



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:54 PM GMT

PDB ID : 1HT5  
Title : THE 2.75 ANGSTROM RESOLUTION MODEL OF OVINE COX-1 COM-  
PLEXED WITH METHYL ESTER FLURBIPROFEN  
Authors : Selinsky, B.S.; Gupta, K.; Sharkey, C.T.; Loll, P.J.  
Deposited on : 2000-12-28  
Resolution : 2.75 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.

---

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

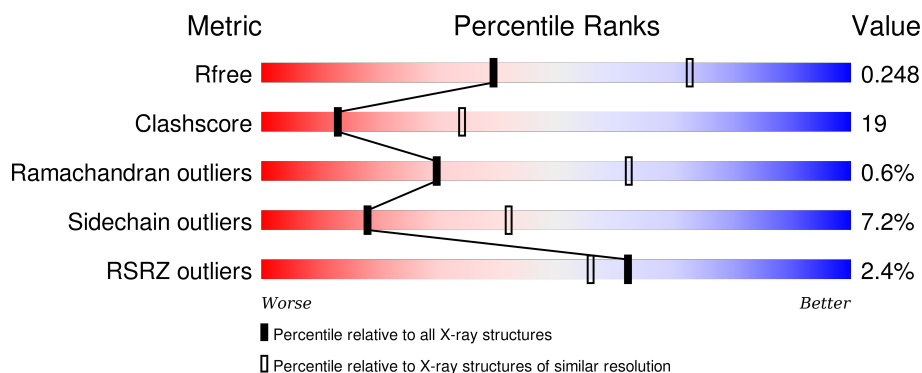
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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>3%</div> <div>62%</div> <div>33%</div> <div>5%</div> </div>
1	B	551	<div> <div>2%</div> <div>65%</div> <div>32%</div> <div>.</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	BOG	A	1802	-	-	-	X
2	BOG	B	2801	-	-	-	X
2	BOG	B	2802	-	-	-	X
3	NAG	A	1671	-	-	X	-
3	NAG	A	1681	-	-	-	X
3	NAG	B	2681	-	-	-	X
5	FL2	A	1701	-	-	-	X
5	FL2	B	2701	-	-	X	X

## 2 Entry composition [i](#)

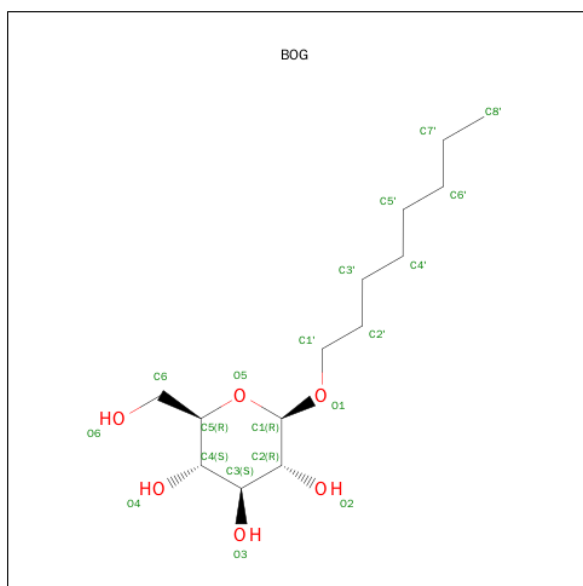
There are 6 unique types of molecules in this entry. The entry contains 9428 atoms, of which 0 are hydrogens and 0 are deuteriums.

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



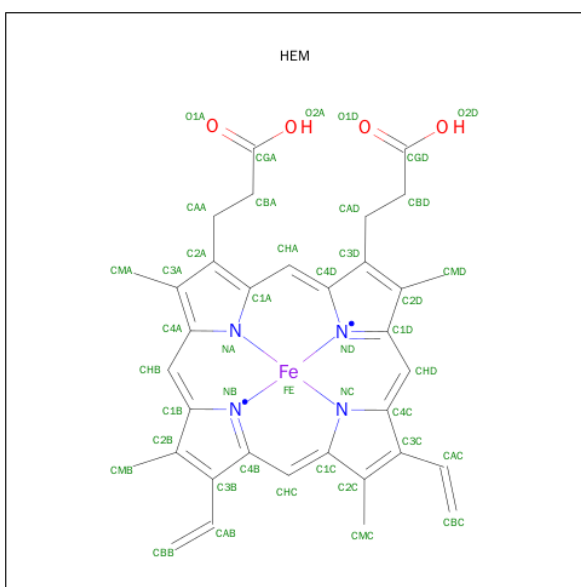
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



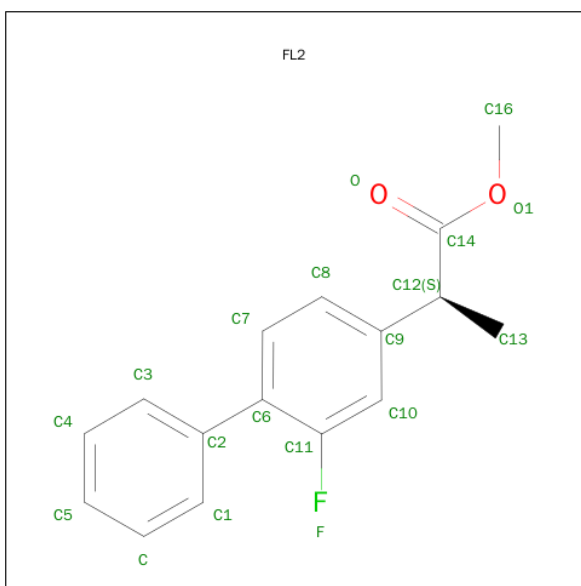
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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 METHYL ESTER (three-letter code: FL2) (formula:  $C_{16}H_{15}FO_2$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O	0	0
			19	16	1	2		
5	B	1	Total	C	F	O	0	0
			19	16	1	2		

