BOG	A	1701	-	-	0/11/31/31	0/1/1/1
3	BOG	A	1702	-	-	0/7/7/31	0/0/0/1
3	BOG	A	1703	-	-	0/11/31/31	0/1/1/1
4	HEM	A	601	1	-	0/10/54/54	0/0/8/8
5	FLP	B	2650	-	-	0/8/12/12	0/2/2/2
3	BOG	B	2802	-	-	0/7/7/31	0/0/0/1
3	BOG	B	2803	-	-	0/7/7/31	0/0/0/1
4	HEM	B	601	1	-	0/10/54/54	0/0/8/8

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C3C-CAC	-7.72	1.36	1.51
4	A	601	HEM	C3C-CAC	-7.56	1.37	1.51
4	A	601	HEM	C3B-CAB	-7.40	1.37	1.51
4	B	601	HEM	C3B-CAB	-6.70	1.38	1.51
4	B	601	HEM	C2D-C3D	-6.37	1.35	1.54
4	B	601	HEM	C3D-C4D	-6.22	1.43	1.51
4	A	601	HEM	C3D-C4D	-6.09	1.43	1.51
4	A	601	HEM	C2C-C1C	-5.90	1.41	1.52
4	A	601	HEM	C2D-C3D	-5.87	1.36	1.54
5	B	2650	FLP	C6-C2	-5.49	1.40	1.49
4	B	601	HEM	C2C-C1C	-5.13	1.42	1.52
4	A	601	HEM	C3B-C4B	-4.30	1.48	1.51
5	A	1650	FLP	C6-C2	-3.93	1.43	1.49
4	B	601	HEM	C3B-C4B	-3.61	1.48	1.51
4	B	601	HEM	C2D-C1D	-2.05	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	CBC-CAC	2.03	1.41	1.29
3	B	2803	BOG	O1-C1'	2.09	1.53	1.40
3	A	1702	BOG	O1-C1	2.10	1.53	1.41
4	B	601	HEM	CBB-CAB	2.19	1.42	1.29
5	B	2650	FLP	C8-C7	2.21	1.42	1.38
4	A	601	HEM	CBB-CAB	2.28	1.42	1.29
3	A	1702	BOG	O1-C1'	2.42	1.55	1.40
4	B	601	HEM	CHD-C4C	2.43	1.42	1.36
3	B	2802	BOG	O1-C1'	2.44	1.55	1.40
4	A	601	HEM	C1C-NC	2.50	1.39	1.36
3	B	2802	BOG	O1-C1	2.95	1.57	1.41
5	B	2650	FLP	C6-C11	3.44	1.43	1.38
5	A	1650	FLP	C6-C11	3.50	1.43	1.38
4	B	601	HEM	C4C-NC	3.89	1.40	1.36
4	B	601	HEM	C1C-NC	4.17	1.41	1.36

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	HEM	CAA-C2A-C3A	-3.23	119.78	129.00
4	A	601	HEM	CAA-C2A-C3A	-3.00	120.43	129.00
5	A	1650	FLP	C10-C11-C6	-2.91	120.58	124.24
4	A	601	HEM	C3C-CAC-CBC	-2.77	120.20	124.46
4	A	601	HEM	CMA-C3A-C4A	-2.21	124.71	128.36
4	B	601	HEM	C3C-CAC-CBC	-2.18	121.11	124.46
3	A	1701	BOG	C4-C3-C2	-2.14	106.81	110.79
3	A	1701	BOG	C6-C5-C4	-2.07	107.92	113.02
5	B	2650	FLP	C10-C11-C6	-2.04	121.67	124.24
3	A	1702	BOG	C1-O1-C1'	2.24	127.79	113.09
4	B	601	HEM	CAD-C3D-C4D	2.59	121.60	112.47
4	A	601	HEM	CAD-C3D-C4D	2.66	121.84	112.47
5	B	2650	FLP	F-C11-C6	2.73	122.87	118.80
3	A	1703	BOG	C1'-O1-C1	2.77	118.78	113.94
4	A	601	HEM	CMD-C2D-C3D	2.93	127.30	114.35
4	B	601	HEM	CMD-C2D-C3D	3.00	127.61	114.35
4	A	601	HEM	CAA-C2A-C1A	3.13	130.40	127.01
5	A	1650	FLP	F-C11-C6	3.22	123.59	118.80
4	B	601	HEM	CAA-C2A-C1A	3.63	130.95	127.01
4	A	601	HEM	CMB-C2B-C3B	3.69	125.74	116.53
4	B	601	HEM	CMC-C2C-C3C	4.14	126.87	116.53
4	B	601	HEM	CMB-C2B-C3B	4.14	126.88	116.53
4	A	601	HEM	CMC-C2C-C3C	4.23	127.08	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	A	601	HEM	C2D-C3D-C4D	4.55	109.22	101.50
4	B	601	HEM	C2D-C3D-C4D	4.65	109.38	101.50
4	A	601	HEM	CAD-C3D-C2D	5.27	128.36	113.22
4	B	601	HEM	CAD-C3D-C2D	5.31	128.48	113.22
4	B	601	HEM	CBA-CAA-C2A	5.42	122.24	112.53
4	A	601	HEM	CBA-CAA-C2A	5.83	122.98	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1650	FLP	1	0
3	A	1701	BOG	1	0
3	A	1702	BOG	2	0
4	A	601	HEM	5	0
3	B	2802	BOG	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.