Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:36 PM GMT

PDB ID	:	1PTH
Title	:	The Structural Basis of Aspirin Activity Inferred from the Crystal Structure of Inactivated Prostaglandin H2 Synthase
Authors	:	Loll, P.J.; Picot, D.; Garavito, R.M.
Deposited on	:	1995-04-11
Resolution	:	3.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	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 (i)

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

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		23
Ramachandran outliers		2.0%
Sidechain outliers		10.1%

Worse　　　　　　　　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
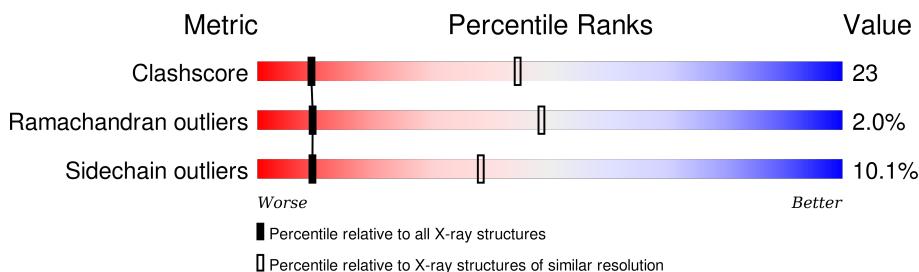
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)

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.

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	576	51%　　38%　　7%　•
1	B	576	52%　　36%　　8%　•
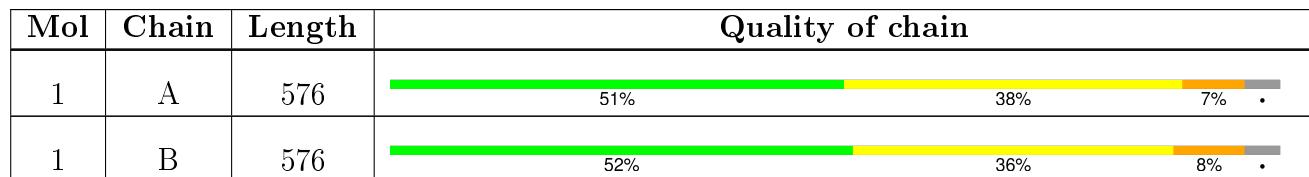
2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9221 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	Br	C	N	O	S	0	0	0
			4481	1	2905	758	789	28			
1	B	551	Total	Br	C	N	O	S	0	0	0
			4481	1	2905	758	789	28			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
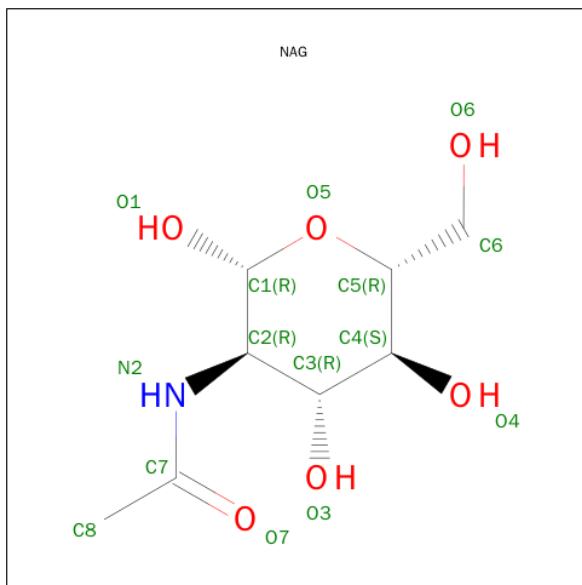
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 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		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).
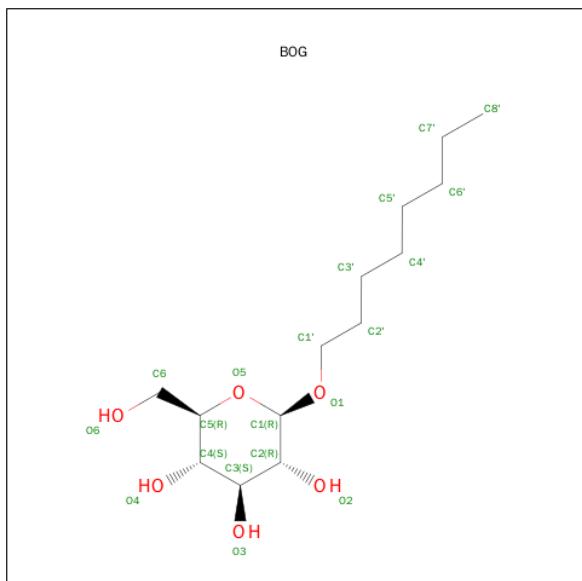
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
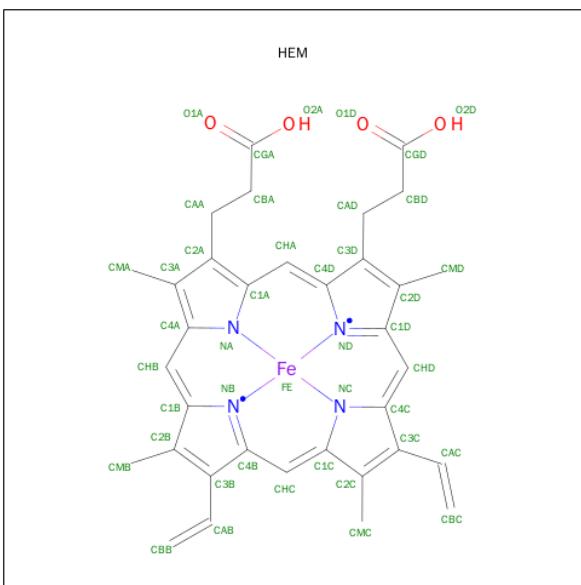
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
5	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 6 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: $C_7H_6O_3$).
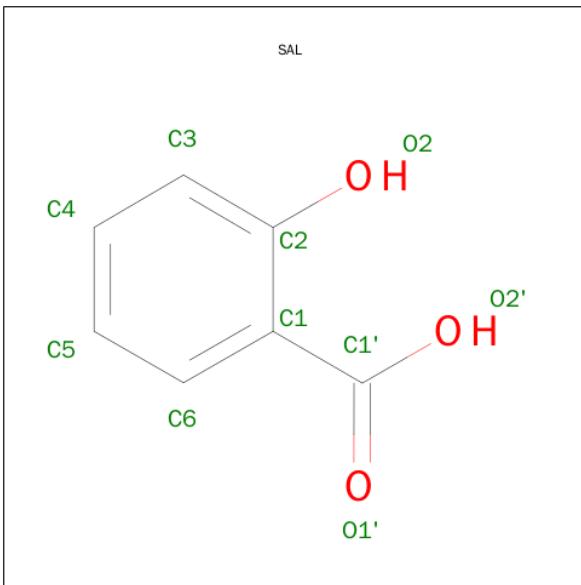
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	7	3		
6	B	1	Total	C	O	0	0
			10	7	3		