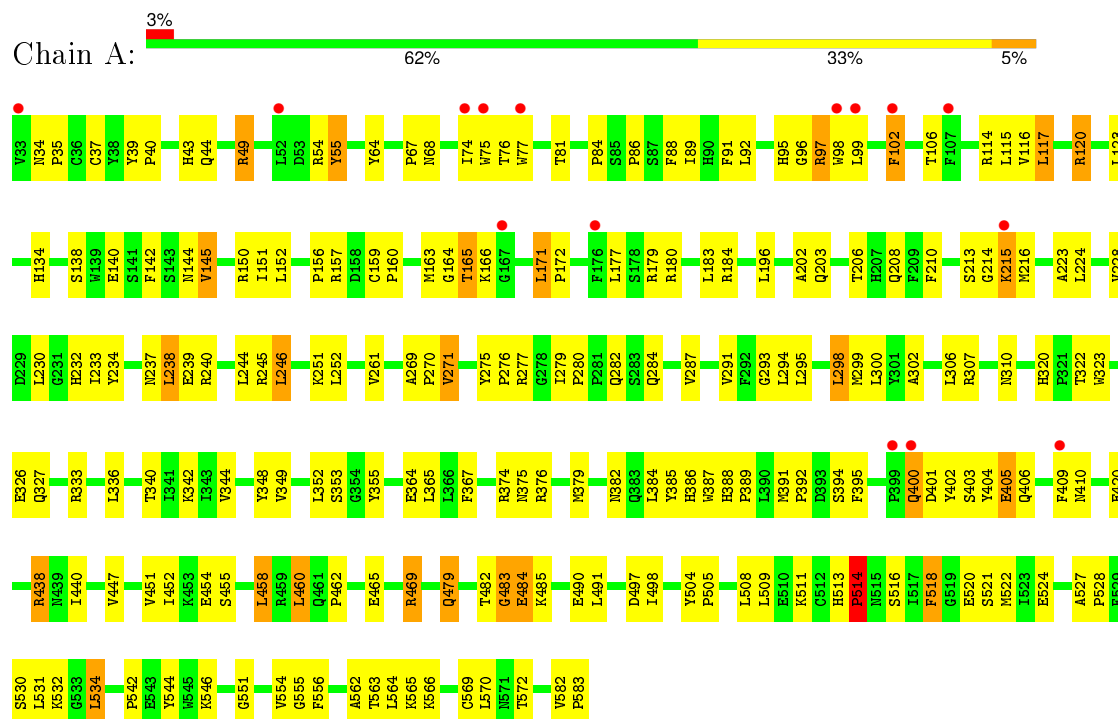
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	79	Total 79	O 79	0	0
6	B	71	Total 71	O 71	0	0

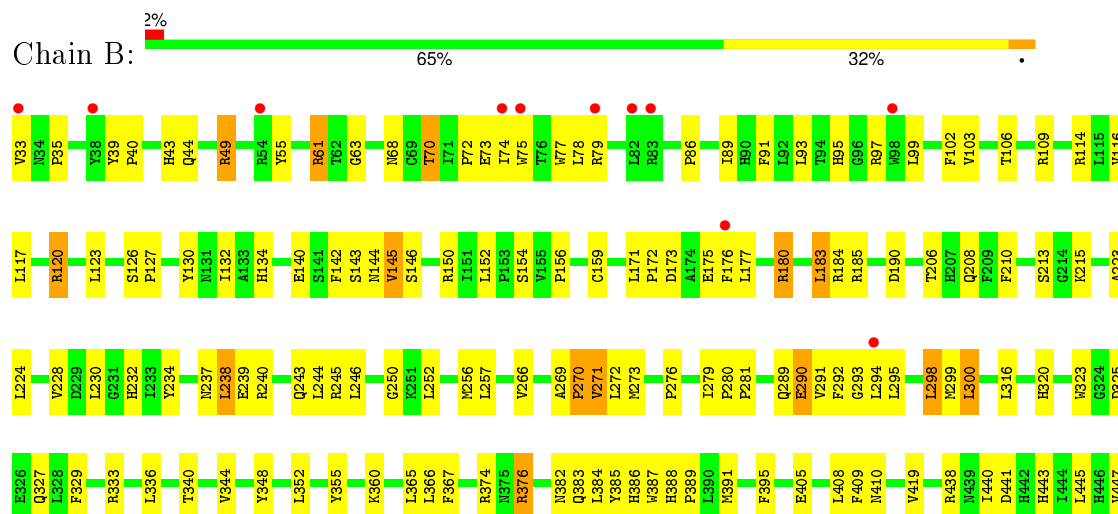
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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.

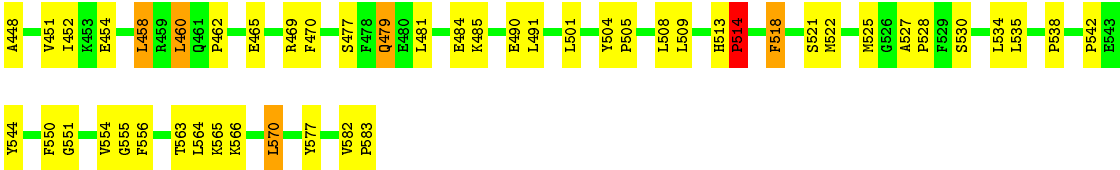
#### • Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



#### • 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, $\alpha$ , $\beta$ , $\gamma$	98.89Å 209.45Å 223.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.89 – 2.75 50.89 – 2.70	Depositor EDS
% Data completeness (in resolution range)	88.2 (50.89-2.75) 88.3 (50.89-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.69Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.223 , 0.252 0.215 , 0.248	Depositor DCC
$R_{free}$ test set	5438 reflections (11.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 57793 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, FL2, 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	0.41	0/4615	0.63	0/6264
1	B	0.39	0/4615	0.64	0/6264
All	All	0.40	0/9230	0.64	0/12528

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	186	0
1	B	4477	0	4386	170	0
2	A	20	0	28	8	0
2	B	40	0	56	6	0
3	A	70	0	65	11	0
3	B	70	0	65	8	0
4	A	43	0	30	5	0
4	B	43	0	30	6	0
5	A	19	0	15	4	0
5	B	19	0	15	7	0
6	A	79	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	71	0	0	0	0
All	All	9428	0	9076	350	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 19.

