Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:50 AM GMT

PDB ID	:	3N8Z
Title	:	Crystal Structure of Cyclooxygenase-1 in Complex with Flurbiprofen
Authors	:	Sidhu, R.S.
Deposited on	:	2010-05-28
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

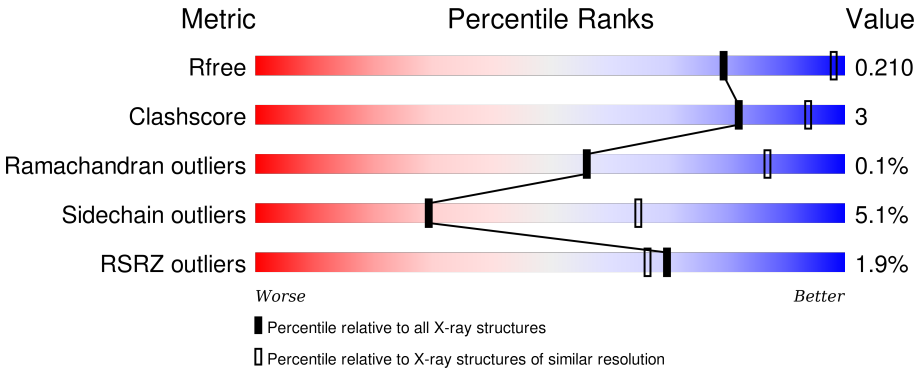
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

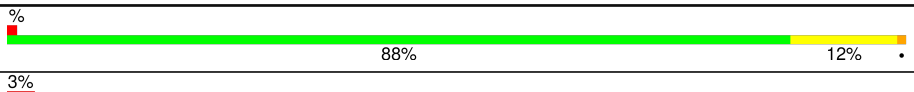
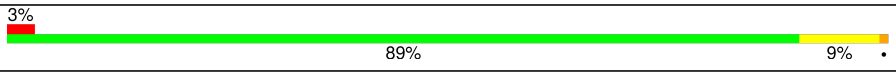
The reported resolution of this entry is 2.90 Å.

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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	553	
1	B	553	

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
4	NAG	A	671	X	-	-	-
5	BOG	A	750	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9437 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.

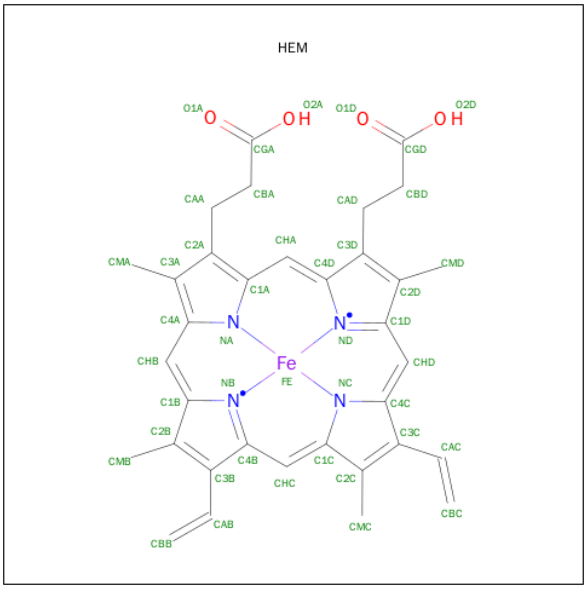
- Molecule 1 is a protein called Prostaglandin G/H synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4451	2886	744	794	27			
1	B	553	Total	C	N	O	S	3	1	0
			4463	2893	752	790	28			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	LEU	MET	CONFLICT	UNP P05979
B	92	LEU	MET	CONFLICT	UNP P05979

