



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:32 PM GMT

PDB ID : 1PGG  
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH 1-(4-IODOBE NZOYL)-5-METHOXY-2-METHYLINDOLE-3-ACETIC ACID (IODOIN-DOMETHACIN), TRANS MODEL  
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.  
Deposited on : 1995-12-02  
Resolution : 4.50 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

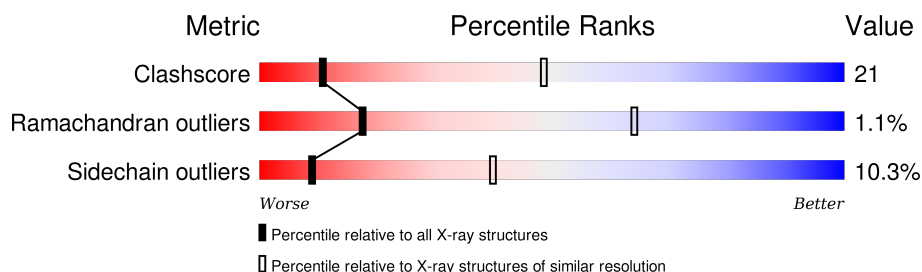
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.50 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	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	
1	B	576	

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
5	IMM	A	1	-	-	X	-
5	IMM	B	1	-	-	X	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9202 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).

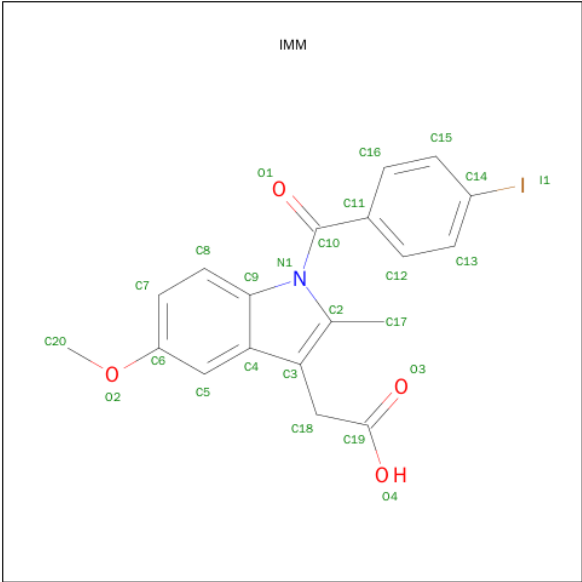
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		

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

- Molecule 5 is 1-(4-IODOBENZOYL)-5-METHOXY-2-METHYL INDOLE-3-ACETIC ACID (three-letter code: IMM) (formula:  $C_{19}H_{16}INO_4$ ).