All (350) 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:144:ASN:HD21	3:B:2671:NAG:C1	1.80	0.94
1:B:410:ASN:HD21	3:B:2681:NAG:C1	1.81	0.94
1:A:391:MET:HG3	4:A:601:HEM:HAB	1.47	0.92
1:B:185:ARG:HH21	1:B:438:ARG:NH1	1.70	0.90
1:A:410:ASN:HD21	3:A:1681:NAG:C1	1.85	0.90
1:B:291:VAL:HG13	1:B:294:LEU:HD12	1.54	0.88
1:A:144:ASN:HD21	3:A:1671:NAG:C1	1.87	0.87
1:A:400:GLN:HE21	1:A:401:ASP:N	1.74	0.85
1:B:180:ARG:HD3	1:B:490:GLU:OE2	1.77	0.83
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.12	0.83
1:A:120:ARG:HG2	5:A:1701:FL2:H161	1.59	0.83
1:B:49:ARG:HH11	1:B:49:ARG:HG3	1.46	0.81
1:B:185:ARG:HH21	1:B:438:ARG:HH11	1.30	0.80
1:B:563:THR:HG22	1:B:565:LYS:H	1.48	0.78
1:B:295:LEU:HD12	1:B:298:LEU:HD22	1.63	0.78
1:B:185:ARG:NH2	1:B:438:ARG:HH11	1.82	0.77
1:B:144:ASN:ND2	3:B:2671:NAG:C1	2.48	0.77
1:A:400:GLN:HE21	1:A:401:ASP:H	1.32	0.77
1:B:295:LEU:HD11	4:B:601:HEM:HBB2	1.65	0.76
1:B:454:GLU:HG2	1:B:458:LEU:HD22	1.68	0.75
1:A:144:ASN:ND2	3:A:1671:NAG:C1	2.49	0.75
1:A:400:GLN:NE2	1:A:401:ASP:H	1.85	0.74
1:B:208:GLN:NE2	1:B:230:LEU:H	1.84	0.74
1:B:150:ARG:HD3	1:B:152:LEU:O	1.87	0.73
1:A:140:GLU:CD	1:A:144:ASN:HD22	1.91	0.73
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.71	0.71
1:B:243:GLN:HG3	1:B:270:PRO:HD2	1.72	0.71
1:A:563:THR:HG22	1:A:565:LYS:H	1.55	0.71
1:A:89:ILE:HD12	2:A:1802:BOG:H62	1.73	0.71
1:A:563:THR:HG22	1:A:565:LYS:N	2.06	0.70
1:A:208:GLN:NE2	1:A:230:LEU:H	1.89	0.70
1:B:272:LEU:HD13	1:B:273:MET:N	2.07	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.74	0.69
1:A:165:THR:HG22	1:A:166:LYS:HD3	1.74	0.69
1:A:462:PRO:HG2	1:A:465:GLU:HG2	1.74	0.69
1:A:374:ARG:NH1	1:B:374:ARG:HB3	2.08	0.69
1:B:237:ASN:ND2	1:B:240:ARG:H	1.92	0.68
1:A:295:LEU:HD11	4:A:601:HEM:HBB2	1.74	0.68
1:B:120:ARG:HG2	5:B:2701:FL2:H161	1.74	0.68
1:B:295:LEU:CD1	4:B:601:HEM:HBB2	2.24	0.67
1:A:114:ARG:HD3	1:A:365:LEU:O	1.95	0.66
1:B:563:THR:HG22	1:B:565:LYS:N	2.10	0.66
1:B:116:VAL:HG13	5:B:2701:FL2:H162	1.77	0.66
1:A:91:PHE:O	1:A:95:HIS:HD2	1.78	0.66
1:A:447:VAL:O	1:A:451:VAL:HG23	1.96	0.66
1:B:185:ARG:HH11	1:B:185:ARG:HG2	1.61	0.65
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.78	0.65
1:A:280:PRO:HB2	1:A:282:GLN:OE1	1.96	0.65
1:A:344:VAL:O	1:A:348:TYR:HB3	1.97	0.65
1:B:120:ARG:NH1	2:B:2802:BOG:H1	2.12	0.64
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.79	0.64
1:A:237:ASN:ND2	1:A:239:GLU:HG2	2.13	0.64
1:A:320:HIS:HD2	1:B:49:ARG:O	1.81	0.64
1:A:482:THR:O	1:A:484:GLU:N	2.31	0.63
1:A:150:ARG:HD3	1:A:152:LEU:O	1.98	0.63
1:A:208:GLN:HE21	1:A:230:LEU:H	1.47	0.63
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.81	0.63
1:A:513:HIS:NE2	1:A:520:GLU:HB3	2.14	0.63
1:B:123:LEU:HD23	1:B:470:PHE:HD1	1.64	0.62
1:A:49:ARG:HG3	1:A:49:ARG:HH11	1.63	0.62
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.81	0.62
1:B:86:PRO:HG3	2:B:2802:BOG:H61	1.82	0.62
1:A:483:GLY:H	1:A:511:LYS:HB3	1.65	0.62
1:B:447:VAL:O	1:B:451:VAL:HG23	2.00	0.61
1:B:410:ASN:ND2	3:B:2681:NAG:C1	2.60	0.61
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.36	0.61
1:A:67:PRO:C	1:A:68:ASN:HD22	2.02	0.61
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.12	0.61
1:B:116:VAL:O	1:B:120:ARG:HB2	2.00	0.61
1:B:554:VAL:HG13	1:B:555:GLY:N	2.16	0.61
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.31	0.61
1:B:213:SER:OG	1:B:215:LYS:HG2	2.01	0.61
1:B:387:TRP:HB2	4:B:601:HEM:HAC	1.83	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:ASN:ND2	3:A:1681:NAG:C1	2.61	0.60
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.82	0.60
1:A:180:ARG:O	1:A:438:ARG:NH1	2.33	0.60
1:B:120:ARG:HE	5:B:2701:FL2:C16	2.15	0.60
1:A:116:VAL:O	1:A:120:ARG:HB2	2.02	0.60
1:B:276:PRO:HD2	1:B:279:ILE:HD12	1.84	0.60
1:B:566:LYS:O	1:B:570:LEU:HB2	2.02	0.59
1:B:185:ARG:CZ	1:B:438:ARG:HD3	2.32	0.59
1:B:237:ASN:ND2	1:B:239:GLU:HG2	2.17	0.59
1:A:387:TRP:HB2	4:A:601:HEM:HAC	1.83	0.59
1:B:293:GLY:HA2	1:B:299:MET:HE2	1.83	0.59
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.65	0.58
1:A:230:LEU:HG	1:A:233:ILE:HD12	1.86	0.58
1:B:120:ARG:HE	5:B:2701:FL2:H161	1.69	0.58
1:A:382:ASN:OD1	1:A:386:HIS:HE1	1.87	0.58
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.43	0.58
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.37	0.58
1:B:294:LEU:O	1:B:295:LEU:HG	2.04	0.58
1:A:86:PRO:HG3	2:A:1802:BOG:H61	1.84	0.57
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.39	0.57
1:A:294:LEU:O	1:A:295:LEU:HG	2.04	0.57
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.34	0.57
1:B:185:ARG:NE	1:B:438:ARG:HD3	2.19	0.57
1:B:116:VAL:CG1	5:B:2701:FL2:H162	2.34	0.57
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.40	0.57
1:B:89:ILE:HD12	2:B:2802:BOG:H62	1.87	0.57
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.35	0.56
1:A:102:PHE:O	1:A:106:THR:HG23	2.05	0.56
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.86	0.56
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.41	0.56
1:A:49:ARG:O	1:B:320:HIS:HD2	1.89	0.56
1:A:295:LEU:HD11	4:A:601:HEM:CBB	2.35	0.56
1:A:379:MET:SD	1:A:458:LEU:HG	2.46	0.55
1:A:183:LEU:HD13	1:A:184:ARG:O	2.07	0.55
1:B:366:LEU:HD12	1:B:535:LEU:HD12	1.86	0.55
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.41	0.55
1:A:120:ARG:NH1	2:A:1802:BOG:H1	2.21	0.55
1:B:132:ILE:HD13	1:B:458:LEU:HD12	1.89	0.55
1:B:462:PRO:HG2	1:B:465:GLU:HG2	1.89	0.55
1:A:306:LEU:HD23	1:A:306:LEU:C	2.26	0.55
1:B:77:TRP:CZ2	2:B:2801:BOG:H7'2	2.41	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:HE3	1:B:395:PHE:HE2	1.71	0.54
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.43	0.54
1:A:524:GLU:OE1	2:A:1802:BOG:H5	2.08	0.54
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.23	0.54
1:A:504:TYR:OH	1:A:508:LEU:HD11	2.08	0.54
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.90	0.54
1:A:388:HIS:N	1:A:389:PRO:CD	2.71	0.54
1:A:240:ARG:NH1	1:A:271:VAL:HG13	2.22	0.53
1:A:563:THR:HB	1:A:566:LYS:HG3	1.89	0.53
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.44	0.53
1:A:374:ARG:HH12	1:B:374:ARG:HB3	1.71	0.53
1:A:554:VAL:HG13	1:A:555:GLY:N	2.23	0.53
1:A:179:ARG:HG2	1:A:179:ARG:HH11	1.74	0.52
1:A:352:LEU:HD11	1:A:387:TRP:HH2	1.74	0.52
1:A:306:LEU:HD23	1:A:306:LEU:O	2.09	0.52
1:A:391:MET:HE1	1:A:395:PHE:HE2	1.75	0.52
1:B:550:PHE:O	1:B:555:GLY:HA3	2.08	0.52
1:B:340:THR:O	1:B:344:VAL:HG23	2.08	0.52
1:A:140:GLU:OE2	1:A:144:ASN:ND2	2.42	0.52
1:B:208:GLN:NE2	1:B:228:VAL:HA	2.25	0.52
1:B:123:LEU:HD23	1:B:470:PHE:CD1	2.43	0.52
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.49	0.52
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.45	0.52
1:B:63:GLY:O	1:B:73:GLU:HG3	2.10	0.52
1:A:144:ASN:OD1	3:A:1671:NAG:C1	2.58	0.52
3:A:1671:NAG:H61	3:B:1672:NAG:HN2	1.75	0.52
1:B:293:GLY:HA2	1:B:299:MET:CE	2.40	0.52
1:B:185:ARG:NH2	1:B:438:ARG:NH1	2.43	0.51
1:B:208:GLN:HE21	1:B:230:LEU:H	1.56	0.51
1:B:477:SER:OG	1:B:479:GLN:HG2	2.10	0.51
1:A:180:ARG:HD3	1:A:490:GLU:OE2	2.10	0.51
1:A:213:SER:OG	1:A:215:LYS:HG2	2.11	0.51
1:B:114:ARG:HD3	1:B:365:LEU:O	2.09	0.51
1:B:49:ARG:NH1	1:B:49:ARG:CG	2.71	0.51
1:A:203:GLN:HA	4:A:601:HEM:HBC2	1.93	0.50
1:B:344:VAL:O	1:B:348:TYR:HB3	2.11	0.50
1:B:491:LEU:HD11	1:B:509:LEU:HD13	1.92	0.50
1:A:269:ALA:O	1:A:271:VAL:N	2.45	0.50
1:B:140:GLU:OE2	1:B:144:ASN:ND2	2.40	0.50
1:B:479:GLN:H	1:B:479:GLN:CD	2.13	0.50
1:B:300:LEU:HD21	1:B:419:VAL:HG13	1.94	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:O	1:A:469:ARG:NH2	2.45	0.50
1:B:513:HIS:HB3	1:B:514:PRO:HD2	1.93	0.50
1:B:140:GLU:CD	1:B:144:ASN:HD22	2.15	0.49
1:A:403:SER:OG	1:A:405:GLU:HG2	2.12	0.49
1:B:35:PRO:HB2	1:B:55:TYR:CD2	2.47	0.49
1:B:582:VAL:HG23	1:B:583:PRO:HD2	1.94	0.49
1:A:400:GLN:HE21	1:A:400:GLN:CA	2.25	0.49
1:A:384:LEU:HD23	1:A:384:LEU:C	2.32	0.49
1:B:49:ARG:HG3	1:B:49:ARG:NH1	2.23	0.49
1:A:291:VAL:O	1:A:291:VAL:HG12	2.12	0.49
1:A:352:LEU:HD11	1:A:387:TRP:CH2	2.48	0.49
1:B:295:LEU:HD12	1:B:298:LEU:CD2	2.36	0.49
1:A:77:TRP:CZ2	1:A:81:THR:HG21	2.48	0.49
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.95	0.48
1:A:179:ARG:HG2	1:A:179:ARG:NH1	2.28	0.48
1:A:117:LEU:HD12	1:A:531:LEU:HD13	1.95	0.48
1:B:291:VAL:O	1:B:291:VAL:HG12	2.13	0.48
1:B:150:ARG:NH1	1:B:154:SER:HA	2.27	0.48
1:B:243:GLN:OE1	1:B:243:GLN:HA	2.13	0.48
1:A:151:ILE:CG2	1:A:469:ARG:NH1	2.76	0.48
1:B:386:HIS:CE1	4:B:601:HEM:HAD2	2.47	0.48
1:A:49:ARG:CG	1:A:49:ARG:HH11	2.25	0.48
1:A:261:VAL:O	1:A:307:ARG:NH1	2.41	0.48
1:A:482:THR:C	1:A:484:GLU:H	2.17	0.48
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.49	0.48
1:A:68:ASN:N	1:A:68:ASN:HD22	2.11	0.48
1:A:35:PRO:CG	1:A:55:TYR:HB3	2.44	0.48
1:B:388:HIS:N	1:B:389:PRO:CD	2.76	0.48
1:A:88:PHE:O	1:A:91:PHE:HB3	2.13	0.48
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.95	0.48
1:A:497:ASP:OD2	1:A:498:ILE:N	2.47	0.48
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.95	0.48
1:B:70:THR:O	1:B:72:PRO:HD3	2.14	0.48
1:A:374:ARG:HB3	1:B:374:ARG:NH1	2.29	0.48
1:A:160:PRO:HD2	1:A:164:GLY:O	2.13	0.48
1:B:116:VAL:HG13	5:B:2701:FL2:C16	2.43	0.48
1:A:134:HIS:HD2	1:A:138:SER:OG	1.96	0.47
1:A:86:PRO:HA	2:A:1802:BOG:H61	1.96	0.47
1:A:214:GLY:H	1:A:215:LYS:HZ1	1.61	0.47
1:B:99:LEU:O	1:B:103:VAL:HG23	2.14	0.47
1:B:352:LEU:HD11	1:B:387:TRP:CH2	2.48	0.47