- 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		

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

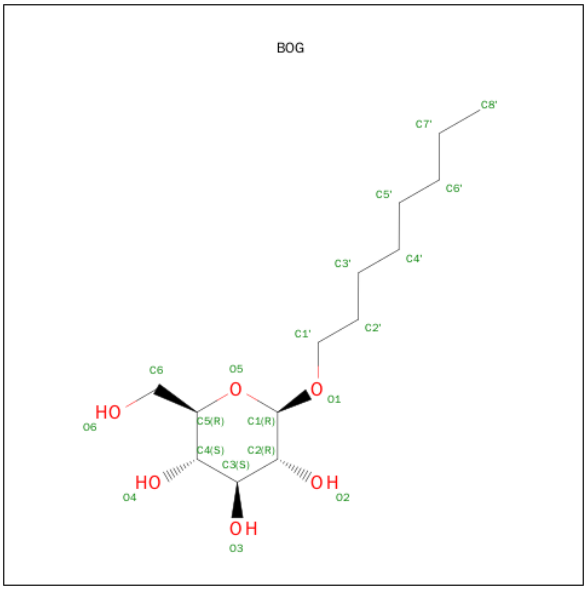
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

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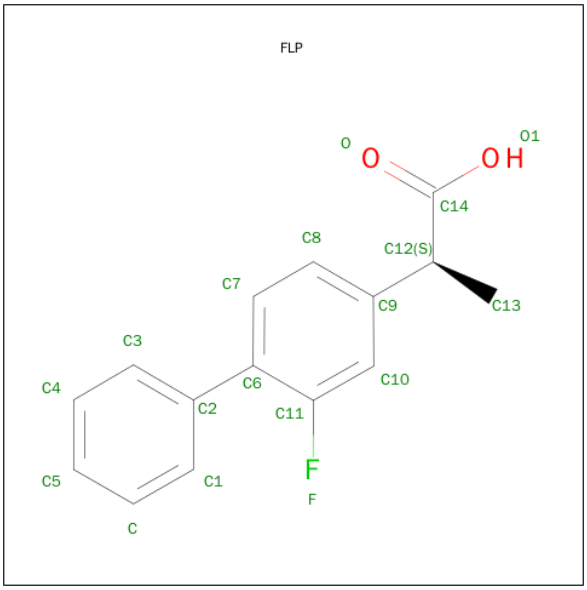
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 7 6	0	0
5	B	1	Total C O 20 14 6	0	0
5	B	1	Total C O 20 14 6	0	0

- Molecule 6 is FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



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

- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	5	Total C N O 61 34 2 25	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	78	Total O 78 78	0	0

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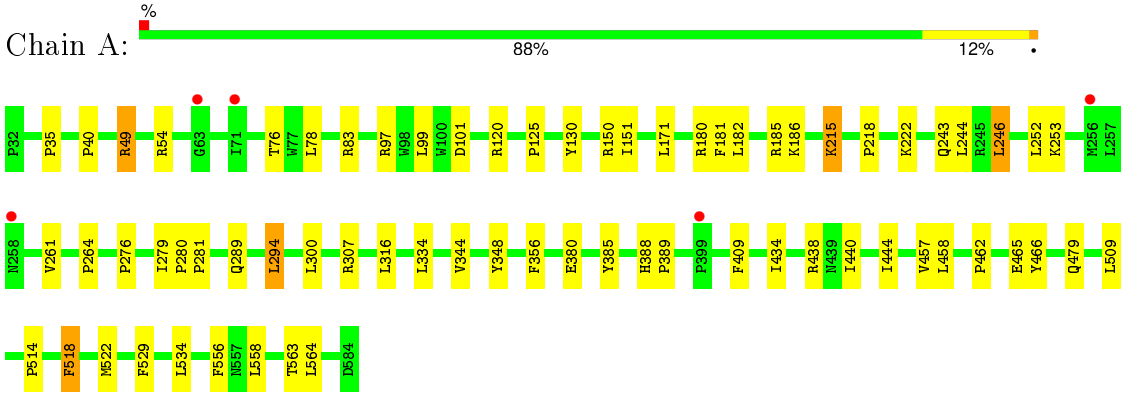
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	57	Total O 57 57	0	0

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.