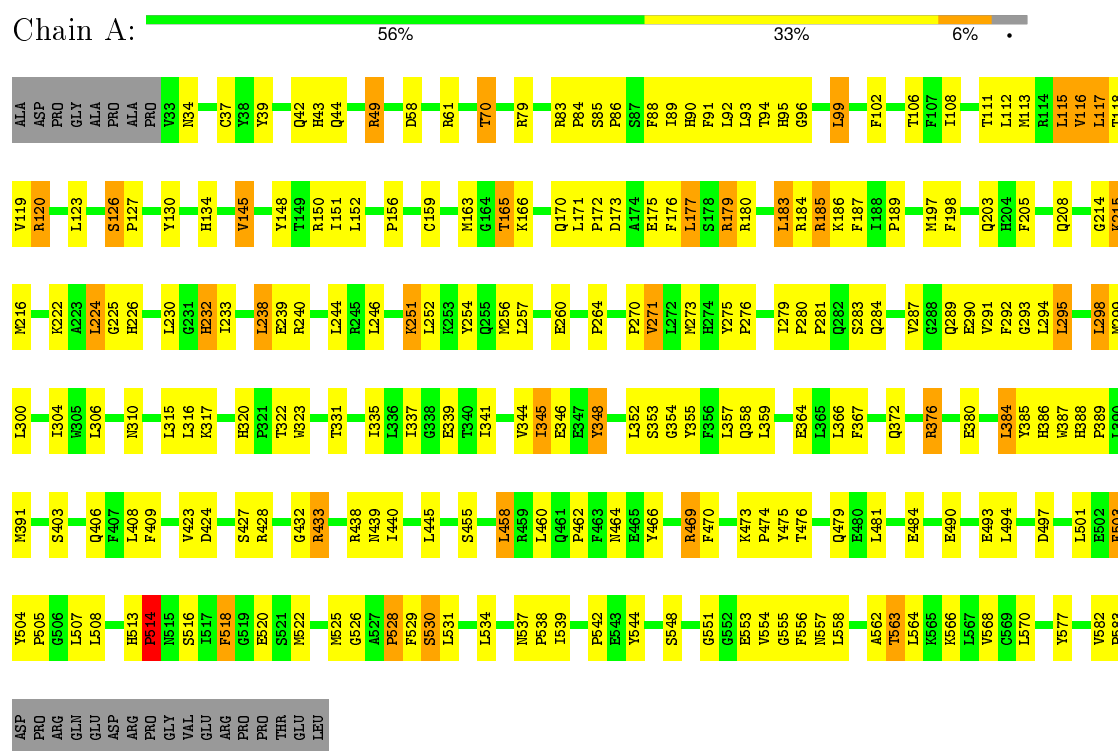
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
5	B	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

### 3 Residue-property plots

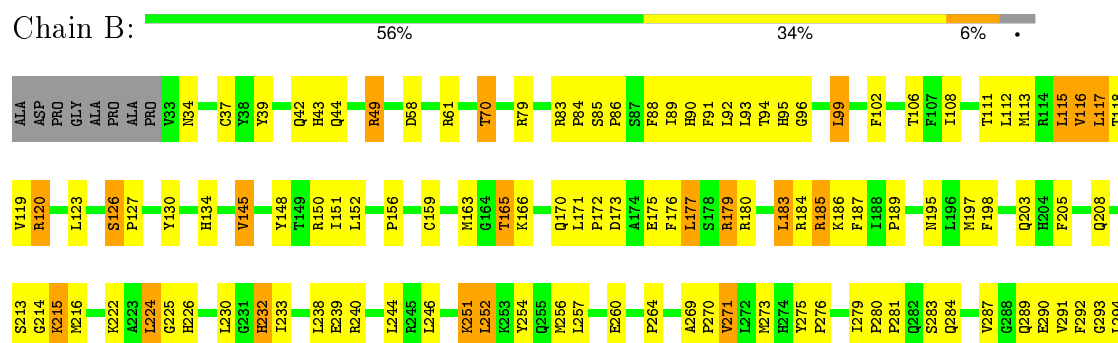
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



P576	L501	W387	L295
Y577	E502	R388	L298
V582	F503	P389	M299
P583	Y504	L390	L300
ASP	E505	M391	
ARG	E506	S403	T304
ARG	L507		M305
GLN	L508	Q406	L306
GLU	H513	F407	M310
ASP	P514	L408	
ARG	N515	F409	L315
PRO	S516		L316
GLY	F517	V423	K317
VAL	F518	D424	
GLU	G519		H320
ARG	E520	S427	P321
PRO	S521	R428	T322
PRO	M522		M323
THR	M525	G432	
GLU	G526	R433	T331
LEU	A527	R438	
	P528	M439	L335
	F529	I440	L336
	S530		L337
	L531	L445	G338
		E339	T340
	L534	S455	L341
	N537	L488	V344
	P538	R459	L345
	L539	L460	E346
		Q461	E347
	P542	P462	Y348
	E543	F463	
	Y544	M464	L352
	S548	E465	S353
		Y466	G354
	G551	R469	Y355
	G552	F470	F356
	E553		L357
	V554	K473	Q358
	G555	P474	L359
	F556	Y475	
	N557	T476	E364
	L558		L365
		Q479	L366
	A562	E480	F367
	L564	L481	
	X565		Q372
	X566	E484	
	X567		R376
	V568	E490	E380
	C569	L494	L384
	L570		Y385
		D497	Z386
	E575		