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:GLN:NE2	1:A:401:ASP:N	2.48	0.47
1:B:291:VAL:CG1	1:B:291:VAL:O	2.61	0.47
1:A:120:ARG:HE	5:A:1701:FL2:C16	2.27	0.47
1:A:120:ARG:HG2	5:A:1701:FL2:C16	2.37	0.47
1:B:240:ARG:NH1	1:B:271:VAL:HG13	2.30	0.47
1:A:513:HIS:HB3	1:A:514:PRO:HD2	1.96	0.47
1:A:77:TRP:CE2	1:A:81:THR:HG21	2.49	0.47
1:B:223:ALA:C	1:B:224:LEU:O	2.46	0.47
1:A:142:PHE:CE2	1:B:538:PRO:HG3	2.49	0.47
1:A:566:LYS:O	1:A:570:LEU:HB2	2.15	0.47
1:A:340:THR:O	1:A:344:VAL:HG23	2.15	0.47
1:A:145:VAL:HG13	1:A:145:VAL:O	2.15	0.47
1:A:180:ARG:HH21	1:A:490:GLU:CD	2.18	0.46
1:B:93:LEU:HD13	1:B:355:TYR:CE1	2.50	0.46
1:A:180:ARG:NH2	1:A:490:GLU:OE1	2.48	0.46
1:A:420:GLU:HG3	1:A:572:THR:HB	1.97	0.46
1:B:513:HIS:O	1:B:514:PRO:C	2.53	0.46
1:A:530:SER:O	1:A:534:LEU:HD22	2.15	0.46
1:B:109:ARG:NH2	1:B:360:LYS:HB2	2.31	0.46
1:B:144:ASN:HD21	3:B:2671:NAG:C2	2.29	0.46
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.81	0.46
1:A:320:HIS:CE1	1:A:551:GLY:O	2.69	0.46
1:B:74:ILE:HG23	1:B:75:TRP:N	2.31	0.46
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.51	0.46
1:A:452:ILE:O	1:A:455:SER:HB3	2.16	0.46
1:A:144:ASN:HD21	3:A:1671:NAG:C2	2.27	0.46
1:B:142:PHE:C	1:B:376:ARG:HH22	2.19	0.46
1:B:530:SER:O	1:B:534:LEU:HD22	2.16	0.46
1:A:151:ILE:HG22	1:A:469:ARG:NH1	2.30	0.46
1:B:126:SER:HA	1:B:127:PRO:C	2.35	0.46
1:A:230:LEU:HD21	1:A:336:LEU:HB3	1.98	0.46
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.56	0.45
1:B:382:ASN:OD1	1:B:386:HIS:HE1	1.98	0.45
1:A:144:ASN:CG	3:A:1671:NAG:C1	2.83	0.45
1:B:538:PRO:HB2	1:B:544:TYR:CE1	2.51	0.45
1:A:163:MET:CE	1:A:171:LEU:HD21	2.46	0.45
1:B:206:THR:HB	1:B:210:PHE:CD2	2.51	0.45
1:B:183:LEU:HD22	1:B:184:ARG:N	2.30	0.45
1:A:513:HIS:HB2	1:A:516:SER:OG	2.16	0.45
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.99	0.45
1:A:520:GLU:HG3	1:A:521:SER:N	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:HIS:O	1:B:44:GLN:HB2	2.16	0.45
1:A:479:GLN:HG3	1:A:485:LYS:HZ2	1.81	0.45
1:B:256:MET:O	1:B:257:LEU:HD23	2.17	0.45
1:A:367:PHE:CE2	1:A:542:PRO:HG3	2.52	0.45
1:B:102:PHE:O	1:B:106:THR:HG23	2.17	0.45
1:A:353:SER:HB2	1:A:355:TYR:CE2	2.52	0.45
1:A:88:PHE:O	1:A:92:LEU:HD13	2.17	0.44
1:A:367:PHE:CD2	1:A:542:PRO:HG3	2.52	0.44
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.51	0.44
1:A:400:GLN:C	1:A:400:GLN:HE21	2.19	0.44
1:B:39:TYR:N	1:B:40:PRO:CD	2.79	0.44
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.53	0.44
1:B:323:TRP:CE3	1:B:327:GLN:HG2	2.52	0.44
1:B:521:SER:O	1:B:525:MET:HB2	2.17	0.44
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.52	0.44
1:A:116:VAL:CG1	5:A:1701:FL2:H162	2.47	0.44
1:A:482:THR:C	1:A:484:GLU:N	2.71	0.44
1:A:554:VAL:HG13	1:A:555:GLY:H	1.82	0.44
1:B:266:VAL:O	1:B:266:VAL:HG12	2.17	0.44
1:A:237:ASN:HD22	1:A:239:GLU:HG2	1.83	0.44
1:B:408:LEU:HB3	1:B:409:PHE:CD1	2.53	0.44
1:B:185:ARG:NH1	1:B:185:ARG:HG2	2.32	0.44
1:B:77:TRP:CZ2	2:B:2801:BOG:H5'2	2.53	0.44
1:A:375:ASN:HD22	1:A:532:LYS:HG3	1.83	0.44
1:B:384:LEU:HG	1:B:522:MET:SD	2.58	0.43
1:A:98:TRP:CG	1:A:99:LEU:N	2.86	0.43
1:A:323:TRP:CD2	1:A:327:GLN:HG2	2.54	0.43
1:B:180:ARG:O	1:B:438:ARG:NH1	2.51	0.43
1:B:185:ARG:NH2	1:B:438:ARG:HD3	2.33	0.43
1:B:237:ASN:HD21	1:B:240:ARG:H	1.66	0.43
1:A:569:CYS:HA	1:A:572:THR:OG1	2.18	0.43
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.91	0.43
1:B:130:TYR:HB3	1:B:134:HIS:O	2.18	0.43
1:A:159:CYS:HB3	1:A:164:GLY:O	2.18	0.43
1:B:74:ILE:HG23	1:B:75:TRP:CD1	2.53	0.43
1:B:91:PHE:O	1:B:95:HIS:HD2	2.01	0.43
1:A:322:THR:OG1	1:B:49:ARG:HG2	2.18	0.43
1:A:367:PHE:HE1	1:B:61:ARG:HH21	1.65	0.43
1:A:74:ILE:HG23	1:A:75:TRP:N	2.34	0.43
1:B:441:ASP:OD2	1:B:443:HIS:CD2	2.72	0.43
1:B:384:LEU:C	1:B:384:LEU:HD23	2.39	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LEU:CD2	1:B:336:LEU:HB3	2.48	0.43
1:A:275:TYR:CD2	1:A:284:GLN:HG2	2.53	0.43
1:A:245:ARG:NH1	1:A:326:GLU:OE2	2.48	0.43
1:A:202:ALA:O	1:A:206:THR:HG23	2.18	0.43
1:A:246:LEU:O	1:A:246:LEU:HD23	2.19	0.43
1:A:544:TYR:O	1:A:546:LYS:N	2.50	0.43
1:B:448:ALA:O	1:B:452:ILE:HG13	2.19	0.43
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.54	0.43
1:A:68:ASN:OD1	3:A:1661:NAG:C1	2.67	0.43
1:A:454:GLU:HG2	1:A:458:LEU:HD22	2.01	0.43
1:B:352:LEU:HD22	1:B:518:PHE:CZ	2.53	0.42
1:A:183:LEU:C	1:A:183:LEU:HD13	2.39	0.42
1:A:479:GLN:HG3	1:A:485:LYS:NZ	2.34	0.42
1:A:391:MET:HB3	1:A:404:TYR:OH	2.18	0.42
1:B:554:VAL:CG1	1:B:555:GLY:N	2.80	0.42
1:A:458:LEU:HB3	1:A:460:LEU:HD13	2.01	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE2	2.01	0.42
1:A:86:PRO:CA	2:A:1802:BOG:H61	2.49	0.42
1:B:206:THR:HB	1:B:210:PHE:HD2	1.84	0.42
1:A:54:ARG:HH11	1:A:54:ARG:HG3	1.84	0.42
1:A:96:GLY:O	1:A:97:ARG:C	2.57	0.42
1:A:287:VAL:HG11	1:A:302:ALA:HB1	2.00	0.42
1:A:43:HIS:O	1:A:44:GLN:HB2	2.20	0.42
1:A:49:ARG:CG	1:A:49:ARG:NH1	2.83	0.42
1:B:367:PHE:CZ	1:B:542:PRO:HA	2.55	0.42
1:A:394:SER:HB2	1:A:402:TYR:O	2.20	0.42
1:B:250:GLY:HA2	1:B:325:ASP:OD1	2.19	0.42
1:A:582:VAL:HG22	1:A:583:PRO:CD	2.46	0.42
1:A:206:THR:HB	1:A:210:PHE:CD2	2.55	0.42
1:B:272:LEU:HD13	1:B:272:LEU:C	2.39	0.42
1:A:295:LEU:HB2	1:A:298:LEU:HD22	2.01	0.42
3:A:1671:NAG:O4	3:B:1672:NAG:C1	2.68	0.42
1:B:504:TYR:OH	1:B:508:LEU:HD11	2.19	0.42
1:B:485:LYS:HD3	1:B:485:LYS:HA	1.90	0.41
1:A:39:TYR:N	1:A:40:PRO:CD	2.83	0.41
1:B:172:PRO:HB2	1:B:177:LEU:HD22	2.02	0.41
1:B:144:ASN:OD1	3:B:2671:NAG:C1	2.68	0.41
1:B:79:ARG:HG2	1:B:79:ARG:HH11	1.85	0.41
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.54	0.41
1:A:196:LEU:HD21	1:A:392:PRO:HD3	2.02	0.41
1:B:210:PHE:HB3	4:B:601:HEM:HBD1	2.02	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:LEU:HD22	1:B:501:LEU:CD2	2.50	0.41
1:A:251:LYS:HB3	1:A:310:ASN:OD1	2.21	0.41
1:B:320:HIS:HE1	1:B:551:GLY:O	2.04	0.41
1:B:145:VAL:HG13	1:B:145:VAL:O	2.19	0.41
1:B:173:ASP:OD2	1:B:175:GLU:HB3	2.21	0.41
1:B:176:PHE:CZ	1:B:180:ARG:HG3	2.56	0.41
1:B:269:ALA:O	1:B:271:VAL:N	2.52	0.41
1:A:344:VAL:O	1:A:349:VAL:HG23	2.21	0.41
1:B:238:LEU:HD23	1:B:238:LEU:HA	1.88	0.41
1:B:292:PHE:CD1	1:B:298:LEU:HG	2.56	0.41
1:B:240:ARG:NH1	1:B:290:GLU:HG3	2.36	0.41
1:B:527:ALA:HB1	5:B:2701:FL2:H163	2.02	0.41
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.56	0.41
1:B:68:ASN:N	1:B:68:ASN:HD22	2.18	0.41
1:A:115:LEU:HD23	2:A:1802:BOG:H5'1	2.03	0.40
1:A:213:SER:HB3	1:A:216:MET:HB2	2.02	0.40
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.80	0.40
1:B:290:GLU:CD	1:B:290:GLU:H	2.25	0.40
1:A:91:PHE:O	1:A:95:HIS:CD2	2.65	0.40
1:A:306:LEU:CD2	1:A:306:LEU:C	2.90	0.40
1:B:383:GLN:HG3	1:B:460:LEU:HD21	2.04	0.40
1:A:406:GLN:HA	3:A:1681:NAG:C8	2.52	0.40
1:A:320:HIS:HE1	1:A:551:GLY:O	2.04	0.40
1:B:116:VAL:HG22	2:B:2802:BOG:H2'1	2.02	0.40
1:A:223:ALA:O	1:A:224:LEU:C	2.59	0.40
1:B:445:LEU:HG	1:B:445:LEU:O	2.22	0.40
1:B:245:ARG:HD2	1:B:329:PHE:CZ	2.57	0.40
1:A:86:PRO:CG	2:A:1802:BOG:H61	2.50	0.40
1:A:206:THR:C	1:A:208:GLN:H	2.25	0.40
1:B:77:TRP:CE3	1:B:78:LEU:HD23	2.56	0.40
1:A:513:HIS:O	1:A:514:PRO:C	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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%)	509 (93%)	36 (7%)	4 (1%)	26	59
1	B	549/551 (100%)	504 (92%)	42 (8%)	3 (0%)	34	67
All	All	1098/1102 (100%)	1013 (92%)	78 (7%)	7 (1%)	30	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	A	483	GLY
1	A	270	PRO
1	B	290	GLU
1	A	157	ARG
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	486/486 (100%)	452 (93%)	34 (7%)	19	44
1	B	486/486 (100%)	450 (93%)	36 (7%)	17	40
All	All	972/972 (100%)	902 (93%)	70 (7%)	18	42