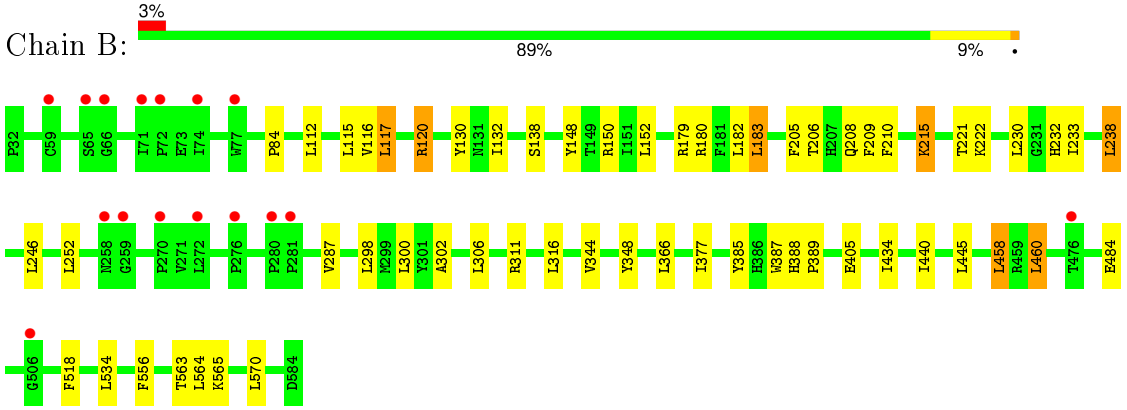
- Molecule 1: Prostaglandin G/H synthase 1

Chain A:



- Molecule 1: Prostaglandin G/H synthase 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	181.49Å 181.49Å 103.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.63 – 2.90 31.63 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (31.63-2.90) 99.9 (31.63-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.176 , 0.207 0.179 , 0.210	Depositor DCC
R_{free} test set	1544 reflections (3.71%)	DCC
Wilson B-factor (Å^2)	64.6	Xtriage
Anisotropy	0.247	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.5	EDS
Estimated twinning fraction	0.502 for H, K, L 0.498 for H+K, -K, -L 0.086 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.502 for H, K, L 0.498 for H+K, -K, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	0 of 43147 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9437	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, FLP, NDG, HEM, BOG, MAN

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	0.33	0/4593	0.47	0/6249
1	B	0.33	0/4602	0.48	0/6257
All	All	0.33	0/9195	0.48	0/12506

