



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:32 PM GMT

PDB ID : 1PGE  
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH P-(2'-IODO-5'-THENOYL)HYDROTROPIC ACID (IODOSUPROFEN)  
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.  
Deposited on : 1995-12-02  
Resolution : 3.50 Å(reported)

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

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

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

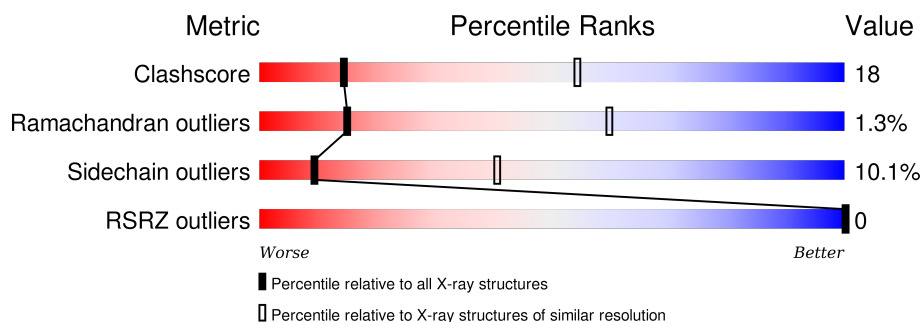
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	576	<div> <div>56%</div> <div>34%</div> <div>5%</div> <div>.</div> </div>
1	B	576	<div> <div>57%</div> <div>34%</div> <div>5%</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	NAG	B	661	-	-	-	X
4	BOG	B	702	-	-	-	X

## 2 Entry composition [i](#)

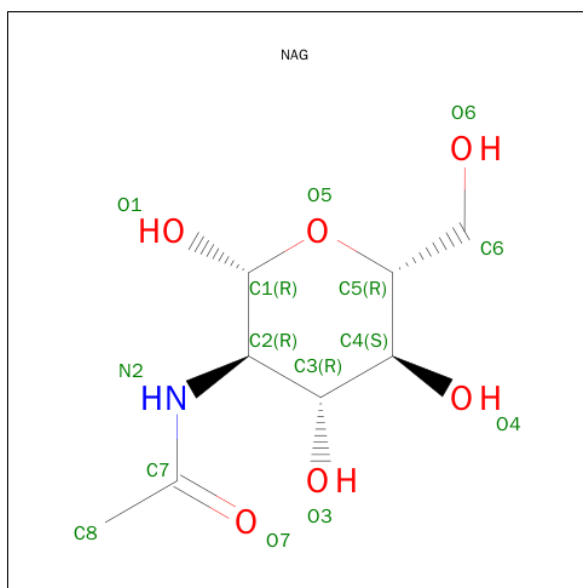
There are 6 unique types of molecules in this entry. The entry contains 9230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

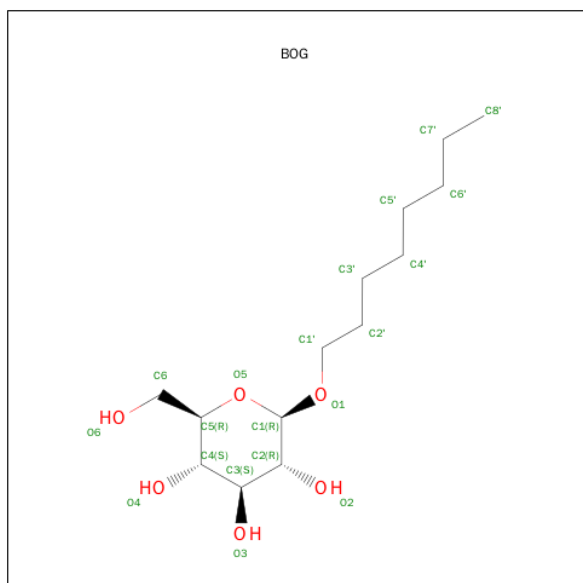


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

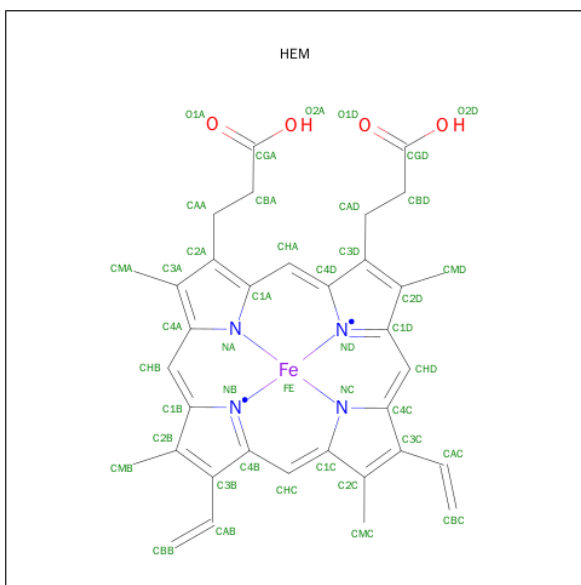
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula:  $C_{14}H_{28}O_6$ ).



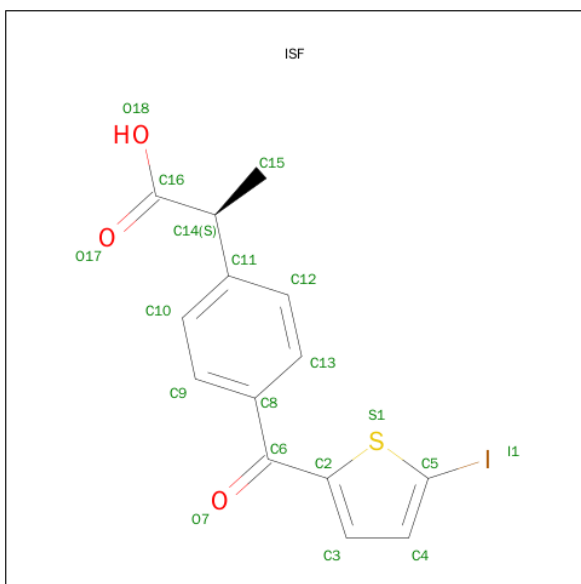
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- 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 43	C 34	Fe 1	N 4	O 4	0	0
5	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 6 is P-(2'-IODO-5'-THENOYL)HYDROTROPIC ACID (three-letter code: ISF) (formula: C<sub>14</sub>H<sub>11</sub>IO<sub>3</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	I	O	S	0	0
			19	14	1	3	1		