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	55	TYR
1	A	97	ARG
1	A	102	PHE
1	A	117	LEU
1	A	120	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	145	VAL
1	A	165	THR
1	A	171	LEU
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	271	VAL
1	A	277	ARG
1	A	298	LEU
1	A	300	LEU
1	A	376	ARG
1	A	385	TYR
1	A	400	GLN
1	A	405	GLU
1	A	438	ARG
1	A	458	LEU
1	A	460	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	564	LEU
1	B	33	VAL
1	B	49	ARG
1	B	61	ARG
1	B	70	THR
1	B	97	ARG
1	B	117	LEU
1	B	120	ARG
1	B	143	SER
1	B	145	VAL
1	B	146	SER
1	B	171	LEU
1	B	180	ARG
1	B	183	LEU
1	B	190	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
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	556	PHE
1	B	564	LEU
1	B	570	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	95	HIS
1	A	134	HIS
1	A	144	ASN
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	320	HIS
1	A	370	GLN
1	A	375	ASN
1	A	386	HIS
1	A	400	GLN
1	A	443	HIS
1	B	68	ASN
1	B	95	HIS
1	B	134	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	320	HIS
1	B	375	ASN
1	B	386	HIS
1	B	400	GLN
1	B	410	ASN
1	B	442	HIS
1	B	443	HIS
1	B	479	GLN
1	B	557	ASN