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	671	NAG	C1

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4451	0	4285	28	0
1	B	4463	0	4323	30	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
3	A	28	0	25	1	0
4	A	56	0	50	1	0
4	B	28	0	25	0	0
5	A	53	0	67	0	0
5	B	40	0	56	3	0
6	A	18	0	12	0	0
6	B	18	0	12	0	0
7	B	61	0	52	1	0
8	A	78	0	0	0	0
8	B	57	0	0	0	0
All	All	9437	0	8967	58	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 3.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LYS:HE2	1:A:215:LYS:H	1.48	0.78
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.70	0.70
1:B:215:LYS:H	1:B:215:LYS:HE2	1.58	0.69
1:A:181:PHE:HB3	1:A:509:LEU:HD21	1.83	0.60
1:B:182:LEU:HB3	1:B:440:ILE:HD12	1.85	0.59
1:B:150:ARG:HD3	1:B:152:LEU:O	2.03	0.57
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.87	0.57
1:A:246:LEU:HD12	1:A:253:LYS:HA	1.85	0.56
1:B:205:PHE:O	1:B:208:GLN:HG2	2.07	0.55
1:B:387:TRP:HB2	2:B:601:HEM:HAC	1.89	0.55
1:B:230:LEU:HG	1:B:233:ILE:HD12	1.89	0.54
1:A:130:TYR:HB2	1:A:150:ARG:HG3	1.88	0.53
1:B:132:ILE:HD13	1:B:458:LEU:HD12	1.90	0.53
4:A:671:NAG:H4	1:B:238:LEU:HD12	1.90	0.53
1:B:115:LEU:HD23	5:B:1751:BOG:H4'2	1.91	0.53
1:B:209:PHE:HB2	1:B:377:ILE:HG13	1.93	0.51
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.25	0.51
1:B:179:ARG:HD3	1:B:183:LEU:HD12	1.93	0.50
1:A:294:LEU:HG	1:A:409:PHE:CE1	2.47	0.50
1:B:130:TYR:HB2	1:B:150:ARG:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:N	1:A:389:PRO:CD	2.74	0.50
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.93	0.50
1:A:444:ILE:HG21	2:A:601:HEM:HBB2	1.95	0.49
1:B:389:PRO:HB2	1:B:434:ILE:HA	1.94	0.49
1:A:334:LEU:HD11	1:B:138:SER:HA	1.95	0.48
1:B:388:HIS:N	1:B:389:PRO:CD	2.76	0.48
1:A:125:PRO:HD2	1:A:151:ILE:HD12	1.95	0.48
1:B:112:LEU:HD22	5:B:1751:BOG:H6'2	1.96	0.48
1:A:261:VAL:H	1:A:307:ARG:HH21	1.63	0.47
1:A:261:VAL:N	1:A:307:ARG:HH21	2.13	0.47
1:B:563:THR:HG22	1:B:565:LYS:H	1.80	0.47
1:A:97:ARG:HG2	1:A:356:PHE:CE2	2.49	0.47
1:B:116:VAL:O	1:B:120:ARG:HB2	2.15	0.46
1:A:389:PRO:HB2	1:A:434:ILE:HA	1.98	0.46
1:A:444:ILE:HD13	2:A:601:HEM:HBB2	1.97	0.46
1:B:311:ARG:NH2	1:B:570:LEU:HD23	2.31	0.46
1:A:35:PRO:HD2	1:A:49:ARG:HD2	1.98	0.45
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.50	0.45
1:A:218:PRO:HG2	1:A:457:VAL:HG11	1.99	0.45
7:B:671:NAG:H62	7:B:672:NAG:C1	2.48	0.44
1:B:458:LEU:HB3	1:B:460:LEU:HD13	1.99	0.44
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.99	0.44
1:B:388:HIS:N	1:B:389:PRO:HD2	2.32	0.44
1:B:206:THR:HB	1:B:210:PHE:HD2	1.82	0.43
1:A:253:LYS:O	1:A:264:PRO:HD3	2.18	0.43
1:B:183:LEU:HG	1:B:445:LEU:HD22	2.01	0.43
1:B:84:PRO:HB3	5:B:1750:BOG:H7'2	2.01	0.42
1:B:148:TYR:CZ	1:B:221:THR:HB	2.54	0.42
1:B:117:LEU:HB3	1:B:366:LEU:HD21	2.00	0.42
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.88	0.42
1:A:40:PRO:HB3	3:A:661:NAG:H61	2.00	0.42
1:A:151:ILE:HD11	1:A:529:PHE:HE2	1.85	0.42
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.83	0.42
1:A:276:PRO:HD2	1:A:279:ILE:HD12	2.02	0.41
1:A:344:VAL:HA	1:A:348:TYR:HB3	2.02	0.41
1:A:185:ARG:HB2	1:A:186:LYS:H	1.73	0.41
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.56	0.41
1:B:252:LEU:HD13	1:B:306:LEU:HG	2.02	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	553/553 (100%)	531 (96%)	21 (4%)	1 (0%)	52 84
1	B	552/553 (100%)	532 (96%)	20 (4%)	0	100 100
All	All	1105/1106 (100%)	1063 (96%)	41 (4%)	1 (0%)	56 87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	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	478/488 (98%)	449 (94%)	29 (6%)	23 56
1	B	480/488 (98%)	460 (96%)	20 (4%)	36 73
All	All	958/976 (98%)	909 (95%)	49 (5%)	29 65

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	54	ARG
1	A	76	THR
1	A	78	LEU
1	A	83	ARG