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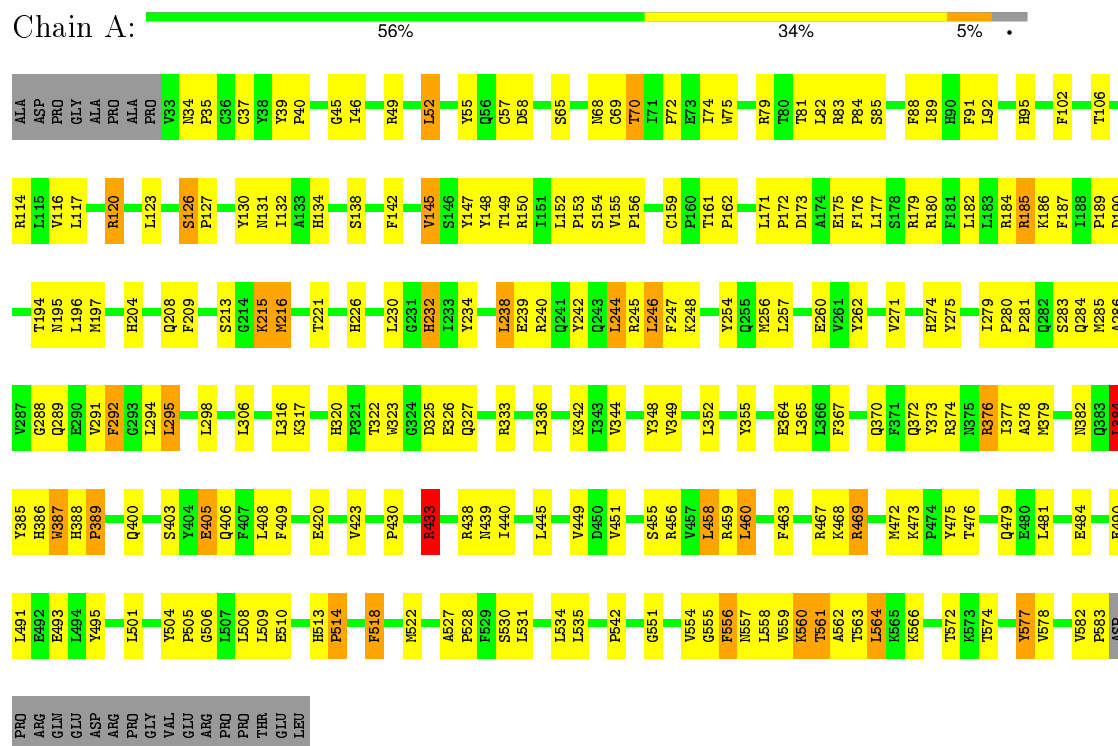
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	I	O	S	0	0
			19	14	1	3	1		

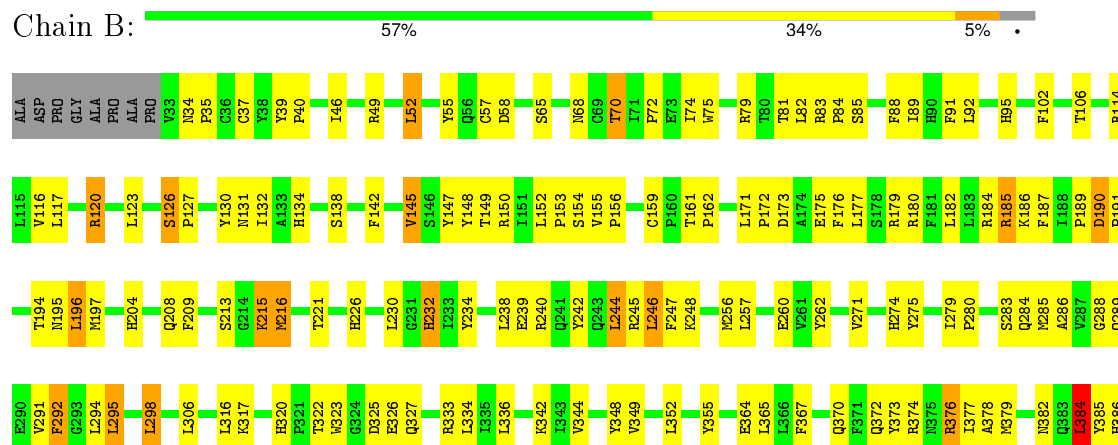
### 3 Residue-property plots

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

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



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







## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.69Å 209.94Å 234.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50 15.11 – 3.50	Depositor EDS
% Data completeness (in resolution range)	90.9 (15.00-3.50) 90.5 (15.11-3.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.73 (at 3.48Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.189 , 0.231 0.180 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	57.2	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 71.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 28057 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9230	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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, BOG, ISF, NAG

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	0.51	0/4615	0.75	5/6264 (0.1%)
1	B	0.51	0/4615	0.75	5/6264 (0.1%)
All	All	0.51	0/9230	0.75	10/12528 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	LEU	CA-CB-CG	6.39	130.00	115.30
1	A	384	LEU	CA-CB-CG	6.37	129.96	115.30
1	B	460	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	460	LEU	CA-CB-CG	5.41	127.73	115.30
1	B	433	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	433	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	A	370	GLN	N-CA-C	-5.08	97.30	111.00
1	A	577	TYR	N-CA-C	-5.07	97.31	111.00
1	B	370	GLN	N-CA-C	-5.06	97.33	111.00
1	B	577	TYR	N-CA-C	-5.06	97.34	111.00

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	4383	166	0
1	B	4477	0	4383	163	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
4	A	20	0	28	1	0
4	B	20	0	28	1	0
5	A	43	0	30	3	0
5	B	43	0	30	3	0
6	A	19	0	10	4	0
6	B	19	0	10	4	0
All	All	9230	0	9004	329	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 18.