• Molecule 7 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total 1	O 1	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: PROSTAGLANDIN H2 SYNTHASE-1
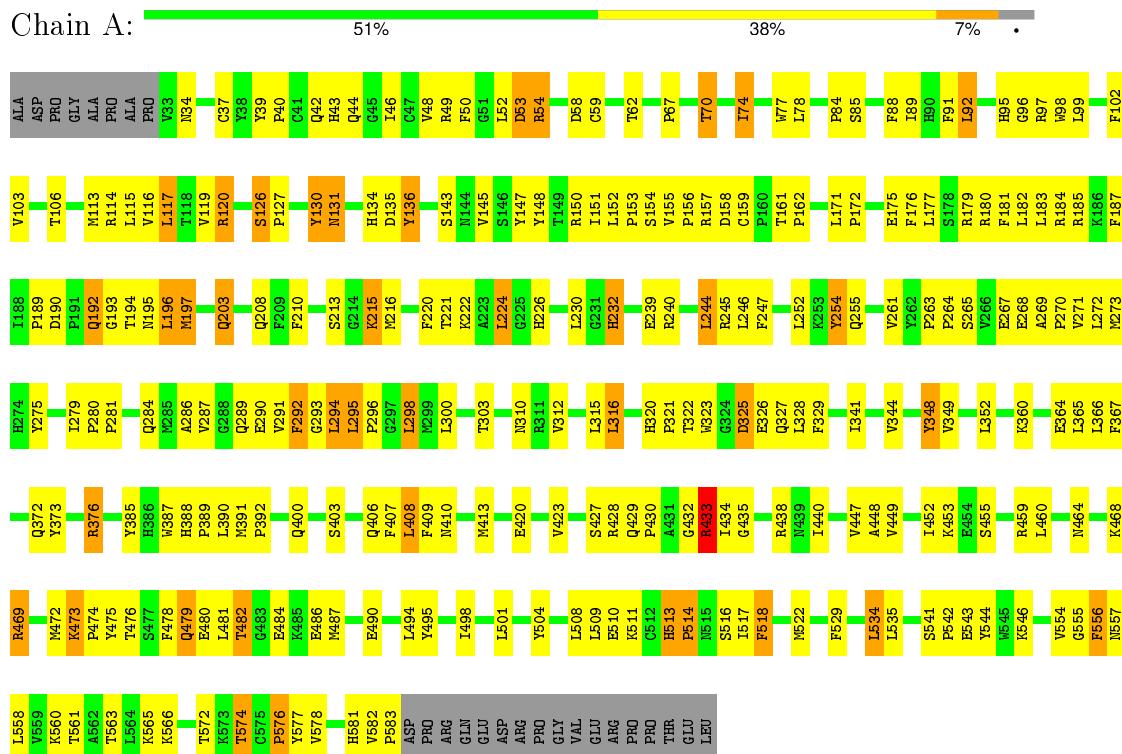
- Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1
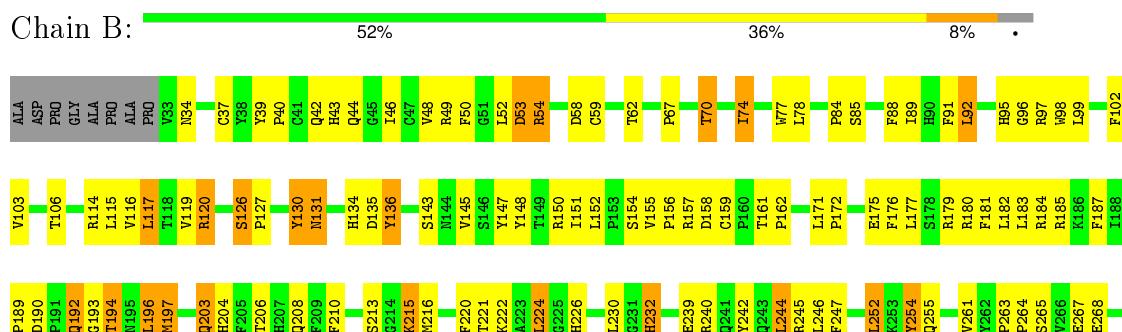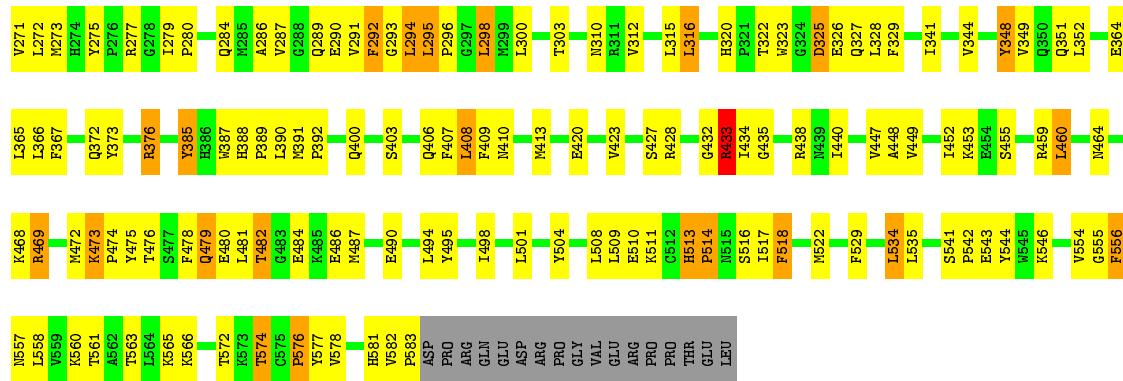
4 Data and refinement statistics (i)

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, α, β, γ	99.57Å 209.80Å 235.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.40	Depositor
% Data completeness (in resolution range)	75.5 (8.00-3.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.186 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9221	wwPDB-VP
Average B, all atoms (Å^2)	20.0	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: 0AH, HEM, BOG, NAG, SAL

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	0.61	0/4608	0.81	5/6253 (0.1%)
1	B	0.61	0/4608	0.81	5/6253 (0.1%)
All	All	0.61	0/9216	0.81	10/12506 (0.1%)

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
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	433	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	B	433	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	408	LEU	N-CA-C	5.31	125.33	111.00
1	B	408	LEU	N-CA-C	5.29	125.30	111.00
1	A	224	LEU	CA-CB-CG	-5.12	103.52	115.30
1	B	224	LEU	CA-CB-CG	-5.11	103.55	115.30
1	B	210	PHE	N-CA-C	-5.08	97.30	111.00
1	A	210	PHE	N-CA-C	-5.07	97.30	111.00
1	B	287	VAL	N-CA-C	5.05	124.65	111.00
1	A	287	VAL	N-CA-C	5.05	124.63	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	TYR	Sidechain
1	A	348	TYR	Sidechain
1	B	136	TYR	Sidechain
1	B	348	TYR	Sidechain

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	4481	0	4381	212	1
1	B	4481	0	4381	213	1
2	A	28	0	26	2	0
2	B	28	0	26	2	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	20	0	28	0	0
4	B	20	0	28	0	0
5	A	43	0	30	6	0
5	B	43	0	30	6	0
6	A	10	0	4	1	0
6	B	10	0	4	1	0
7	A	1	0	0	0	0
All	All	9221	0	8988	417	1

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 23.