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Mol	Chain	Res	Type
1	A	99	LEU
1	A	101	ASP
1	A	120	ARG
1	A	171	LEU
1	A	180	ARG
1	A	215	LYS
1	A	222	LYS
1	A	243	GLN
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	289	GLN
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	385	TYR
1	A	458	LEU
1	A	479	GLN
1	A	518	PHE
1	A	534	LEU
1	A	556	PHE
1	A	558	LEU
1	A	563	THR
1	A	564	LEU
1	B	117	LEU
1	B	120	ARG
1	B	180	ARG
1	B	183	LEU
1	B	215	LYS
1	B	222	LYS
1	B	238	LEU
1	B	246	LEU
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	385	TYR
1	B	405	GLU
1	B	458	LEU
1	B	460	LEU
1	B	484	GLU
1	B	518	PHE
1	B	534	LEU

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Mol	Chain	Res	Type
1	B	556	PHE
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

13 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	$\#\|Z\| > 2$
3	NAG	A	661	1,3	14,14,15	0.49	0	15,19,21	0.97	2 (13%)
3	NDG	A	662	3	14,14,15	0.49	0	15,19,21	0.82	1 (6%)
4	NAG	A	671	1,4	14,14,15	0.42	0	15,19,21	1.18	1 (6%)
4	NAG	A	672	4	14,14,15	0.48	0	15,19,21	0.83	0
4	NAG	A	681	1,4	14,14,15	0.51	0	15,19,21	0.74	0
4	NAG	A	682	4	14,14,15	0.48	0	15,19,21	0.78	1 (6%)
7	NAG	B	671	1,7	14,14,15	0.46	0	15,19,21	1.47	1 (6%)
7	NAG	B	672	7	14,14,15	0.54	0	15,19,21	0.86	0
7	BMA	B	673	7	11,11,12	0.53	0	14,15,17	1.21	2 (14%)
7	BMA	B	674	7	11,11,12	0.70	0	14,15,17	0.78	0
7	MAN	B	675	7	11,11,12	0.60	0	14,15,17	1.31	2 (14%)
4	NAG	B	681	4	14,14,15	0.57	0	15,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	682	4	14,14,15	0.43	0	15,19,21	1.02	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
3	NAG	A	661	1,3	-	0/6/23/26	0/1/1/1
3	NDG	A	662	3	-	0/6/23/26	0/1/1/1
4	NAG	A	671	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	672	4	-	0/6/23/26	0/1/1/1
4	NAG	A	681	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	682	4	-	0/6/23/26	0/1/1/1
7	NAG	B	671	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	672	7	-	0/6/23/26	0/1/1/1
7	BMA	B	673	7	-	0/2/19/22	0/1/1/1
7	BMA	B	674	7	-	0/2/19/22	0/1/1/1
7	MAN	B	675	7	-	0/2/19/22	0/1/1/1
4	NAG	B	681	4	-	0/6/23/26	0/1/1/1
4	NAG	B	682	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	661	NAG	C1-O5-C5	2.05	114.84	112.25
4	A	682	NAG	C1-O5-C5	2.16	114.99	112.25
3	A	661	NAG	O4-C4-C3	2.18	115.24	110.34
3	A	662	NDG	C1-O-C5	2.23	115.08	112.25
7	B	673	BMA	C1-C2-C3	2.49	112.48	109.54
7	B	675	MAN	C3-C4-C5	2.54	114.63	110.20
7	B	673	BMA	C1-O5-C5	3.16	116.26	112.25
4	B	682	NAG	C1-O5-C5	3.39	116.55	112.25
7	B	675	MAN	C1-O5-C5	3.43	116.60	112.25
4	A	671	NAG	C1-O5-C5	3.65	116.88	112.25
7	B	671	NAG	C1-O5-C5	4.94	118.52	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	671	NAG	C1

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	661	NAG	1	0
4	A	671	NAG	1	0
7	B	671	NAG	1	0
7	B	672	NAG	1	0