All (329) 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:84:PRO:HG2	1:B:89:ILE:HD11	1.48	0.95
1:A:384:LEU:HD23	6:A:800:ISF:I1	2.39	0.93
1:B:384:LEU:HD23	6:B:800:ISF:I1	2.39	0.92
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.48	0.91
1:B:294:LEU:HD22	1:B:409:PHE:CE2	2.09	0.88
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.09	0.87
1:B:433:ARG:HB3	1:B:433:ARG:HH11	1.47	0.79
1:A:433:ARG:HH11	1:A:433:ARG:HB3	1.46	0.79
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.50	0.77
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.50	0.77
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.20	0.76
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.20	0.75
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.18	0.74
1:A:294:LEU:HD22	1:A:409:PHE:HE2	1.52	0.74
1:A:563:THR:HG22	1:A:566:LYS:HD3	1.70	0.74
1:B:294:LEU:HD22	1:B:409:PHE:HE2	1.52	0.74
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.18	0.73
1:B:563:THR:HG22	1:B:566:LYS:HD3	1.70	0.72
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.72	0.72
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.25	0.72
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.30	0.72
1:A:387:TRP:HB2	5:A:601:HEM:HAC	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.30	0.72
1:B:116:VAL:O	1:B:120:ARG:HB2	1.90	0.72
1:B:563:THR:HG23	1:B:566:LYS:H	1.56	0.71
1:A:116:VAL:O	1:A:120:ARG:HB2	1.90	0.71
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.25	0.70
1:B:384:LEU:CD2	6:B:800:ISF:I1	3.09	0.70
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.72	0.70
1:A:384:LEU:CD2	6:A:800:ISF:I1	3.09	0.70
1:A:563:THR:HG23	1:A:566:LYS:H	1.56	0.70
1:B:387:TRP:HB2	5:B:601:HEM:HAC	1.72	0.69
1:A:245:ARG:HH22	1:A:326:GLU:HG2	1.59	0.68
1:B:245:ARG:HH22	1:B:326:GLU:HG2	1.59	0.66
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.78	0.66
1:B:182:LEU:HB3	1:B:440:ILE:HD12	1.78	0.65
1:A:154:SER:HB2	1:A:459:ARG:HB2	1.78	0.65
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.32	0.65
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.32	0.64
1:A:403:SER:OG	1:A:406:GLN:HG3	1.97	0.64
1:B:403:SER:OG	1:B:406:GLN:HG3	1.97	0.64
1:B:274:HIS:O	1:B:294:LEU:HD21	1.99	0.63
1:B:154:SER:HB2	1:B:459:ARG:HB2	1.78	0.63
1:A:274:HIS:O	1:A:294:LEU:HD21	1.99	0.61
1:A:91:PHE:HD2	1:A:92:LEU:HD12	1.66	0.61
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.61
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.83	0.61
1:A:213:SER:HB3	1:A:216:MET:HB2	1.83	0.61
1:B:120:ARG:NH1	4:B:702:BOG:H1'2	2.16	0.60
1:B:91:PHE:HD2	1:B:92:LEU:HD12	1.66	0.60
1:A:491:LEU:HD11	1:A:509:LEU:HD13	1.84	0.60
1:A:230:LEU:CD2	1:A:336:LEU:HB3	2.32	0.60
1:A:120:ARG:NH1	4:A:702:BOG:H1'2	2.16	0.59
1:B:213:SER:HB3	1:B:216:MET:HB2	1.83	0.59
1:B:230:LEU:CD2	1:B:336:LEU:HB3	2.32	0.59
1:B:491:LEU:HD11	1:B:509:LEU:HD13	1.84	0.59
1:B:149:THR:O	1:B:378:ALA:HA	2.02	0.59
1:A:171:LEU:HD23	1:A:456:ARG:NE	2.18	0.59
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.38	0.59
1:B:171:LEU:HD23	1:B:456:ARG:NE	2.18	0.59
1:A:149:THR:O	1:A:378:ALA:HA	2.02	0.59
1:A:459:ARG:HG2	1:A:459:ARG:HH11	1.68	0.59
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:HB	1:B:58:ASP:HB3	1.85	0.58
1:B:459:ARG:HH11	1:B:459:ARG:HG2	1.68	0.58
1:A:52:LEU:HD12	1:A:52:LEU:H	1.69	0.58
1:B:52:LEU:HD12	1:B:52:LEU:H	1.69	0.58
1:A:132:ILE:HD13	1:A:458:LEU:HD12	1.86	0.57
1:A:215:LYS:H	1:A:215:LYS:HE2	1.70	0.57
1:B:132:ILE:HD13	1:B:458:LEU:HD12	1.86	0.57
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.40	0.57
1:B:176:PHE:CZ	1:B:180:ARG:HD2	2.40	0.56
1:A:239:GLU:CD	1:A:239:GLU:H	2.08	0.56
1:A:433:ARG:HH11	1:A:433:ARG:CB	2.18	0.56
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.40	0.56
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.41	0.56
1:A:46:ILE:HB	1:A:58:ASP:HB3	1.85	0.56