All (417) 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:156:PRO:HG2	1:B:159:CYS:SG	1.79	1.23
1:A:156:PRO:HG2	1:A:159:CYS:SG	1.79	1.22
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.42	1.01
1:B:203:GLN:HG2	1:B:298:LEU:HD11	1.43	1.00
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.54	0.88
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.57	0.85
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.57	0.84
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.16	0.81
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.16	0.79
1:B:245:ARG:HH22	1:B:326:GLU:HG2	1.47	0.79
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.47	0.78
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.50	0.76
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.50	0.76
1:B:197:MET:HE1	1:B:423:VAL:HG13	1.68	0.75
1:A:563:THR:HG22	1:A:565:LYS:H	1.53	0.74
1:A:197:MET:HE1	1:A:423:VAL:HG13	1.70	0.73
1:B:116:VAL:O	1:B:120:ARG:HB2	1.90	0.72
1:A:116:VAL:O	1:A:120:ARG:HB2	1.90	0.72
1:B:563:THR:HG22	1:B:565:LYS:N	2.05	0.72
1:A:563:THR:HG22	1:A:565:LYS:N	2.05	0.72
1:A:433:ARG:HH11	1:A:433:ARG:HB3	1.55	0.72
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.25	0.71
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.25	0.71
1:B:563:THR:HG22	1:B:565:LYS:H	1.53	0.71
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.26	0.70
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.26	0.70
1:B:48:VAL:HB	1:B:50:PHE:HE1	1.57	0.70
1:A:177:LEU:HD21	1:A:495:TYR:OH	1.92	0.70
1:B:433:ARG:HB3	1:B:433:ARG:HH11	1.55	0.70
1:A:222:LYS:HE2	1:A:222:LYS:HA	1.73	0.70
1:B:177:LEU:HD21	1:B:495:TYR:OH	1.92	0.70
1:A:48:VAL:HB	1:A:50:PHE:HE1	1.57	0.70
1:B:222:LYS:HE2	1:B:222:LYS:HA	1.73	0.69
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.28	0.69
1:B:43:HIS:O	1:B:44:GLN:HB2	1.93	0.69
1:B:478:PHE:O	1:B:482:THR:HG23	1.94	0.68
1:A:187:PHE:HE1	1:A:189:PRO:HB3	1.58	0.68
1:B:349:VAL:HG13	6:B:711:SAL:C3	2.23	0.68
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.23	0.68
1:A:349:VAL:HG13	6:A:710:SAL:C3	2.23	0.68
1:A:176:PHE:CZ	1:A:180:ARG:HG3	2.29	0.68
1:A:43:HIS:O	1:A:44:GLN:HB2	1.93	0.68
1:B:187:PHE:HE1	1:B:189:PRO:HB3	1.58	0.68
1:A:478:PHE:O	1:A:482:THR:HG23	1.94	0.68
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.28	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:ARG:HA	1:B:438:ARG:O	1.94	0.68
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.23	0.67
1:A:184:ARG:HA	1:A:438:ARG:O	1.94	0.67
1:B:176:PHE:CZ	1:B:180:ARG:HG3	2.29	0.67
1:B:131:ASN:ND2	1:B:134:HIS:H	1.94	0.66
1:B:49:ARG:HG3	1:B:50:PHE:N	2.11	0.65
1:B:130:TYR:HB3	1:B:134:HIS:O	1.97	0.64
1:A:131:ASN:ND2	1:A:134:HIS:H	1.94	0.64
1:A:49:ARG:HG3	1:A:50:PHE:N	2.11	0.64
1:A:130:TYR:HB3	1:A:134:HIS:O	1.97	0.63
1:B:91:PHE:HD2	1:B:92:LEU:HD12	1.63	0.63
1:B:239:GLU:H	1:B:239:GLU:CD	2.02	0.63
1:A:91:PHE:HD2	1:A:92:LEU:HD12	1.63	0.63
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.64	0.62
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.39	0.62
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.34	0.62
1:A:289:GLN:OE1	1:A:291:VAL:HG12	1.99	0.62
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.34	0.61
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.64	0.61
1:A:420:GLU:HG2	1:A:574:THR:HG23	1.83	0.61
1:B:289:GLN:OE1	1:B:291:VAL:HG12	1.99	0.61
1:A:239:GLU:CD	1:A:239:GLU:H	2.02	0.61
1:B:420:GLU:HG2	1:B:574:THR:HG23	1.83	0.61
1:A:263:PRO:HD3	1:A:303:THR:OG1	2.02	0.60
1:A:187:PHE:CE1	1:A:189:PRO:HB3	2.37	0.60
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.37	0.60
1:B:187:PHE:CE1	1:B:189:PRO:HB3	2.37	0.59
1:A:42:GLN:HG3	1:A:70:THR:HG23	1.83	0.59
1:B:344:VAL:O	1:B:348:TYR:HB3	2.02	0.59
1:A:388:HIS:N	1:A:389:PRO:HD2	2.18	0.59
1:B:42:GLN:HG3	1:B:70:THR:HG23	1.83	0.59
1:A:344:VAL:O	1:A:348:TYR:HB3	2.02	0.59
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.37	0.59
1:B:263:PRO:HD3	1:B:303:THR:OG1	2.02	0.59
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.37	0.59
1:B:388:HIS:N	1:B:389:PRO:HD2	2.18	0.59
1:B:88:PHE:CE1	1:B:92:LEU:HD11	2.38	0.59
1:B:240:ARG:O	1:B:244:LEU:HD22	2.03	0.59
1:B:289:GLN:HG3	1:B:292:PHE:CZ	2.37	0.58
1:A:240:ARG:O	1:A:244:LEU:HD22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:208:GLN:HE22	1:B:230:LEU:H	1.52	0.58
1:B:39:TYR:N	1:B:40:PRO:HD3	2.19	0.58
1:A:448:ALA:O	1:A:452:ILE:HG12	2.03	0.58
1:A:88:PHE:CE1	1:A:92:LEU:HD11	2.38	0.57
1:A:208:GLN:HE22	1:A:230:LEU:H	1.52	0.57
1:B:448:ALA:O	1:B:452:ILE:HG12	2.03	0.57
1:B:387:TRP:HB2	5:B:602:HEM:HBC2	1.86	0.57
1:B:341:ILE:HG23	1:B:534:LEU:HG	1.86	0.57
1:B:473:LYS:HA	1:B:473:LYS:HE2	1.87	0.57
1:A:387:TRP:HB2	5:A:601:HEM:CBC	2.35	0.57
1:B:389:PRO:HD3	1:B:440:ILE:HG12	1.86	0.57