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
2	HEM	A	601	-	30,50,50	2.19	12 (40%)	24,82,82	2.35	12 (50%)
6	FLP	A	701	-	16,19,19	5.19	13 (81%)	21,26,26	1.46	2 (9%)
5	BOG	A	750	-	20,20,20	0.76	0	25,25,25	1.66	4 (16%)
5	BOG	A	751	-	20,20,20	0.74	0	25,25,25	1.40	3 (12%)
5	BOG	A	752	-	13,13,20	0.86	0	18,18,25	1.88	5 (27%)
6	FLP	B	1701	-	16,19,19	5.19	13 (81%)	21,26,26	1.37	2 (9%)
5	BOG	B	1750	-	20,20,20	0.72	0	25,25,25	1.43	4 (16%)
5	BOG	B	1751	-	20,20,20	0.73	0	25,25,25	1.51	4 (16%)
2	HEM	B	601	1	30,50,50	2.13	12 (40%)	24,82,82	2.33	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	601	-	-	0/10/54/54	0/0/8/8
6	FLP	A	701	-	-	0/8/12/12	0/2/2/2
5	BOG	A	750	-	-	0/11/31/31	0/1/1/1
5	BOG	A	751	-	-	0/11/31/31	0/1/1/1
5	BOG	A	752	-	-	0/4/24/31	0/1/1/1
6	FLP	B	1701	-	-	0/8/12/12	0/2/2/2
5	BOG	B	1750	-	-	0/11/31/31	0/1/1/1
5	BOG	B	1751	-	-	0/11/31/31	0/1/1/1
2	HEM	B	601	1	-	0/10/54/54	0/0/8/8

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C3B-C4B	-6.92	1.45	1.51
2	B	601	HEM	C3B-C4B	-6.46	1.46	1.51
2	B	601	HEM	C3D-C4D	-4.73	1.45	1.51
6	B	1701	FLP	C6-C11	-4.66	1.32	1.38
2	A	601	HEM	C3D-C4D	-4.60	1.45	1.51
6	A	701	FLP	C6-C11	-4.53	1.33	1.38
6	B	1701	FLP	C10-C9	-3.84	1.32	1.39
6	A	701	FLP	C10-C9	-3.72	1.32	1.39
6	A	701	FLP	C8-C7	-3.62	1.32	1.38
6	B	1701	FLP	C8-C7	-3.62	1.32	1.38
2	A	601	HEM	C2C-C1C	-3.51	1.45	1.52
2	B	601	HEM	C2C-C1C	-3.42	1.46	1.52
6	A	701	FLP	C-C1	-3.16	1.32	1.38
6	B	1701	FLP	C-C1	-3.08	1.32	1.38
6	B	1701	FLP	C3-C2	-3.08	1.32	1.39
6	A	701	FLP	C3-C2	-3.06	1.32	1.39
6	A	701	FLP	C5-C4	-2.13	1.32	1.38
6	B	1701	FLP	C5-C4	-2.13	1.32	1.38
2	A	601	HEM	C2D-C1D	-2.04	1.45	1.51
2	B	601	HEM	C2B-C1B	-2.02	1.45	1.51
2	A	601	HEM	C3B-CAB	2.02	1.55	1.51
2	B	601	HEM	C3C-CAC	2.04	1.55	1.51
2	B	601	HEM	CAA-C2A	2.05	1.55	1.52
2	B	601	HEM	C3B-CAB	2.07	1.55	1.51
2	A	601	HEM	CAA-C2A	2.13	1.55	1.52
2	A	601	HEM	FE-NB	2.15	2.08	1.97
2	B	601	HEM	FE-ND	2.16	2.08	1.97
2	A	601	HEM	C3C-CAC	2.16	1.55	1.51
2	B	601	HEM	C4C-NC	2.29	1.38	1.36
2	B	601	HEM	FE-NC	2.29	2.04	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	HEM	C4C-NC	2.33	1.38	1.36
6	A	701	FLP	C6-C2	2.40	1.53	1.49
2	B	601	HEM	C1C-NC	2.40	1.39	1.36
2	A	601	HEM	C1C-NC	2.41	1.39	1.36
6	B	1701	FLP	C6-C2	2.45	1.53	1.49
2	A	601	HEM	FE-ND	2.72	2.11	1.97
2	B	601	HEM	FE-NB	2.78	2.12	1.97
2	A	601	HEM	FE-NC	2.91	2.07	1.95
6	B	1701	FLP	C5-C	5.93	1.53	1.38
6	A	701	FLP	C5-C	6.00	1.53	1.38
6	A	701	FLP	C1-C2	6.69	1.53	1.39
6	B	1701	FLP	C1-C2	6.71	1.53	1.39
6	A	701	FLP	C4-C3	7.11	1.53	1.38
6	B	1701	FLP	C4-C3	7.18	1.53	1.38
6	B	1701	FLP	C7-C6	7.99	1.53	1.39
6	A	701	FLP	C7-C6	8.13	1.53	1.39
6	A	701	FLP	C8-C9	8.83	1.53	1.39
6	B	1701	FLP	C8-C9	8.84	1.53	1.39
6	B	1701	FLP	C10-C11	8.85	1.53	1.37
6	A	701	FLP	C10-C11	8.85	1.53	1.37