1:B:215:LYS:H	1:B:215:LYS:HE2	1.69	0.56
1:B:239:GLU:H	1:B:239:GLU:CD	2.08	0.56
1:A:577:TYR:HE2	1:A:583:PRO:HD3	1.71	0.56
1:A:176:PHE:CZ	1:A:180:ARG:HD2	2.40	0.56
1:A:102:PHE:O	1:A:106:THR:HG23	2.06	0.55
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.41	0.55
1:B:275:TYR:CE1	1:B:284:GLN:HB3	2.42	0.55
1:B:102:PHE:O	1:B:106:THR:HG23	2.06	0.55
1:A:39:TYR:OH	1:A:155:VAL:HG22	2.08	0.54
1:A:554:VAL:HG23	1:A:555:GLY:N	2.22	0.54
1:B:39:TYR:OH	1:B:155:VAL:HG22	2.08	0.54
1:B:554:VAL:HG23	1:B:555:GLY:N	2.22	0.54
1:A:130:TYR:HB3	1:A:134:HIS:O	2.08	0.54
1:B:379:MET:SD	1:B:458:LEU:HG	2.48	0.54
1:B:294:LEU:HD22	1:B:409:PHE:CD2	2.43	0.54
1:A:275:TYR:CE1	1:A:284:GLN:HB3	2.42	0.54
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.43	0.53
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.48	0.53
1:B:126:SER:HA	1:B:127:PRO:C	2.29	0.53
1:B:156:PRO:HD2	1:B:159:CYS:SG	2.48	0.53
1:B:577:TYR:HE2	1:B:583:PRO:HD3	1.71	0.53
1:A:490:GLU:HA	1:A:493:GLU:HG2	1.91	0.53
1:A:344:VAL:O	1:A:349:VAL:HG23	2.08	0.53
1:B:344:VAL:O	1:B:349:VAL:HG23	2.08	0.53
1:B:433:ARG:CB	1:B:433:ARG:HH11	2.18	0.53
1:A:171:LEU:HD23	1:A:456:ARG:HE	1.74	0.53
1:A:379:MET:SD	1:A:458:LEU:HG	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:TYR:HB3	1:B:134:HIS:O	2.08	0.53
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.39	0.52
1:A:126:SER:HA	1:A:127:PRO:C	2.29	0.52
1:B:187:PHE:CE2	1:B:189:PRO:HB3	2.44	0.52
1:A:195:ASN:HA	1:A:430:PRO:HA	1.91	0.52
1:B:582:VAL:CG2	1:B:583:PRO:HD2	2.39	0.52
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.45	0.52
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.45	0.52
1:A:342:LYS:HD2	1:A:559:VAL:O	2.09	0.52
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.45	0.52
1:B:342:LYS:HD2	1:B:559:VAL:O	2.09	0.52
1:A:256:MET:O	1:A:257:LEU:HD23	2.09	0.52
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.45	0.52
1:B:468:LYS:HA	1:B:472:MET:O	2.11	0.51
1:B:246:LEU:HD13	1:B:248:LYS:HB3	1.92	0.51
1:B:171:LEU:HD23	1:B:456:ARG:HE	1.74	0.51
1:B:490:GLU:HA	1:B:493:GLU:HG2	1.91	0.51
1:B:195:ASN:HA	1:B:430:PRO:HA	1.91	0.51
1:A:187:PHE:CE2	1:A:189:PRO:HB3	2.44	0.51
1:A:561:THR:HB	1:A:566:LYS:NZ	2.26	0.51
1:A:91:PHE:CE1	1:A:95:HIS:CD2	2.99	0.51
1:B:91:PHE:CE1	1:B:95:HIS:CD2	2.99	0.51
1:A:271:VAL:CG1	1:A:286:ALA:HB1	2.41	0.51
1:A:468:LYS:HA	1:A:472:MET:O	2.10	0.51
5:B:601:HEM:HMB1	5:B:601:HEM:HBB2	1.92	0.51
1:B:256:MET:O	1:B:257:LEU:HD23	2.09	0.51
1:B:271:VAL:CG1	1:B:286:ALA:HB1	2.41	0.50
1:B:561:THR:HB	1:B:566:LYS:NZ	2.26	0.50
1:B:389:PRO:HG3	1:B:440:ILE:HG12	1.93	0.50
1:B:52:LEU:HD12	1:B:52:LEU:N	2.27	0.50
1:A:289:GLN:OE1	1:A:291:VAL:HG12	2.12	0.50
1:A:150:ARG:HD3	1:A:152:LEU:O	2.12	0.50
1:A:463:PHE:CE2	1:A:467:ARG:HD3	2.47	0.50
1:A:389:PRO:HG3	1:A:440:ILE:HG12	1.92	0.50
1:A:372:GLN:HE22	1:B:373:TYR:H	1.59	0.50
5:A:601:HEM:HBB2	5:A:601:HEM:HMB1	1.93	0.50
1:A:246:LEU:HD13	1:A:248:LYS:HB3	1.92	0.50
1:A:52:LEU:N	1:A:52:LEU:HD12	2.27	0.49
1:A:208:GLN:NE2	1:A:230:LEU:H	2.11	0.49
1:B:150:ARG:HD3	1:B:152:LEU:O	2.12	0.49
1:B:463:PHE:CE2	1:B:467:ARG:HD3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:LEU:HB3	1:A:460:LEU:HD22	1.95	0.49
1:B:320:HIS:HE1	1:B:551:GLY:O	1.95	0.49
1:B:262:TYR:HB3	1:B:285:MET:CE	2.43	0.49
1:B:458:LEU:HB3	1:B:460:LEU:HD22	1.95	0.49
1:A:320:HIS:HE1	1:A:551:GLY:O	1.95	0.49
1:B:123:LEU:O	1:B:469:ARG:NH2	2.46	0.49
1:B:289:GLN:OE1	1:B:291:VAL:HG12	2.12	0.49
1:A:522:MET:O	6:A:800:ISF:H4	2.13	0.49
1:A:123:LEU:O	1:A:469:ARG:NH2	2.46	0.49
1:A:262:TYR:HB3	1:A:285:MET:CE	2.43	0.49
1:B:280:PRO:HG2	1:B:283:SER:OG	2.14	0.48
1:A:306:LEU:HD23	1:A:306:LEU:C	2.34	0.48
1:A:35:PRO:HB2	1:A:55:TYR:CD2	2.49	0.48
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.49	0.48
1:B:522:MET:O	6:B:800:ISF:H4	2.13	0.48
1:B:148:TYR:CZ	1:B:221:THR:HB	2.49	0.48
1:B:295:LEU:HD11	5:B:601:HEM:CAB	2.44	0.48