1:A:389:PRO:HD3	1:A:440:ILE:HG12	1.86	0.57
1:A:39:TYR:N	1:A:40:PRO:HD3	2.19	0.57
1:A:387:TRP:HB2	5:A:601:HEM:HBC2	1.86	0.57
1:A:433:ARG:HG2	1:A:435:GLY:O	2.05	0.57
1:B:582:VAL:HG23	1:B:583:PRO:HD2	1.86	0.57
1:B:126:SER:HA	1:B:127:PRO:C	2.25	0.57
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.86	0.56
1:A:400:GLN:NE2	1:A:400:GLN:HA	2.20	0.56
1:B:433:ARG:HG2	1:B:435:GLY:O	2.05	0.56
1:A:126:SER:HA	1:A:127:PRO:C	2.25	0.56
1:B:449:VAL:O	1:B:453:LYS:HG3	2.05	0.56
1:B:208:GLN:NE2	1:B:230:LEU:H	2.03	0.56
1:A:449:VAL:O	1:A:453:LYS:HG3	2.06	0.56
1:B:387:TRP:HB2	5:B:602:HEM:CBC	2.35	0.56
1:A:341:ILE:HG23	1:A:534:LEU:HG	1.86	0.56
1:B:150:ARG:HD3	1:B:152:LEU:O	2.05	0.56
1:A:473:LYS:HE2	1:A:473:LYS:HA	1.87	0.56
1:A:254:TYR:HD2	1:A:310:ASN:ND2	2.04	0.56
1:B:403:SER:OG	1:B:406:GLN:HG3	2.06	0.56
1:B:296:PRO:HG2	1:B:407:PHE:CZ	2.41	0.55
1:A:150:ARG:HD3	1:A:152:LEU:O	2.05	0.55
1:A:179:ARG:HG3	1:A:183:LEU:HD12	1.89	0.55
1:A:403:SER:OG	1:A:406:GLN:HG3	2.06	0.55
1:A:296:PRO:HG2	1:A:407:PHE:CZ	2.41	0.55
1:A:130:TYR:HD2	1:A:136:TYR:N	2.05	0.55
1:A:556:PHE:CD2	1:A:560:LYS:HD2	2.41	0.55
1:B:556:PHE:CD2	1:B:560:LYS:HD2	2.41	0.55
1:B:131:ASN:ND2	1:B:134:HIS:N	2.54	0.55
1:A:208:GLN:NE2	1:A:230:LEU:H	2.03	0.55
1:A:131:ASN:ND2	1:A:134:HIS:N	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:HD2	1:B:310:ASN:ND2	2.04	0.55
1:B:130:TYR:HD2	1:B:136:TYR:N	2.05	0.55
1:B:400:GLN:NE2	1:B:400:GLN:HA	2.20	0.55
1:B:179:ARG:HG3	1:B:183:LEU:HD12	1.89	0.54
1:B:433:ARG:CB	1:B:433:ARG:HH11	2.20	0.53
1:A:203:GLN:HA	5:A:601:HEM:HAC	1.91	0.53
1:B:88:PHE:O	1:B:92:LEU:HD13	2.09	0.53
1:B:91:PHE:CE1	1:B:95:HIS:CD2	2.97	0.53
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.44	0.53
1:A:88:PHE:O	1:A:92:LEU:HD13	2.09	0.52
1:A:433:ARG:HH11	1:A:433:ARG:CB	2.20	0.52
1:B:481:LEU:HD22	1:B:501:LEU:CD2	2.40	0.52
1:B:203:GLN:HA	5:B:602:HEM:HAC	1.91	0.52
1:A:102:PHE:O	1:A:106:THR:HG23	2.10	0.52
1:A:91:PHE:CE1	1:A:95:HIS:CD2	2.97	0.52
1:B:102:PHE:O	1:B:106:THR:HG23	2.10	0.52
1:A:181:PHE:HB3	1:A:509:LEU:HD21	1.92	0.52
1:A:372:GLN:HE22	1:B:373:TYR:H	1.58	0.52
1:A:481:LEU:HD22	1:A:501:LEU:CD2	2.40	0.52
1:A:197:MET:CE	1:A:423:VAL:HG13	2.40	0.52
1:B:213:SER:HB3	1:B:216:MET:HB2	1.91	0.52
1:B:88:PHE:O	1:B:91:PHE:HB3	2.10	0.51
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.44	0.51
1:A:88:PHE:O	1:A:91:PHE:HB3	2.10	0.51
1:A:145:VAL:HG23	1:A:224:LEU:HD23	1.92	0.51
1:B:433:ARG:CG	1:B:433:ARG:HH11	2.24	0.51
1:B:145:VAL:HG23	1:B:224:LEU:HD23	1.92	0.51
1:A:544:TYR:CE1	1:B:127:PRO:HB2	2.45	0.51
1:B:254:TYR:CD2	1:B:310:ASN:ND2	2.79	0.51
1:A:254:TYR:CD1	1:A:254:TYR:C	2.84	0.51
1:B:197:MET:CE	1:B:423:VAL:HG13	2.40	0.51
1:A:213:SER:HB3	1:A:216:MET:HB2	1.91	0.51
1:B:43:HIS:O	1:B:62:THR:HG23	2.11	0.51
1:A:413:MET:HA	2:A:681:NAG:O6	2.11	0.51
1:B:151:ILE:HD11	1:B:529:PHE:HE1	1.76	0.51
1:A:127:PRO:HB2	1:B:544:TYR:CE1	2.46	0.50
1:B:413:MET:HA	2:B:681:NAG:O6	2.11	0.50
1:B:181:PHE:HB3	1:B:509:LEU:HD21	1.92	0.50
1:A:203:GLN:HG2	1:A:298:LEU:CD1	2.29	0.50
1:A:480:GLU:O	1:A:511:LYS:NZ	2.43	0.50
1:A:312:VAL:HG12	1:A:316:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:CD2	1:A:310:ASN:ND2	2.79	0.50
1:B:312:VAL:HG12	1:B:316:LEU:CD2	2.41	0.50
1:A:433:ARG:CG	1:A:433:ARG:HH11	2.24	0.50
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.94	0.50
1:A:151:ILE:HD11	1:A:529:PHE:HE1	1.76	0.50
1:B:344:VAL:HG12	1:B:534:LEU:HD21	1.93	0.50
1:B:185:ARG:NE	1:B:438:ARG:HD3	2.22	0.49
1:A:43:HIS:O	1:A:62:THR:HG23	2.11	0.49
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.47	0.49
1:B:323:TRP:CD2	1:B:327:GLN:HG3	2.47	0.49
1:B:464:ASN:O	1:B:468:LYS:HG3	2.12	0.49
1:B:96:GLY:O	1:B:99:LEU:N	2.45	0.49
1:B:130:TYR:CD1	1:B:130:TYR:N	2.80	0.49
1:A:215:LYS:H	1:A:215:LYS:NZ	2.11	0.49
1:A:157:ARG:HG2	1:A:459:ARG:HD2	1.94	0.49
1:B:182:LEU:HB3	1:B:440:ILE:HD12	1.94	0.49
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.47	0.49
1:A:344:VAL:HG12	1:A:534:LEU:HD21	1.93	0.49
1:A:481:LEU:HD11	1:A:510:GLU:HB2	1.95	0.49
1:B:145:VAL:HG23	1:B:224:LEU:CD2	2.43	0.49
1:A:464:ASN:O	1:A:468:LYS:HG3	2.12	0.49
1:B:203:GLN:HG2	1:B:298:LEU:CD1	2.29	0.49
1:B:254:TYR:C	1:B:254:TYR:CD1	2.84	0.49
1:A:96:GLY:O	1:A:97:ARG:C	2.51	0.49
1:A:130:TYR:N	1:A:130:TYR:CD1	2.80	0.49
1:A:323:TRP:CD2	1:A:327:GLN:HG3	2.47	0.49
1:B:157:ARG:HG2	1:B:459:ARG:HD2	1.94	0.49
1:B:215:LYS:H	1:B:215:LYS:NZ	2.11	0.48
1:A:52:LEU:N	1:A:52:LEU:HD12	2.28	0.48
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.46	0.48
1:A:272:LEU:HD22	1:A:273:MET:N	2.28	0.48
1:A:96:GLY:O	1:A:99:LEU:N	2.45	0.48
1:B:52:LEU:HD12	1:B:52:LEU:N	2.28	0.48
1:A:175:GLU:HG3	1:A:179:ARG:HH21	1.78	0.48
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.46	0.48
1:B:161:THR:HB	1:B:162:PRO:HD2	1.95	0.48