### 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](#)

17 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	$\# Z  > 2$
3	NAG	A	1661	-	14,14,15	1.27	2 (14%)	15,19,21	1.05	1 (6%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	1662	-	14,14,15	1.56	4 (28%)	15,19,21	1.04	1 (6%)
3	NAG	A	1671	-	14,14,15	1.13	1 (7%)	15,19,21	0.86	1 (6%)
3	NAG	A	1681	-	14,14,15	1.60	3 (21%)	15,19,21	0.93	0
5	FL2	A	1701	-	20,20,20	3.09	12 (60%)	27,27,27	2.64	4 (14%)
2	BOG	A	1802	-	20,20,20	1.51	4 (20%)	25,25,25	0.96	2 (8%)
3	NAG	A	2672	-	14,14,15	1.76	6 (42%)	15,19,21	1.15	1 (6%)
4	HEM	A	601	1	30,50,50	2.38	9 (30%)	24,82,82	2.66	10 (41%)
3	NAG	B	1672	-	14,14,15	1.43	3 (21%)	15,19,21	1.15	1 (6%)
3	NAG	B	2661	-	14,14,15	1.33	2 (14%)	15,19,21	1.06	1 (6%)
3	NAG	B	2662	-	14,14,15	1.60	5 (35%)	15,19,21	1.10	1 (6%)
3	NAG	B	2671	-	14,14,15	1.03	1 (7%)	15,19,21	0.94	1 (6%)
3	NAG	B	2681	-	14,14,15	1.48	3 (21%)	15,19,21	1.03	1 (6%)
5	FL2	B	2701	-	20,20,20	3.14	14 (70%)	27,27,27	2.65	4 (14%)
2	BOG	B	2801	-	20,20,20	1.66	6 (30%)	25,25,25	1.07	1 (4%)
2	BOG	B	2802	-	20,20,20	1.47	4 (20%)	25,25,25	0.97	2 (8%)
4	HEM	B	601	1	30,50,50	2.20	7 (23%)	24,82,82	2.79	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
3	NAG	A	1661	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1662	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1671	-	-	0/6/23/26	0/1/1/1
3	NAG	A	1681	-	-	0/6/23/26	0/1/1/1
5	FL2	A	1701	-	-	1/14/14/14	0/2/2/2
2	BOG	A	1802	-	-	0/11/31/31	0/1/1/1
3	NAG	A	2672	-	-	0/6/23/26	0/1/1/1
4	HEM	A	601	1	-	0/10/54/54	0/0/8/8
3	NAG	B	1672	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2661	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2662	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2671	-	-	0/6/23/26	0/1/1/1
3	NAG	B	2681	-	-	0/6/23/26	0/1/1/1
5	FL2	B	2701	-	-	1/14/14/14	0/2/2/2
2	BOG	B	2801	-	-	0/11/31/31	0/1/1/1
2	BOG	B	2802	-	-	0/11/31/31	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	B	601	1	-	0/10/54/54	0/0/8/8