1:A:280:PRO:O	1:A:284:GLN:HG3	2.14	0.48
1:A:320:HIS:CE1	1:A:551:GLY:O	2.67	0.48
1:A:256:MET:HA	1:A:260:GLU:O	2.14	0.48
1:B:209:PHE:HB2	1:B:377:ILE:HG13	1.95	0.48
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.49	0.48
1:B:320:HIS:CE1	1:B:551:GLY:O	2.67	0.48
1:B:35:PRO:HB2	1:B:55:TYR:CD2	2.49	0.48
1:B:208:GLN:NE2	1:B:230:LEU:H	2.11	0.48
1:A:148:TYR:CZ	1:A:221:THR:HB	2.49	0.48
1:B:306:LEU:HD23	1:B:306:LEU:C	2.34	0.47
1:A:74:ILE:HG23	1:A:75:TRP:N	2.29	0.47
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.49	0.47
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.95	0.47
1:A:280:PRO:HG2	1:A:283:SER:OG	2.14	0.47
1:B:256:MET:HA	1:B:260:GLU:O	2.14	0.47
1:A:295:LEU:HD11	5:A:601:HEM:CAB	2.43	0.47
1:B:280:PRO:O	1:B:284:GLN:HG3	2.14	0.47
1:B:240:ARG:HE	1:B:288:GLY:HA2	1.80	0.47
1:B:74:ILE:HG23	1:B:75:TRP:N	2.29	0.47
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.49	0.47
1:B:323:TRP:CE3	1:B:327:GLN:HG2	2.50	0.46
1:A:81:THR:O	1:A:82:LEU:HD12	2.15	0.46
1:A:531:LEU:HD11	6:A:800:ISF:H10	1.98	0.46
1:B:177:LEU:HD21	1:B:495:TYR:OH	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:TRP:CD2	1:A:327:GLN:HG2	2.51	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.50	0.46
1:A:240:ARG:HE	1:A:288:GLY:HA2	1.80	0.46
1:B:230:LEU:HA	1:B:230:LEU:HD12	1.69	0.46
1:A:177:LEU:HD21	1:A:495:TYR:OH	2.15	0.46
1:A:150:ARG:HB3	1:A:379:MET:CE	2.46	0.46
1:B:323:TRP:CD2	1:B:327:GLN:HG2	2.51	0.46
1:B:81:THR:O	1:B:82:LEU:HD12	2.15	0.46
1:A:176:PHE:CE1	1:A:180:ARG:HD2	2.51	0.46
1:A:491:LEU:HD11	1:A:509:LEU:CD1	2.46	0.45
1:A:475:TYR:CE2	1:A:481:LEU:HD12	2.52	0.45
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.98	0.45
1:A:386:HIS:CD2	1:A:451:VAL:HG21	2.51	0.45
1:B:531:LEU:HD11	6:B:800:ISF:H10	1.98	0.45
1:B:240:ARG:HG3	1:B:271:VAL:HG21	1.98	0.45
1:B:386:HIS:CD2	1:B:451:VAL:HG21	2.51	0.45
1:A:420:GLU:HG3	1:A:572:THR:HB	1.99	0.45
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.51	0.45
1:A:215:LYS:H	1:A:215:LYS:CE	2.29	0.45
1:B:176:PHE:CE1	1:B:180:ARG:HD2	2.51	0.45
1:A:564:LEU:HD13	1:A:578:VAL:HG22	1.99	0.45
1:A:187:PHE:HE2	1:A:189:PRO:HB3	1.82	0.45
1:A:173:ASP:OD1	1:A:175:GLU:HB3	2.17	0.45
1:B:187:PHE:HE2	1:B:189:PRO:HB3	1.82	0.45
1:B:150:ARG:HB3	1:B:379:MET:CE	2.46	0.45
1:B:420:GLU:HG3	1:B:572:THR:HB	1.99	0.45
1:B:242:TYR:CD1	1:B:247:PHE:HZ	2.35	0.45
1:A:403:SER:OG	1:A:405:GLU:HG2	2.17	0.45
1:B:213:SER:CB	1:B:216:MET:HB2	2.46	0.45
1:B:215:LYS:CE	1:B:215:LYS:H	2.29	0.45
1:A:373:TYR:H	1:B:372:GLN:HE22	1.64	0.45
1:B:403:SER:OG	1:B:405:GLU:HG2	2.17	0.44
1:A:244:LEU:HD11	1:A:271:VAL:HG11	1.99	0.44
1:B:244:LEU:HD11	1:B:271:VAL:HG11	1.99	0.44
1:B:40:PRO:O	1:B:68:ASN:HB3	2.18	0.44
1:A:81:THR:C	1:A:82:LEU:HD12	2.38	0.44
1:B:247:PHE:HD1	1:B:325:ASP:OD2	2.00	0.44
1:B:535:LEU:HD13	1:B:535:LEU:HA	1.66	0.44
1:B:173:ASP:OD1	1:B:175:GLU:HB3	2.17	0.44
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.69	0.44
1:B:491:LEU:HD11	1:B:509:LEU:CD1	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:VAL:O	1:A:145:VAL:HG13	2.17	0.44
1:A:184:ARG:HA	1:A:438:ARG:O	2.17	0.44
1:B:564:LEU:HD13	1:B:578:VAL:HG22	1.99	0.44
1:B:81:THR:C	1:B:82:LEU:HD12	2.38	0.44
1:A:213:SER:CB	1:A:216:MET:HB2	2.46	0.44
1:A:262:TYR:HB3	1:A:285:MET:HE1	2.00	0.44
1:B:184:ARG:HA	1:B:438:ARG:O	2.18	0.44
1:A:70:THR:O	1:A:72:PRO:HD3	2.16	0.44
1:B:142:PHE:CG	1:B:142:PHE:O	2.71	0.44
1:B:70:THR:O	1:B:72:PRO:HD3	2.16	0.44
1:B:185:ARG:NE	1:B:438:ARG:HD3	2.26	0.44
1:A:247:PHE:HD1	1:A:325:ASP:OD2	2.00	0.44
1:B:114:ARG:HD3	1:B:365:LEU:O	2.18	0.44
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.86	0.44
1:B:563:THR:HG22	1:B:566:LYS:HB2	1.99	0.43
1:A:242:TYR:CD1	1:A:247:PHE:HZ	2.35	0.43
1:A:40:PRO:O	1:A:68:ASN:HB3	2.18	0.43
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.43
1:B:145:VAL:HG13	1:B:145:VAL:O	2.17	0.43
1:B:130:TYR:CE2	1:B:153:PRO:HD3	2.54	0.43