1:B:175:GLU:HG3	1:B:179:ARG:HH21	1.78	0.48
1:A:475:TYR:CE1	1:A:481:LEU:HA	2.48	0.48
1:B:272:LEU:HD22	1:B:273:MET:N	2.28	0.48
1:B:275:TYR:CE2	1:B:284:GLN:HB3	2.49	0.48
1:B:114:ARG:HB2	1:B:365:LEU:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:THR:HB	1:A:162:PRO:HD2	1.94	0.48
1:B:423:VAL:HG11	1:B:578:VAL:HG12	1.95	0.48
1:A:423:VAL:HG11	1:A:578:VAL:HG12	1.95	0.48
1:A:145:VAL:HG23	1:A:224:LEU:CD2	2.43	0.48
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.49	0.48
1:A:373:TYR:H	1:B:372:GLN:HE22	1.60	0.47
1:A:420:GLU:HG2	1:A:574:THR:O	2.15	0.47
1:B:344:VAL:CG1	1:B:534:LEU:HD21	2.44	0.47
1:B:481:LEU:HD11	1:B:510:GLU:HB2	1.95	0.47
1:B:475:TYR:CE1	1:B:481:LEU:HA	2.48	0.47
1:B:312:VAL:HA	1:B:315:LEU:HD12	1.95	0.47
1:A:215:LYS:HZ2	1:A:215:LYS:H	1.60	0.47
1:A:98:TRP:CD2	1:A:99:LEU:N	2.82	0.47
1:B:294:LEU:O	1:B:294:LEU:HD12	2.15	0.47
1:B:420:GLU:HG2	1:B:574:THR:O	2.15	0.47
1:A:312:VAL:HA	1:A:315:LEU:HD12	1.96	0.47
1:A:53:ASP:O	1:A:54:ARG:O	2.32	0.47
1:A:91:PHE:CD1	1:A:95:HIS:CD2	3.03	0.47
1:B:96:GLY:O	1:B:97:ARG:C	2.51	0.47
1:B:504:TYR:OH	1:B:508:LEU:HD11	2.15	0.47
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.49	0.47
1:B:53:ASP:O	1:B:54:ARG:O	2.32	0.47
1:A:185:ARG:NE	1:A:438:ARG:HD3	2.22	0.47
1:B:91:PHE:CD1	1:B:95:HIS:CD2	3.03	0.47
1:A:372:GLN:HE22	1:B:372:GLN:HA	1.80	0.47
1:B:98:TRP:CD2	1:B:99:LEU:N	2.82	0.47
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.49	0.47
1:A:255:GLN:HG2	1:A:263:PRO:O	2.15	0.47
1:A:344:VAL:CG1	1:A:534:LEU:HD21	2.44	0.47
1:B:99:LEU:O	1:B:103:VAL:HG23	2.15	0.47
1:A:504:TYR:OH	1:A:508:LEU:HD11	2.15	0.47
1:A:114:ARG:HB2	1:A:365:LEU:HB3	1.96	0.47
1:A:294:LEU:O	1:A:294:LEU:HD12	2.15	0.46
1:B:255:GLN:HG2	1:B:263:PRO:O	2.15	0.46
1:A:372:GLN:HA	1:B:372:GLN:HE22	1.80	0.46
1:A:291:VAL:O	1:A:293:GLY:N	2.49	0.46
1:B:316:LEU:HB3	1:B:328:LEU:HD23	1.97	0.46
1:A:85:SER:O	1:A:89:ILE:HD13	2.15	0.46
1:B:323:TRP:CE3	1:B:327:GLN:HG3	2.50	0.46
1:B:265:SER:OG	1:B:267:GLU:HB3	2.16	0.46
1:A:498:ILE:HD12	1:A:498:ILE:HA	1.72	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:VAL:CG1	1:B:578:VAL:HG12	2.45	0.46
1:A:423:VAL:CG1	1:A:578:VAL:HG12	2.45	0.46
1:B:279:ILE:O	1:B:284:GLN:NE2	2.48	0.46
1:A:543:GLU:O	1:A:546:LYS:HD2	2.16	0.46
1:B:291:VAL:O	1:B:293:GLY:N	2.49	0.46
1:A:99:LEU:O	1:A:103:VAL:HG23	2.15	0.46
1:A:197:MET:HE1	1:A:423:VAL:HG22	1.97	0.46
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.46	0.46
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.46	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG3	2.50	0.46
1:B:479:GLN:H	1:B:479:GLN:CD	2.19	0.46
1:A:181:PHE:CE1	1:A:487:MET:HB2	2.51	0.46
1:B:181:PHE:CE1	1:B:487:MET:HB2	2.51	0.46
1:A:265:SER:OG	1:A:267:GLU:HB3	2.16	0.46
1:B:391:MET:HG3	5:B:602:HEM:HAB	1.99	0.45
1:A:152:LEU:HA	1:A:153:PRO:HD2	1.75	0.45
1:A:316:LEU:HB3	1:A:328:LEU:HD23	1.97	0.45
1:A:479:GLN:H	1:A:479:GLN:CD	2.19	0.45
1:B:247:PHE:HA	1:B:325:ASP:OD2	2.16	0.45
1:A:279:ILE:O	1:A:284:GLN:NE2	2.48	0.45
1:A:247:PHE:HA	1:A:325:ASP:OD2	2.16	0.45
1:A:196:LEU:HD11	1:A:392:PRO:HG3	1.99	0.45
1:B:196:LEU:HD11	1:B:392:PRO:HG3	1.99	0.45
1:A:147:TYR:CE1	1:A:220:PHE:CZ	3.05	0.45
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.98	0.45
1:A:391:MET:HG3	5:A:601:HEM:HAB	1.99	0.45
1:B:85:SER:O	1:B:89:ILE:HD13	2.15	0.45
1:B:192:GLN:OE1	1:B:517:ILE:N	2.49	0.45
1:A:518:PHE:CE2	1:A:522:MET:HG2	2.52	0.45
1:B:464:ASN:ND2	1:B:474:PRO:HB2	2.32	0.45
1:B:89:ILE:HD12	1:B:89:ILE:N	2.32	0.45
1:A:420:GLU:HG3	1:A:572:THR:HB	1.98	0.45
1:B:400:GLN:NE2	1:B:400:GLN:CA	2.80	0.45
1:B:480:GLU:O	1:B:511:LYS:NZ	2.43	0.45
1:A:156:PRO:HB2	1:A:158:ASP:OD1	2.17	0.44
1:B:98:TRP:CG	1:B:99:LEU:N	2.85	0.44
1:A:98:TRP:CG	1:A:99:LEU:N	2.85	0.44
1:B:543:GLU:O	1:B:546:LYS:HD2	2.16	0.44
1:A:192:GLN:OE1	1:A:517:ILE:N	2.49	0.44
1:B:390:LEU:HD21	1:B:434:ILE:HD11	2.00	0.44
1:B:176:PHE:HE2	1:B:494:LEU:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:SER:HB2	1:B:542:PRO:HD2	2.00	0.44
1:A:130:TYR:HD2	1:A:135:ASP:C	2.21	0.44
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.47	0.44
1:B:154:SER:HB2	1:B:459:ARG:HB2	1.98	0.44
1:B:147:TYR:CE1	1:B:220:PHE:CZ	3.05	0.44
1:B:518:PHE:CE2	1:B:522:MET:HG2	2.52	0.44
1:A:176:PHE:HE2	1:A:494:LEU:HD11	1.82	0.44
1:B:189:PRO:HA	1:B:432:GLY:HA2	2.00	0.44
1:A:390:LEU:HD21	1:A:434:ILE:HD11	1.99	0.44
1:A:541:SER:HB2	1:A:542:PRO:HD2	2.00	0.44
1:B:156:PRO:HB2	1:B:158:ASP:OD1	2.17	0.44
1:B:176:PHE:CE1	1:B:180:ARG:HG3	2.53	0.44
1:B:420:GLU:HG3	1:B:572:THR:HB	1.98	0.44
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.47	0.44
1:A:117:LEU:HD12	1:A:117:LEU:HA	1.78	0.44
1:B:130:TYR:HD2	1:B:135:ASP:C	2.21	0.44
1:B:117:LEU:HA	1:B:117:LEU:HD12	1.78	0.44
1:B:534:LEU:HA	1:B:534:LEU:HD12	1.88	0.43
1:A:89:ILE:N	1:A:89:ILE:HD12	2.32	0.43