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C3D-C4D	-5.87	1.44	1.51
4	B	601	HEM	C2D-C3D	-5.86	1.36	1.54
4	A	601	HEM	C2D-C3D	-5.65	1.37	1.54
4	A	601	HEM	C3B-C4B	-4.66	1.47	1.51
4	B	601	HEM	C3D-C4D	-4.65	1.45	1.51
4	B	601	HEM	C3B-C4B	-4.10	1.48	1.51
4	A	601	HEM	C2C-C1C	-3.20	1.46	1.52
4	B	601	HEM	C2C-C1C	-3.02	1.46	1.52
2	A	1802	BOG	C4-C5	-2.81	1.47	1.53
2	B	2802	BOG	C4-C5	-2.61	1.47	1.53
2	B	2801	BOG	C4-C5	-2.44	1.47	1.53
2	B	2801	BOG	C3'-C2'	-2.37	1.37	1.51
2	B	2802	BOG	C3'-C2'	-2.26	1.38	1.51
4	A	601	HEM	C2B-C1B	-2.24	1.44	1.51
2	A	1802	BOG	C3'-C2'	-2.22	1.38	1.51
4	B	601	HEM	C2B-C1B	-2.18	1.44	1.51
3	B	2662	NAG	C4-C3	2.02	1.57	1.52
5	A	1701	FL2	C9-C12	2.02	1.55	1.52
3	A	1662	NAG	O5-C5	2.07	1.48	1.43
5	B	2701	FL2	C10-C11	2.09	1.41	1.37
3	B	1672	NAG	C4-C3	2.11	1.57	1.52
3	B	2662	NAG	C4-C5	2.11	1.57	1.53
4	A	601	HEM	C4C-NC	2.13	1.38	1.36
2	B	2801	BOG	C3-C2	2.16	1.58	1.52
3	A	1662	NAG	C1-C2	2.18	1.55	1.52
5	B	2701	FL2	C10-C9	2.18	1.42	1.39
5	A	1701	FL2	C12-C14	2.22	1.55	1.52
2	B	2801	BOG	C4-C3	2.26	1.58	1.52
3	B	1672	NAG	C4-C5	2.26	1.57	1.53
3	A	2672	NAG	C4-C5	2.27	1.57	1.53
3	B	2661	NAG	C4-C5	2.28	1.57	1.53
3	B	2662	NAG	C1-C2	2.29	1.55	1.52
3	B	2671	NAG	C3-C2	2.30	1.57	1.52
3	A	1661	NAG	C4-C5	2.30	1.58	1.53
3	A	2672	NAG	C4-C3	2.31	1.58	1.52
3	B	2681	NAG	C3-C2	2.32	1.57	1.52
3	B	2662	NAG	O5-C5	2.35	1.48	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1662	NAG	C4-C5	2.36	1.58	1.53
3	A	2672	NAG	C2-N2	2.36	1.50	1.46
5	B	2701	FL2	C12-C14	2.38	1.55	1.52
3	A	2672	NAG	O5-C5	2.39	1.48	1.43
3	A	2672	NAG	C3-C2	2.46	1.58	1.52
2	A	1802	BOG	O5-C5	2.48	1.50	1.44
3	B	1672	NAG	C3-C2	2.49	1.58	1.52
5	B	2701	FL2	C5-C4	2.51	1.44	1.38
3	B	2681	NAG	O5-C5	2.53	1.49	1.43
5	A	1701	FL2	C5-C4	2.55	1.44	1.38
3	A	1681	NAG	C3-C2	2.68	1.58	1.52
5	B	2701	FL2	O-C14	2.68	1.27	1.21
3	A	1671	NAG	C4-C5	2.70	1.58	1.53
3	B	2661	NAG	C3-C2	2.72	1.58	1.52
3	A	1681	NAG	C4-C5	2.72	1.58	1.53
3	A	1661	NAG	C3-C2	2.72	1.58	1.52
2	B	2802	BOG	O5-C5	2.80	1.51	1.44
5	B	2701	FL2	C9-C12	2.83	1.57	1.52
3	B	2681	NAG	C4-C5	2.84	1.59	1.53
5	A	1701	FL2	O-C14	2.86	1.28	1.21
2	B	2801	BOG	O5-C5	2.87	1.51	1.44
5	A	1701	FL2	C3-C2	2.91	1.45	1.39
3	A	1681	NAG	O5-C5	2.95	1.49	1.43
5	B	2701	FL2	C3-C2	2.96	1.45	1.39
5	A	1701	FL2	C-C1	2.97	1.45	1.38
3	A	1662	NAG	C3-C2	2.99	1.59	1.52
3	B	2662	NAG	C3-C2	3.14	1.59	1.52
4	A	601	HEM	C1C-NC	3.14	1.39	1.36
2	B	2802	BOG	O5-C1	3.17	1.50	1.41
3	A	2672	NAG	C1-C2	3.21	1.56	1.52
2	A	1802	BOG	O5-C1	3.25	1.50	1.41
5	B	2701	FL2	C4-C3	3.30	1.45	1.38
5	B	2701	FL2	C-C1	3.30	1.45	1.38
5	A	1701	FL2	C4-C3	3.35	1.45	1.38
2	B	2801	BOG	O5-C1	3.69	1.51	1.41
5	B	2701	FL2	C8-C7	3.74	1.45	1.38
4	B	601	HEM	CBB-CAB	3.88	1.51	1.29
4	A	601	HEM	CBC-CAC	3.90	1.51	1.29
5	A	1701	FL2	C8-C7	3.95	1.45	1.38
4	A	601	HEM	CBB-CAB	4.02	1.52	1.29
4	B	601	HEM	CBC-CAC	4.03	1.52	1.29
5	B	2701	FL2	C1-C2	4.12	1.48	1.39