1:A:85:SER:O	1:A:89:ILE:HG12	2.19	0.43
1:A:185:ARG:NE	1:A:438:ARG:HD3	2.26	0.43
1:B:262:TYR:HB3	1:B:285:MET:HE2	2.01	0.43
1:A:114:ARG:HD3	1:A:365:LEU:O	2.18	0.43
1:A:445:LEU:O	1:A:449:VAL:HG23	2.19	0.43
1:B:85:SER:O	1:B:89:ILE:HG12	2.19	0.43
1:A:563:THR:HG22	1:A:566:LYS:HB2	1.99	0.43
1:A:130:TYR:CE2	1:A:153:PRO:HD3	2.54	0.43
1:B:240:ARG:NH1	1:B:271:VAL:HG22	2.34	0.43
1:A:481:LEU:HD11	1:A:510:GLU:HB2	2.01	0.43
1:B:382:ASN:OD1	1:B:386:HIS:HE1	2.02	0.43
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.86	0.43
1:A:535:LEU:HA	1:A:535:LEU:HD13	1.66	0.43
1:B:555:GLY:O	1:B:558:LEU:HB2	2.19	0.43
1:A:134:HIS:HD2	1:A:138:SER:OG	2.01	0.43
1:A:142:PHE:O	1:A:142:PHE:CG	2.71	0.43
1:B:134:HIS:HD2	1:B:138:SER:OG	2.01	0.43
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.54	0.42
1:B:197:MET:CE	1:B:423:VAL:HG13	2.49	0.42
1:A:388:HIS:N	1:A:389:PRO:CD	2.81	0.42
1:B:459:ARG:NH1	1:B:459:ARG:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ILE:O	1:B:57:CYS:HA	2.20	0.42
1:A:555:GLY:O	1:A:558:LEU:HB2	2.19	0.42
1:B:557:ASN:O	1:B:558:LEU:C	2.58	0.42
1:B:204:HIS:ND1	1:B:292:PHE:CE2	2.88	0.42
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.54	0.42
1:A:557:ASN:O	1:A:558:LEU:C	2.58	0.42
1:B:481:LEU:HD11	1:B:510:GLU:HB2	2.01	0.42
1:A:197:MET:CE	1:A:423:VAL:HG13	2.49	0.42
1:A:91:PHE:CD1	1:A:95:HIS:CD2	3.08	0.42
1:B:91:PHE:CD1	1:B:95:HIS:CD2	3.08	0.42
1:B:334:LEU:HA	1:B:334:LEU:HD23	1.89	0.42
1:A:501:LEU:HD21	1:A:506:GLY:HA2	2.02	0.42
1:B:445:LEU:O	1:B:449:VAL:HG23	2.19	0.42
1:A:46:ILE:O	1:A:57:CYS:HA	2.20	0.42
1:B:184:ARG:HB2	1:B:439:ASN:C	2.41	0.42
1:A:518:PHE:CG	1:A:522:MET:HG2	2.55	0.41
1:A:184:ARG:HB2	1:A:439:ASN:C	2.41	0.41
1:B:226:HIS:HB3	1:B:376:ARG:HA	2.02	0.41
1:A:382:ASN:OD1	1:A:386:HIS:HE1	2.02	0.41
1:A:355:TYR:CD1	1:A:355:TYR:N	2.88	0.41
1:A:238:LEU:HA	1:A:238:LEU:HD23	1.75	0.41
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.86	0.41
1:A:226:HIS:HB3	1:A:376:ARG:HA	2.02	0.41
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.93	0.41
1:B:279:ILE:O	1:B:284:GLN:NE2	2.53	0.41
1:B:518:PHE:CG	1:B:522:MET:HG2	2.55	0.41
1:B:501:LEU:HD21	1:B:506:GLY:HA2	2.02	0.41
1:B:155:VAL:O	1:B:459:ARG:NE	2.53	0.41
1:B:556:PHE:CD1	1:B:560:LYS:HD2	2.56	0.41
1:A:279:ILE:O	1:A:284:GLN:NE2	2.53	0.41
1:A:240:ARG:NH1	1:A:271:VAL:HG22	2.34	0.41
1:A:344:VAL:O	1:A:348:TYR:HB3	2.21	0.41
1:A:238:LEU:HD13	3:B:672:NAG:H62	2.02	0.41
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.81	0.41
1:A:504:TYR:HB3	1:A:505:PRO:HD3	2.03	0.41
1:A:556:PHE:CD1	1:A:560:LYS:HD2	2.56	0.41
1:A:161:THR:HB	1:A:162:PRO:CD	2.50	0.41
1:B:120:ARG:NH2	1:B:524:GLU:OE1	2.54	0.41
1:A:459:ARG:HG2	1:A:459:ARG:NH1	2.34	0.41
1:B:582:VAL:HG22	1:B:583:PRO:HD2	2.02	0.41
1:A:582:VAL:HG22	1:A:583:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:O	1:A:91:PHE:HB3	2.21	0.41
1:B:180:ARG:NH1	1:B:490:GLU:OE1	2.54	0.41
1:A:204:HIS:ND1	1:A:292:PHE:CE2	2.88	0.41
1:B:161:THR:HB	1:B:162:PRO:CD	2.50	0.41
1:B:232:HIS:ND1	1:B:232:HIS:N	2.68	0.41
1:B:355:TYR:N	1:B:355:TYR:CD1	2.87	0.41
1:A:154:SER:HB2	1:A:459:ARG:CB	2.48	0.40
1:B:88:PHE:O	1:B:92:LEU:HD13	2.22	0.40
1:A:197:MET:HE2	1:A:423:VAL:HG13	2.04	0.40
1:B:344:VAL:O	1:B:348:TYR:HB3	2.21	0.40
1:A:45:GLY:HA3	1:A:69:CYS:SG	2.61	0.40
1:B:433:ARG:CG	1:B:433:ARG:HH11	2.35	0.40
1:A:88:PHE:O	1:A:92:LEU:HD13	2.21	0.40
1:B:292:PHE:HA	1:B:298:LEU:HD23	2.03	0.40
1:A:254:TYR:C	1:A:254:TYR:CD1	2.95	0.40
1:B:79:ARG:O	1:B:83:ARG:HG3	2.22	0.40
1:A:180:ARG:NH1	1:A:490:GLU:OE1	2.54	0.40
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.62	0.40
1:A:79:ARG:O	1:A:83:ARG:HG3	2.22	0.40
1:B:196:LEU:HA	1:B:196:LEU:HD22	1.97	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	15	60
1	B	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	15	60
All	All	1098/1152 (95%)	980 (89%)	104 (10%)	14 (1%)	15	60