1:A:563:THR:HB	1:A:566:LYS:HB2	1.99	0.43
1:B:91:PHE:O	1:B:95:HIS:CD2	2.72	0.43
1:B:152:LEU:HD21	1:B:469:ARG:HG3	2.00	0.43
1:A:447:VAL:HG22	5:A:601:HEM:HMA3	2.00	0.43
1:B:563:THR:HB	1:B:566:LYS:HB2	1.99	0.43
1:B:581:HIS:ND1	1:B:582:VAL:O	2.51	0.43
1:A:581:HIS:ND1	1:A:582:VAL:O	2.51	0.43
1:A:152:LEU:HD21	1:A:469:ARG:HG3	2.00	0.43
1:A:176:PHE:CE1	1:A:180:ARG:HG3	2.53	0.43
1:A:400:GLN:NE2	1:A:400:GLN:CA	2.80	0.43
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.32	0.43
1:A:91:PHE:O	1:A:95:HIS:CD2	2.71	0.43
1:A:320:HIS:HA	1:A:321:PRO:HD2	1.90	0.43
1:B:272:LEU:HD22	1:B:273:MET:H	1.84	0.43
1:A:513:HIS:HB2	1:A:516:SER:HB2	2.00	0.43
1:A:264:PRO:HG2	1:A:286:ALA:HB3	2.01	0.43
1:B:447:VAL:HG22	5:B:602:HEM:HMA3	2.00	0.43
1:A:189:PRO:HA	1:A:432:GLY:HA2	2.00	0.43
1:B:498:ILE:HD12	1:B:498:ILE:HA	1.72	0.43
1:B:428:ARG:O	1:B:582:VAL:HG23	2.19	0.43
1:B:555:GLY:HA2	1:B:558:LEU:HD13	2.01	0.43
1:A:148:TYR:CZ	1:A:221:THR:HB	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ASN:O	1:A:561:THR:HG23	2.19	0.42
1:B:67:PRO:HG2	2:B:661:NAG:H82	2.01	0.42
1:A:429:GLN:HA	1:A:430:PRO:HD3	1.85	0.42
1:A:534:LEU:HA	1:A:534:LEU:HD12	1.89	0.42
1:A:162:PRO:HG2	1:A:171:LEU:HD21	2.01	0.42
1:B:513:HIS:HB2	1:B:516:SER:HB2	2.00	0.42
1:A:428:ARG:O	1:A:582:VAL:HG23	2.19	0.42
1:B:264:PRO:HG2	1:B:286:ALA:HB3	2.00	0.42
1:A:555:GLY:HA2	1:A:558:LEU:HD13	2.00	0.42
1:B:460:LEU:HD12	1:B:460:LEU:HA	1.83	0.42
1:A:291:VAL:HG13	1:A:292:PHE:N	2.35	0.42
1:B:148:TYR:CZ	1:B:221:THR:HB	2.54	0.42
1:B:557:ASN:O	1:B:561:THR:HG23	2.19	0.42
1:A:77:TRP:CE3	1:A:78:LEU:N	2.88	0.42
1:B:254:TYR:HD1	1:B:254:TYR:C	2.22	0.42
1:B:291:VAL:HG13	1:B:292:PHE:N	2.35	0.42
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.74	0.42
1:B:366:LEU:HD23	1:B:366:LEU:HA	1.73	0.42
1:B:34:ASN:HB2	1:B:158:ASP:OD2	2.20	0.42
1:A:216:MET:HE2	1:A:222:LYS:HE3	2.01	0.42
1:B:180:ARG:NH2	1:B:490:GLU:OE1	2.53	0.42
1:B:162:PRO:HG2	1:B:171:LEU:HD21	2.01	0.42
1:A:39:TYR:OH	1:A:155:VAL:HB	2.20	0.42
1:B:46:ILE:HB	1:B:58:ASP:HB3	2.02	0.42
1:B:74:ILE:HA	1:B:74:ILE:HD13	1.66	0.42
1:A:193:GLY:O	1:A:582:VAL:HG12	2.20	0.41
1:B:39:TYR:OH	1:B:155:VAL:HB	2.20	0.41
1:B:77:TRP:CE3	1:B:78:LEU:N	2.88	0.41
1:A:155:VAL:HA	1:A:156:PRO:HD2	1.82	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.93	0.41
1:A:46:ILE:HB	1:A:58:ASP:HB3	2.02	0.41
1:A:34:ASN:HB2	1:A:158:ASP:OD2	2.20	0.41
1:B:197:MET:HE1	1:B:423:VAL:HG22	2.01	0.41
1:A:272:LEU:HD22	1:A:273:MET:H	1.84	0.41
1:A:433:ARG:NH1	1:A:433:ARG:HB3	2.30	0.41
1:B:433:ARG:HB3	1:B:433:ARG:NH1	2.30	0.41
1:A:74:ILE:HD13	1:A:74:ILE:HA	1.66	0.41
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.90	0.41
1:A:254:TYR:HD1	1:A:254:TYR:C	2.22	0.41
1:B:295:LEU:HD11	5:B:602:HEM:CBB	2.50	0.41
1:A:180:ARG:NH2	1:A:490:GLU:OE1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASN:HD22	1:B:131:ASN:H	1.69	0.41
1:B:289:GLN:HB3	1:B:292:PHE:CG	2.56	0.41
1:B:42:GLN:HG3	1:B:70:THR:CG2	2.50	0.41
1:A:254:TYR:HD2	1:A:310:ASN:HD21	1.67	0.41
1:B:245:ARG:NH1	1:B:329:PHE:CD2	2.89	0.41
1:B:115:LEU:O	1:B:119:VAL:HG13	2.21	0.41
1:B:48:VAL:HB	1:B:50:PHE:CE1	2.47	0.41
1:A:213:SER:CB	1:A:216:MET:HB2	2.51	0.41
1:B:213:SER:CB	1:B:216:MET:HB2	2.51	0.41
1:B:289:GLN:HG3	1:B:292:PHE:CE1	2.56	0.41
1:B:226:HIS:HB3	1:B:376:ARG:HA	2.03	0.41
1:B:252:LEU:HD12	1:B:252:LEU:HA	1.88	0.41
1:A:245:ARG:NH1	1:A:329:PHE:CD2	2.89	0.41
1:B:193:GLY:O	1:B:582:VAL:HG12	2.20	0.41
1:A:289:GLN:HB3	1:A:292:PHE:CG	2.56	0.41
1:A:388:HIS:N	1:A:389:PRO:CD	2.84	0.41
1:A:372:GLN:HA	1:B:372:GLN:NE2	2.36	0.41
1:A:372:GLN:NE2	1:B:372:GLN:HA	2.36	0.41
1:A:226:HIS:HB3	1:A:376:ARG:HA	2.03	0.41
1:A:67:PRO:HG2	2:A:661:NAG:H82	2.01	0.41
1:B:204:HIS:HB2	1:B:298:LEU:HD12	2.03	0.40
1:A:563:THR:CG2	1:A:565:LYS:HB3	2.51	0.40
1:B:216:MET:HE2	1:B:222:LYS:HE3	2.01	0.40
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.56	0.40
1:B:240:ARG:NH1	1:B:271:VAL:HG22	2.36	0.40
1:B:215:LYS:H	1:B:215:LYS:HZ2	1.69	0.40
1:A:59:CYS:HA	1:A:62:THR:OG1	2.21	0.40
1:B:254:TYR:HD2	1:B:310:ASN:HD21	1.67	0.40
1:A:115:LEU:O	1:A:119:VAL:HG13	2.21	0.40
1:B:185:ARG:HE	1:B:438:ARG:HH11	1.68	0.40
1:B:280:PRO:O	1:B:284:GLN:HG3	2.21	0.40
1:B:194:THR:HG23	1:B:351:GLN:HE21	1.86	0.40
1:A:295:LEU:HD11	5:A:601:HEM:CBB	2.50	0.40
1:B:59:CYS:HA	1:B:62:THR:OG1	2.21	0.40
1:A:240:ARG:NH1	1:A:271:VAL:HG22	2.36	0.40
1:A:468:LYS:HA	1:A:472:MET:O	2.21	0.40
1:B:242:TYR:CD1	1:B:247:PHE:HZ	2.40	0.40
1:A:113:MET:HG2	1:A:360:LYS:HB3	2.04	0.40
1:A:269:ALA:HA	1:A:270:PRO:HD2	1.92	0.40
1:A:183:LEU:HD23	1:A:184:ARG:N	2.37	0.40
1:B:468:LYS:HA	1:B:472:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ASN:HA	1:A:430:PRO:HA	2.04	0.40
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:PHE:CE1	1:B:277:ARG:NH1[8_456]	2.18	0.02