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	750	BOG	O5-C1-C2	-4.59	100.87	110.28
5	A	750	BOG	C1'-O1-C1	-4.28	106.46	113.94
5	A	751	BOG	O5-C1-C2	-4.23	101.60	110.28
5	A	752	BOG	C1'-O1-C1	-4.05	106.67	113.29
5	A	752	BOG	O5-C1-C2	-4.02	102.03	110.28
5	B	1751	BOG	C1'-O1-C1	-3.97	107.00	113.94
6	A	701	FLP	C10-C11-C6	-3.59	119.72	124.24
5	B	1750	BOG	O5-C1-C2	-3.37	103.35	110.28
6	B	1701	FLP	C10-C11-C6	-3.37	120.00	124.24
5	B	1751	BOG	O5-C1-C2	-3.27	103.56	110.28
5	A	751	BOG	C1'-O1-C1	-3.19	108.38	113.94
5	B	1750	BOG	O5-C5-C4	-3.14	103.78	109.68
5	A	752	BOG	C4-C3-C2	-3.12	104.97	110.79
5	B	1751	BOG	O5-C5-C4	-2.99	104.07	109.68
5	A	750	BOG	C1-C2-C3	-2.67	104.71	109.97
5	A	750	BOG	C4-C3-C2	-2.66	105.82	110.79
2	A	601	HEM	C3B-CAB-CBB	-2.66	120.38	124.46
5	B	1750	BOG	C4-C3-C2	-2.65	105.85	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	752	BOG	O5-C5-C4	-2.61	104.78	109.68
2	B	601	HEM	C3C-CAC-CBC	-2.52	120.59	124.46
5	B	1751	BOG	C4-C3-C2	-2.47	106.18	110.79
2	B	601	HEM	C3B-CAB-CBB	-2.37	120.82	124.46
2	A	601	HEM	CAA-CBA-CGA	-2.36	108.42	112.75
5	A	751	BOG	O5-C5-C4	-2.31	105.34	109.68
5	B	1750	BOG	C1'-O1-C1	-2.29	109.94	113.94
2	A	601	HEM	CAA-C2A-C1A	-2.28	124.53	127.01
5	A	752	BOG	C1-C2-C3	-2.13	105.78	109.97
2	A	601	HEM	C3B-C4B-NB	-2.07	107.67	111.63
2	A	601	HEM	CMA-C3A-C4A	-2.03	125.01	128.36
2	B	601	HEM	C3B-C4B-NB	-2.01	107.79	111.63
2	B	601	HEM	C2C-C1C-CHC	2.14	126.93	123.68
2	B	601	HEM	C2D-C3D-C4D	2.26	105.33	101.50
2	A	601	HEM	C2D-C3D-C4D	2.26	105.34	101.50
2	A	601	HEM	C3B-C4B-CHC	2.66	126.91	123.16
2	B	601	HEM	CMD-C2D-C3D	2.92	127.25	114.35
2	A	601	HEM	CMD-C2D-C3D	2.95	127.41	114.35
2	B	601	HEM	C3B-C4B-CHC	3.07	127.48	123.16
2	B	601	HEM	CMC-C2C-C3C	3.60	125.52	116.53
2	A	601	HEM	CMC-C2C-C3C	3.81	126.04	116.53
6	B	1701	FLP	C7-C6-C11	3.97	119.84	115.90
2	A	601	HEM	CMB-C2B-C3B	4.00	126.52	116.53
2	B	601	HEM	CMB-C2B-C3B	4.19	126.98	116.53
6	A	701	FLP	C7-C6-C11	4.22	120.09	115.90
2	B	601	HEM	CAD-C3D-C4D	4.22	127.37	112.47
2	A	601	HEM	CAD-C3D-C4D	4.31	127.69	112.47
2	A	601	HEM	CAD-C3D-C2D	4.78	126.97	113.22
2	B	601	HEM	CAD-C3D-C2D	4.90	127.31	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	HEM	2	0
5	B	1750	BOG	1	0
5	B	1751	BOG	2	0
2	B	601	HEM	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	553/553 (100%)	-0.25	5 (0%)	85	84	52, 67, 82, 91	0
1	B	553/553 (100%)	-0.15	16 (2%)	55	49	50, 65, 82, 98	2 (0%)
All	All	1106/1106 (100%)	-0.20	21 (1%)	70	66	50, 66, 82, 98	2 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	258	ASN	4.3
1	B	259	GLY	4.0
1	A	258	ASN	3.8
1	B	65	SER	3.6
1	B	71	ILE	2.9
1	A	256	MET	2.6
1	B	280	PRO	2.5
1	B	272	LEU	2.5
1	A	63	GLY	2.4
1	B	476	THR	2.4
1	B	270	PRO	2.3
1	B	72	PRO	2.3
1	B	59	CYS	2.3
1	B	276	PRO	2.3
1	B	74	ILE	2.3
1	B	77	TRP	2.2
1	B	281	PRO	2.2
1	B	66	GLY	2.2
1	A	71	ILE	2.2
1	A	399	PRO	2.1
1	B	506	GLY	2.1