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	295	LEU
1	A	514	PRO
1	B	295	LEU
1	B	514	PRO
1	A	387	TRP
1	B	387	TRP
1	A	292	PHE
1	A	408	LEU
1	A	562	ALA
1	B	292	PHE
1	B	408	LEU
1	B	562	ALA
1	A	384	LEU
1	B	384	LEU

### 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	486/506 (96%)	437 (90%)	49 (10%)	9	40
1	B	486/506 (96%)	437 (90%)	49 (10%)	9	40
All	All	972/1012 (96%)	874 (90%)	98 (10%)	9	40

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

Mol	Chain	Res	Type
1	A	49	ARG
1	A	52	LEU
1	A	65	SER
1	A	70	THR
1	A	117	LEU
1	A	120	ARG
1	A	126	SER
1	A	145	VAL
1	A	179	ARG
1	A	185	ARG

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Mol	Chain	Res	Type
1	A	186	LYS
1	A	190	ASP
1	A	194	THR
1	A	196	LEU
1	A	215	LYS
1	A	216	MET
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	298	LEU
1	A	316	LEU
1	A	317	LYS
1	A	322	THR
1	A	352	LEU
1	A	374	ARG
1	A	376	ARG
1	A	385	TYR
1	A	389	PRO
1	A	400	GLN
1	A	405	GLU
1	A	433	ARG
1	A	455	SER
1	A	458	LEU
1	A	469	ARG
1	A	473	LYS
1	A	476	THR
1	A	479	GLN
1	A	484	GLU
1	A	513	HIS
1	A	514	PRO
1	A	518	PHE
1	A	530	SER
1	A	534	LEU
1	A	556	PHE
1	A	560	LYS
1	A	561	THR
1	A	564	LEU
1	A	574	THR
1	B	49	ARG
1	B	52	LEU
1	B	65	SER

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Mol	Chain	Res	Type
1	B	70	THR
1	B	117	LEU
1	B	120	ARG
1	B	126	SER
1	B	145	VAL
1	B	179	ARG
1	B	185	ARG
1	B	186	LYS
1	B	190	ASP
1	B	194	THR
1	B	196	LEU
1	B	215	LYS
1	B	216	MET
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	298	LEU
1	B	316	LEU
1	B	317	LYS
1	B	322	THR
1	B	352	LEU
1	B	374	ARG
1	B	376	ARG
1	B	385	TYR
1	B	389	PRO
1	B	400	GLN
1	B	405	GLU
1	B	433	ARG
1	B	455	SER
1	B	458	LEU
1	B	469	ARG
1	B	473	LYS
1	B	476	THR
1	B	479	GLN
1	B	484	GLU
1	B	513	HIS
1	B	514	PRO
1	B	518	PHE
1	B	530	SER
1	B	534	LEU
1	B	556	PHE

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Mol	Chain	Res	Type
1	B	560	LYS
1	B	561	THR
1	B	564	LEU
1	B	574	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	134	HIS
1	A	203	GLN
1	A	208	GLN
1	A	241	GLN
1	A	320	HIS
1	A	372	GLN
1	A	375	ASN
1	A	386	HIS
1	A	443	HIS
1	B	95	HIS
1	B	134	HIS
1	B	203	GLN
1	B	208	GLN
1	B	241	GLN
1	B	320	HIS
1	B	372	GLN
1	B	375	ASN
1	B	386	HIS
1	B	443	HIS

### 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 ⓘ

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	0.53	0	15,19,21	1.08	1 (6%)
3	NAG	A	672	3	14,14,15	0.68	0	15,19,21	1.00	1 (6%)
3	NAG	B	671	1,3	14,14,15	0.54	0	15,19,21	1.08	1 (6%)
3	NAG	B	672	3	14,14,15	0.68	0	15,19,21	0.99	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(°)	Ideal(°)
3	A	672	NAG	C4-C3-C2	-2.34	107.59	111.23
3	A	671	NAG	C2-N2-C7	-2.34	120.04	123.04
3	B	672	NAG	C4-C3-C2	-2.32	107.62	111.23
3	B	671	NAG	C2-N2-C7	-2.31	120.07	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	672	NAG	1	0