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	548/576 (95%)	488 (89%)	49 (9%)	11 (2%)	9	48
1	B	548/576 (95%)	488 (89%)	49 (9%)	11 (2%)	9	48
All	All	1096/1152 (95%)	976 (89%)	98 (9%)	22 (2%)	9	48

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ARG
1	A	295	LEU
1	A	408	LEU
1	A	514	PRO
1	B	54	ARG
1	B	295	LEU
1	B	408	LEU
1	B	514	PRO
1	A	410	ASN
1	B	410	ASN
1	A	292	PHE

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Mol	Chain	Res	Type
1	A	325	ASP
1	B	292	PHE
1	B	325	ASP
1	A	290	GLU
1	A	486	GLU
1	A	554	VAL
1	B	290	GLU
1	B	486	GLU
1	B	554	VAL
1	A	576	PRO
1	B	576	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	485/505 (96%)	436 (90%)	49 (10%)	9	38
1	B	485/505 (96%)	436 (90%)	49 (10%)	9	38
All	All	970/1010 (96%)	872 (90%)	98 (10%)	9	38

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASP
1	A	70	THR
1	A	74	ILE
1	A	92	LEU
1	A	117	LEU
1	A	120	ARG
1	A	126	SER
1	A	130	TYR
1	A	131	ASN
1	A	143	SER
1	A	190	ASP
1	A	192	GLN

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Mol	Chain	Res	Type
1	A	194	THR
1	A	196	LEU
1	A	197	MET
1	A	203	GLN
1	A	215	LYS
1	A	232	HIS
1	A	244	LEU
1	A	246	LEU
1	A	252	LEU
1	A	254	TYR
1	A	261	VAL
1	A	268	GLU
1	A	294	LEU
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	322	THR
1	A	352	LEU
1	A	376	ARG
1	A	385	TYR
1	A	433	ARG
1	A	455	SER
1	A	460	LEU
1	A	469	ARG
1	A	473	LYS
1	A	476	THR
1	A	479	GLN
1	A	482	THR
1	A	484	GLU
1	A	513	HIS
1	A	514	PRO
1	A	518	PHE
1	A	534	LEU
1	A	535	LEU
1	A	556	PHE
1	A	574	THR
1	A	576	PRO
1	B	53	ASP
1	B	70	THR
1	B	74	ILE
1	B	92	LEU
1	B	117	LEU

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Mol	Chain	Res	Type
1	B	120	ARG
1	B	126	SER
1	B	130	TYR
1	B	131	ASN
1	B	143	SER
1	B	190	ASP
1	B	192	GLN
1	B	194	THR
1	B	196	LEU
1	B	197	MET
1	B	203	GLN
1	B	215	LYS
1	B	232	HIS
1	B	244	LEU
1	B	246	LEU
1	B	252	LEU
1	B	254	TYR
1	B	261	VAL
1	B	268	GLU
1	B	294	LEU
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	322	THR
1	B	352	LEU
1	B	376	ARG
1	B	385	TYR
1	B	433	ARG
1	B	455	SER
1	B	460	LEU
1	B	469	ARG
1	B	473	LYS
1	B	476	THR
1	B	479	GLN
1	B	482	THR
1	B	484	GLU
1	B	513	HIS
1	B	514	PRO
1	B	518	PHE
1	B	534	LEU
1	B	535	LEU
1	B	556	PHE

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Mol	Chain	Res	Type
1	B	574	THR
1	B	576	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	131	ASN
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	351	GLN
1	A	358	GLN
1	A	372	GLN
1	A	375	ASN
1	A	400	GLN
1	A	443	HIS
1	B	95	HIS
1	B	131	ASN
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	358	GLN
1	B	372	GLN
1	B	375	ASN
1	B	400	GLN
1	B	443	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