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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NAG	B	681	14/15	0.92	0.18	0.99	100,105,108,109	0
3	NAG	A	661	14/15	0.95	0.21	-0.17	74,76,79,80	0
4	NAG	A	681	14/15	0.89	0.18	-0.20	86,90,92,92	0
4	NAG	A	671	14/15	0.95	0.13	-0.98	63,65,67,69	0
7	NAG	B	671	14/15	0.95	0.12	-1.04	66,68,71,74	0
7	NAG	B	672	14/15	0.92	0.20	-	75,78,83,86	0
4	NAG	A	682	14/15	0.87	0.41	-	94,96,99,100	0
7	BMA	B	673	11/12	0.94	0.24	-	88,91,94,96	0
4	NAG	A	672	14/15	0.90	0.30	-	71,73,76,76	0
7	BMA	B	674	11/12	0.88	0.21	-	96,99,103,105	0
3	NDG	A	662	14/15	0.91	0.20	-	81,82,85,86	0
7	MAN	B	675	11/12	0.90	0.37	-	104,107,111,112	0
4	NAG	B	682	14/15	0.83	0.30	-	109,112,115,115	0

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	BOG	A	750	20/20	0.85	0.25	2.38	119,119,119,119	0
5	BOG	A	751	20/20	0.95	0.16	1.01	67,68,68,69	0
2	HEM	A	601	43/43	0.90	0.21	1.00	86,91,96,97	0
5	BOG	B	1751	20/20	0.94	0.15	0.01	73,73,74,74	0
6	FLP	B	1701	18/18	0.98	0.16	-0.04	54,54,54,54	0
2	HEM	B	601	43/43	0.93	0.17	-0.22	75,80,85,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	FLP	A	701	18/18	0.96	0.15	-0.78	62,63,63,63	0
5	BOG	B	1750	20/20	0.84	0.26	-	73,73,75,75	0
5	BOG	A	752	13/20	0.89	0.26	-	96,96,97,97	0

6.5 Other polymers (i)

There are no such residues in this entry.