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1701	FL2	C1-C2	4.43	1.48	1.39
5	B	2701	FL2	C8-C9	4.94	1.47	1.39
5	B	2701	FL2	C7-C6	5.17	1.48	1.39
5	A	1701	FL2	C8-C9	5.17	1.47	1.39
5	A	1701	FL2	C7-C6	5.26	1.48	1.39
5	A	1701	FL2	C6-C11	5.82	1.46	1.38
5	B	2701	FL2	C6-C11	6.27	1.47	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	601	HEM	C3B-CAB-CBB	-6.70	114.18	124.46
4	A	601	HEM	C3B-CAB-CBB	-5.18	116.52	124.46
4	A	601	HEM	C3C-CAC-CBC	-4.09	118.19	124.46
5	A	1701	FL2	O-C14-C12	-3.95	109.95	123.91
5	B	2701	FL2	O-C14-C12	-3.93	110.03	123.91
4	B	601	HEM	C3C-CAC-CBC	-3.62	118.90	124.46
4	B	601	HEM	CBA-CAA-C2A	-3.25	106.70	112.53
3	A	2672	NAG	O7-C7-C8	-2.61	117.27	122.06
3	B	1672	NAG	O7-C7-C8	-2.46	117.54	122.06
3	B	2662	NAG	O7-C7-C8	-2.31	117.82	122.06
3	A	1662	NAG	O7-C7-C8	-2.20	118.02	122.06
3	A	1671	NAG	C4-C3-C2	-2.16	107.87	111.23
3	B	2661	NAG	O7-C7-C8	-2.10	118.20	122.06
4	A	601	HEM	CBA-CAA-C2A	-2.06	108.83	112.53
3	B	2671	NAG	O7-C7-C8	-2.05	118.30	122.06
3	B	2681	NAG	O7-C7-C8	-2.04	118.31	122.06
3	A	1661	NAG	O7-C7-C8	-2.01	118.37	122.06
2	A	1802	BOG	C1'-O1-C1	2.14	117.68	113.94
4	A	601	HEM	CAA-CBA-CGA	2.19	116.76	112.75
2	B	2802	BOG	O1-C1-C2	2.20	110.82	108.04
4	B	601	HEM	CAA-CBA-CGA	2.40	117.14	112.75
5	A	1701	FL2	C16-O1-C14	2.66	122.23	115.99
5	B	2701	FL2	C16-O1-C14	2.67	122.25	115.99
4	A	601	HEM	CMD-C2D-C3D	3.14	128.24	114.35
4	B	601	HEM	CMD-C2D-C3D	3.26	128.78	114.35
4	B	601	HEM	C2D-C3D-C4D	3.35	107.17	101.50
4	A	601	HEM	CAD-C3D-C4D	3.37	124.34	112.47
4	A	601	HEM	C2D-C3D-C4D	3.45	107.35	101.50
2	A	1802	BOG	O1-C1-C2	3.50	112.46	108.04
2	B	2802	BOG	C1'-O1-C1	3.55	120.15	113.94
4	B	601	HEM	CAD-C3D-C4D	3.60	125.17	112.47

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2701	FL2	C13-C12-C14	3.65	118.90	111.36
5	A	1701	FL2	C13-C12-C14	3.82	119.27	111.36
2	B	2801	BOG	C1'-O1-C1	4.19	121.26	113.94
4	B	601	HEM	CMC-C2C-C3C	4.67	128.18	116.53
4	A	601	HEM	CMC-C2C-C3C	4.68	128.21	116.53
4	B	601	HEM	CMB-C2B-C3B	4.79	128.49	116.53
4	B	601	HEM	CAD-C3D-C2D	5.02	127.66	113.22
4	A	601	HEM	CMB-C2B-C3B	5.19	129.49	116.53
4	A	601	HEM	CAD-C3D-C2D	5.25	128.30	113.22
5	A	1701	FL2	O1-C14-C12	11.48	128.83	111.41
5	B	2701	FL2	O1-C14-C12	11.62	129.04	111.41

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	2701	FL2	C16-O1-C14-C12
5	A	1701	FL2	C16-O1-C14-C12

There are no ring outliers.

13 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1661	NAG	1	0
3	A	1671	NAG	7	0
3	A	1681	NAG	3	0
5	A	1701	FL2	4	0
2	A	1802	BOG	8	0
4	A	601	HEM	5	0
3	B	1672	NAG	2	0
3	B	2671	NAG	4	0
3	B	2681	NAG	2	0
5	B	2701	FL2	7	0
2	B	2801	BOG	2	0
2	B	2802	BOG	4	0
4	B	601	HEM	6	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<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%)	0.13	15 (2%) 58 51	22, 37, 53, 64	0
1	B	551/551 (100%)	0.08	11 (1%) 68 63	23, 37, 53, 64	0
All	All	1102/1102 (100%)	0.11	26 (2%) 62 56	22, 37, 53, 64	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TRP	5.5
1	B	33	VAL	4.9
1	A	102	PHE	4.2
1	A	107	PHE	3.6
1	A	33	VAL	3.2
1	A	99	LEU	3.1
1	A	52	LEU	2.9
1	B	82	LEU	2.9
1	B	74	ILE	2.7
1	B	54	ARG	2.7
1	A	215	LYS	2.7
1	A	167	GLY	2.6
1	B	75	TRP	2.5
1	B	83	ARG	2.4
1	B	79	ARG	2.3
1	A	409	PHE	2.3
1	B	294	LEU	2.2
1	B	176	PHE	2.2
1	B	98	TRP	2.2
1	A	75	TRP	2.2
1	A	77	TRP	2.2
1	A	176	PHE	2.2
1	B	38	TYR	2.1
1	A	399	PRO	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	400	GLN	2.1
1	A	74	ILE	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](#)

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
2	BOG	B	2801	20/20	0.52	1.24	8.88	37,63,68,68	0
5	FL2	B	2701	19/19	0.92	0.26	4.83	50,52,56,59	0
2	BOG	A	1802	20/20	0.83	0.37	4.72	37,54,64,67	0
5	FL2	A	1701	19/19	0.90	0.26	3.81	50,51,56,59	0
3	NAG	B	2681	14/15	0.81	0.28	3.04	31,36,42,42	0
2	BOG	B	2802	20/20	0.83	0.40	3.03	37,54,64,67	0
3	NAG	A	1681	14/15	0.80	0.30	2.39	31,36,42,42	0
3	NAG	B	2661	14/15	0.87	0.30	1.63	50,60,64,78	0
3	NAG	A	1661	14/15	0.79	0.28	1.58	50,60,64,78	0
4	HEM	A	601	43/43	0.95	0.19	0.90	36,41,53,61	0
4	HEM	B	601	43/43	0.94	0.19	0.78	36,40,55,65	0
3	NAG	A	1671	14/15	0.94	0.14	-1.18	6,16,23,25	0
3	NAG	B	2671	14/15	0.96	0.12	-2.05	6,16,23,25	0
3	NAG	A	1662	14/15	0.55	0.61	-	63,84,96,96	0
3	NAG	B	2662	14/15	0.70	0.74	-	63,84,96,96	0
3	NAG	B	1672	14/15	0.81	0.25	-	32,39,65,76	0
3	NAG	A	2672	14/15	0.80	0.26	-	32,39,65,76	0



## 6.5 Other polymers

There are no such residues in this entry.