## 5.6 Ligand geometry

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	2.74	9 (30%)	24,82,82	2.06	8 (33%)
2	NAG	A	661	1	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
2	NAG	A	681	1	14,14,15	0.49	0	15,19,21	1.24	2 (13%)
4	BOG	A	702	-	20,20,20	1.00	1 (5%)	25,25,25	1.31	5 (20%)
6	ISF	A	800	-	15,20,20	1.70	3 (20%)	15,28,28	0.80	0
5	HEM	B	601	1	30,50,50	2.74	10 (33%)	24,82,82	2.06	8 (33%)
2	NAG	B	661	1	14,14,15	0.51	0	15,19,21	0.96	1 (6%)
2	NAG	B	681	1	14,14,15	0.50	0	15,19,21	1.24	2 (13%)
4	BOG	B	702	-	20,20,20	1.01	1 (5%)	25,25,25	1.31	5 (20%)
6	ISF	B	800	-	15,20,20	1.69	3 (20%)	15,28,28	0.79	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	ISF	A	800	-	-	0/8/16/16	0/2/2/2
5	HEM	B	601	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	ISF	B	800	-	-	0/8/16/16	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	HEM	C2D-C3D	-7.28	1.32	1.54
5	B	601	HEM	C2D-C3D	-7.26	1.32	1.54
5	A	601	HEM	C3C-CAC	-6.87	1.38	1.51
5	B	601	HEM	C3C-CAC	-6.83	1.38	1.51
5	B	601	HEM	C3B-CAB	-5.75	1.40	1.51
5	A	601	HEM	C3B-CAB	-5.74	1.40	1.51
5	A	601	HEM	C2C-C1C	-4.73	1.43	1.52
5	B	601	HEM	C2C-C1C	-4.73	1.43	1.52
6	A	800	ISF	C2-C6	-4.58	1.38	1.49
6	B	800	ISF	C2-C6	-4.56	1.38	1.49
5	B	601	HEM	C3D-C4D	-4.48	1.45	1.51
5	A	601	HEM	C3D-C4D	-4.46	1.45	1.51
6	B	800	ISF	C8-C6	-2.88	1.44	1.49
6	A	800	ISF	C8-C6	-2.88	1.44	1.49
5	B	601	HEM	C2D-C1D	-2.87	1.42	1.51
5	A	601	HEM	C2D-C1D	-2.86	1.42	1.51
6	A	800	ISF	C5-S1	-2.26	1.68	1.72
6	B	800	ISF	C5-S1	-2.19	1.68	1.72
5	B	601	HEM	C2A-C3A	-2.01	1.31	1.37
5	B	601	HEM	CBC-CAC	2.52	1.43	1.29
5	A	601	HEM	CBC-CAC	2.52	1.43	1.29
5	A	601	HEM	CBB-CAB	2.82	1.45	1.29
5	B	601	HEM	CBB-CAB	2.82	1.45	1.29
4	A	702	BOG	C4-C5	3.07	1.59	1.53
4	B	702	BOG	C4-C5	3.09	1.59	1.53
5	B	601	HEM	C4C-NC	3.62	1.40	1.36
5	A	601	HEM	C4C-NC	3.62	1.40	1.36

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	681	NAG	C2-N2-C7	-3.21	118.92	123.04
2	A	681	NAG	C2-N2-C7	-3.21	118.92	123.04
2	B	661	NAG	C2-N2-C7	-2.71	119.55	123.04
2	A	661	NAG	C2-N2-C7	-2.69	119.58	123.04
4	B	702	BOG	C1-C2-C3	-2.36	105.33	109.97
4	A	702	BOG	C1-C2-C3	-2.35	105.35	109.97
5	A	601	HEM	C3B-C4B-CHC	2.00	125.98	123.16
5	B	601	HEM	C3B-C4B-CHC	2.01	125.99	123.16
4	B	702	BOG	C1'-O1-C1	2.20	117.78	113.94
4	A	702	BOG	C1'-O1-C1	2.20	117.79	113.94
2	A	681	NAG	C6-C5-C4	2.37	118.85	113.02
2	B	681	NAG	C6-C5-C4	2.38	118.89	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	HEM	CMD-C2D-C3D	2.43	125.08	114.35
5	A	601	HEM	CMD-C2D-C3D	2.43	125.10	114.35
4	A	702	BOG	O1-C1-C2	2.45	111.13	108.04
4	B	702	BOG	O1-C1-C2	2.45	111.14	108.04
5	A	601	HEM	CMC-C2C-C3C	2.58	122.97	116.53
5	B	601	HEM	CMC-C2C-C3C	2.59	122.99	116.53
5	B	601	HEM	CAA-C2A-C1A	2.66	129.90	127.01
5	A	601	HEM	CAA-C2A-C1A	2.67	129.91	127.01
4	B	702	BOG	C3-C4-C5	2.73	114.95	110.20
4	A	702	BOG	C3-C4-C5	2.74	114.98	110.20
5	A	601	HEM	CBA-CAA-C2A	2.93	117.77	112.53
4	B	702	BOG	O5-C5-C4	2.93	115.19	109.68
5	B	601	HEM	CBA-CAA-C2A	2.94	117.81	112.53
4	A	702	BOG	O5-C5-C4	2.95	115.21	109.68
5	B	601	HEM	CMB-C2B-C3B	3.67	125.70	116.53
5	A	601	HEM	CMB-C2B-C3B	3.68	125.71	116.53
5	A	601	HEM	CAD-C3D-C2D	4.16	125.17	113.22
5	B	601	HEM	CAD-C3D-C2D	4.16	125.17	113.22
5	A	601	HEM	CAD-C3D-C4D	5.06	130.31	112.47
5	B	601	HEM	CAD-C3D-C4D	5.06	130.31	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	601	HEM	3	0
4	A	702	BOG	1	0
6	A	800	ISF	4	0
5	B	601	HEM	3	0
4	B	702	BOG	1	0
6	B	800	ISF	4	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 [i](#)

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

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	551/576 (95%)	-0.97	0 100 100	4, 18, 53, 91	0
1	B	551/576 (95%)	-0.96	0 100 100	4, 18, 53, 91	0
All	All	1102/1152 (95%)	-0.96	0 100 100	4, 18, 53, 91	0

There are no RSRZ outliers to report.

### 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<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	A	671	14/15	0.95	0.14	-0.06	4,22,31,34	0
3	NAG	B	671	14/15	0.94	0.14	-0.24	4,22,31,34	0
3	NAG	A	672	14/15	0.94	0.24	-	19,37,47,59	0
3	NAG	B	672	14/15	0.93	0.30	-	19,37,47,59	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<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	NAG	B	661	14/15	0.91	0.25	2.56	33,43,61,66	0
4	BOG	B	702	20/20	0.91	0.28	2.21	15,15,15,15	0
2	NAG	A	661	14/15	0.92	0.20	1.48	33,43,61,66	0
4	BOG	A	702	20/20	0.91	0.23	1.44	15,15,15,15	0
2	NAG	A	681	14/15	0.90	0.25	0.89	15,22,38,44	0
5	HEM	A	601	43/43	0.96	0.15	0.89	7,17,43,67	0
5	HEM	B	601	43/43	0.97	0.14	0.60	7,17,43,67	0
2	NAG	B	681	14/15	0.93	0.18	0.19	15,22,38,44	0
6	ISF	A	800	19/19	0.99	0.09	-1.09	15,15,15,15	0
6	ISF	B	800	19/19	0.99	0.08	-1.66	15,15,15,15	0

## 6.5 Other polymers

There are no such residues in this entry.