2 non-standard protein/DNA/RNA residues 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

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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	#$|Z| > 2$
1	0AH	A	530	1	8,9,10	0.99	0	6,10,12	5.13	1 (16%)
1	0AH	B	530	1	8,9,10	0.99	0	6,10,12	5.13	1 (16%)

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
1	0AH	A	530	1	-	0/7/9/11	0/0/0/0
1	0AH	B	530	1	-	0/7/9/11	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	530	0AH	O2-CB-CA	12.23	144.79	108.73
1	B	530	0AH	O2-CB-CA	12.23	144.81	108.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

4 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	671	1,3	14,14,15	0.65	0	15,19,21	1.30	1 (6%)
3	NAG	A	672	3	14,14,15	0.80	0	15,19,21	1.16	1 (6%)
3	NAG	B	671	1,3	14,14,15	0.65	0	15,19,21	1.30	1 (6%)
3	NAG	B	672	3	14,14,15	0.79	0	15,19,21	1.16	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	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	NAG	B	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	672	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	671	NAG	C2-N2-C7	-3.05	119.13	123.04
3	A	671	NAG	C2-N2-C7	-3.01	119.17	123.04
3	A	672	NAG	C4-C3-C2	-2.53	107.29	111.23
3	B	672	NAG	C4-C3-C2	-2.52	107.31	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

10 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	HEM	A	601	1	30,50,50	2.95	11 (36%)	24,82,82	3.06	11 (45%)
2	NAG	A	661	1	14,14,15	0.50	0	15,19,21	0.84	1 (6%)
2	NAG	A	681	1	14,14,15	0.52	0	15,19,21	1.12	1 (6%)
4	BOG	A	702	-	20,20,20	0.62	0	25,25,25	0.79	1 (4%)
6	SAL	A	710	-	7,10,10	0.39	0	10,13,13	0.67	0
5	HEM	B	602	1	30,50,50	2.96	11 (36%)	24,82,82	3.06	11 (45%)
2	NAG	B	661	1	14,14,15	0.49	0	15,19,21	0.84	1 (6%)
2	NAG	B	681	1	14,14,15	0.52	0	15,19,21	1.12	1 (6%)
4	BOG	B	702	-	20,20,20	0.61	0	25,25,25	0.79	1 (4%)
6	SAL	B	711	-	7,10,10	0.40	0	10,13,13	0.67	0

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	HEM	A	601	1	-	0/10/54/54	0/0/8/8
2	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
4	BOG	A	702	-	-	0/11/31/31	0/1/1/1
6	SAL	A	710	-	-	0/0/4/4	0/1/1/1
5	HEM	B	602	1	-	0/10/54/54	0/0/8/8
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
4	BOG	B	702	-	-	0/11/31/31	0/1/1/1
6	SAL	B	711	-	-	0/0/4/4	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	C3C-CAC	-8.76	1.34	1.51
5	B	602	HEM	C3C-CAC	-8.74	1.34	1.51
5	A	601	HEM	C2D-C3D	-6.70	1.34	1.54
5	B	602	HEM	C2D-C3D	-6.68	1.34	1.54
5	A	601	HEM	C2C-C1C	-6.14	1.40	1.52
5	B	602	HEM	C2C-C1C	-6.10	1.41	1.52
5	B	602	HEM	C3D-C4D	-5.87	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	C3D-C4D	-5.78	1.44	1.51
5	B	602	HEM	C3B-CAB	-4.83	1.42	1.51
5	A	601	HEM	C3B-CAB	-4.82	1.42	1.51
5	A	601	HEM	C2A-C3A	-2.29	1.30	1.37
5	B	602	HEM	C2A-C3A	-2.28	1.30	1.37
5	B	602	HEM	C2D-C1D	-2.08	1.45	1.51
5	A	601	HEM	C2D-C1D	-2.07	1.45	1.51
5	A	601	HEM	CBC-CAC	2.09	1.41	1.29
5	B	602	HEM	CBC-CAC	2.10	1.41	1.29
5	A	601	HEM	C1C-NC	2.12	1.38	1.36
5	B	602	HEM	C1C-NC	2.16	1.38	1.36
5	B	602	HEM	C4C-NC	2.51	1.39	1.36
5	A	601	HEM	C4C-NC	2.52	1.39	1.36
5	A	601	HEM	CBB-CAB	3.01	1.46	1.29
5	B	602	HEM	CBB-CAB	3.01	1.46	1.29

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	602	HEM	C3C-CAC-CBC	-6.80	114.03	124.46
5	A	601	HEM	C3C-CAC-CBC	-6.76	114.08	124.46
5	A	601	HEM	CMA-C3A-C2A	-3.24	118.46	125.24
5	B	602	HEM	CMA-C3A-C2A	-3.24	118.47	125.24
2	A	681	NAG	C2-N2-C7	-3.04	119.14	123.04
2	B	681	NAG	C2-N2-C7	-3.03	119.14	123.04
2	B	661	NAG	C2-N2-C7	-2.29	120.09	123.04
2	A	661	NAG	C2-N2-C7	-2.28	120.11	123.04
5	A	601	HEM	C2D-C3D-C4D	2.05	104.97	101.50
5	B	602	HEM	C2D-C3D-C4D	2.05	104.98	101.50
4	A	702	BOG	C1'-O1-C1	2.45	118.23	113.94
4	B	702	BOG	C1'-O1-C1	2.46	118.24	113.94
5	A	601	HEM	CMD-C2D-C3D	2.73	126.41	114.35
5	B	602	HEM	CMD-C2D-C3D	2.73	126.44	114.35
5	B	602	HEM	CMB-C2B-C3B	3.50	125.28	116.53
5	A	601	HEM	CMB-C2B-C3B	3.52	125.31	116.53
5	A	601	HEM	CAD-C3D-C4D	3.87	126.12	112.47
5	B	602	HEM	CAD-C3D-C4D	3.88	126.15	112.47
5	A	601	HEM	C3B-CAB-CBB	4.14	130.81	124.46
5	B	602	HEM	C3B-CAB-CBB	4.15	130.82	124.46
5	A	601	HEM	CMC-C2C-C3C	4.38	127.46	116.53
5	B	602	HEM	CMC-C2C-C3C	4.39	127.50	116.53
5	B	602	HEM	CAA-C2A-C1A	4.59	132.00	127.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	HEM	CAA-C2A-C1A	4.59	132.00	127.01
5	B	602	HEM	CAD-C3D-C2D	5.27	128.37	113.22
5	A	601	HEM	CAD-C3D-C2D	5.28	128.41	113.22
5	A	601	HEM	CBA-CAA-C2A	5.46	122.31	112.53
5	B	602	HEM	CBA-CAA-C2A	5.47	122.33	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	HEM	6	0
2	A	661	NAG	1	0
2	A	681	NAG	1	0
6	A	710	SAL	1	0
5	B	602	HEM	6	0
2	B	661	NAG	1	0
2	B	681	NAG	1	0
6	B	711	SAL	1	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.