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.22Å 208.99Å 232.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.50	Depositor
% Data completeness (in resolution range)	79.2 (8.00-4.50)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.254 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, IMM, 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	0.70	0/4615	0.86	8/6264 (0.1%)
1	B	0.70	0/4615	0.86	8/6264 (0.1%)
All	All	0.70	0/9230	0.86	16/12528 (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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	433	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	433	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	408	LEU	N-CA-C	6.29	127.97	111.00
1	B	408	LEU	N-CA-C	6.28	127.96	111.00
1	A	148	TYR	N-CA-C	-5.82	95.30	111.00
1	B	148	TYR	N-CA-C	-5.80	95.34	111.00
1	A	225	GLY	N-CA-C	-5.51	99.32	113.10
1	B	225	GLY	N-CA-C	-5.51	99.33	113.10
1	A	224	LEU	N-CA-C	-5.47	96.23	111.00
1	B	224	LEU	N-CA-C	-5.46	96.25	111.00
1	B	460	LEU	CA-CB-CG	5.17	127.20	115.30
1	A	460	LEU	CA-CB-CG	5.17	127.19	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	LEU	CA-CB-CG	5.13	127.11	115.30
1	A	177	LEU	CA-CB-CG	5.11	127.05	115.30
1	B	99	LEU	CA-CB-CG	-5.03	103.73	115.30
1	A	99	LEU	CA-CB-CG	-5.03	103.74	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	Sidechain
1	B	39	TYR	Sidechain

## 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	188	0
1	B	4477	0	4383	197	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0
3	A	28	0	25	1	0
3	B	28	0	25	1	0
4	A	43	0	30	7	0
4	B	43	0	30	7	0
5	A	25	0	15	15	0
5	B	25	0	15	16	0
All	All	9202	0	8958	383	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 21.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:MET:HG3	4:A:601:HEM:HAB	1.41	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.41	0.98
5:B:1:IMM:H172	5:B:1:IMM:H16	1.52	0.90
5:A:1:IMM:H16	5:A:1:IMM:H172	1.52	0.89
1:A:91:PHE:HD1	1:A:92:LEU:HD12	1.38	0.89
1:B:91:PHE:HD1	1:B:92:LEU:HD12	1.38	0.88
1:A:359:LEU:HD13	5:A:1:IMM:H203	1.56	0.87
1:B:359:LEU:HD13	5:B:1:IMM:H203	1.56	0.85
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.60	0.84
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.14	0.83
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.60	0.83
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.14	0.83
1:A:530:SER:CB	5:A:1:IMM:H12	2.10	0.82
1:B:530:SER:CB	5:B:1:IMM:H12	2.10	0.82
1:A:344:VAL:O	1:A:348:TYR:HB3	1.84	0.78
1:A:563:THR:HG22	1:A:566:LYS:H	1.50	0.77
1:B:344:VAL:O	1:B:348:TYR:HB3	1.84	0.77
1:B:563:THR:HG22	1:B:566:LYS:H	1.49	0.77
1:B:352:LEU:HD11	1:B:387:TRP:CH2	2.21	0.76
1:A:352:LEU:HD11	1:A:387:TRP:CH2	2.21	0.76
1:B:294:LEU:HD22	1:B:409:PHE:CD1	2.22	0.75
1:B:150:ARG:HD3	1:B:152:LEU:O	1.87	0.75
1:A:150:ARG:HD3	1:A:152:LEU:O	1.87	0.75
1:A:294:LEU:HD22	1:A:409:PHE:CD1	2.22	0.74
1:A:88:PHE:O	1:A:92:LEU:HD13	1.88	0.74
1:B:352:LEU:HD11	1:B:387:TRP:HH2	1.51	0.74
1:B:88:PHE:O	1:B:92:LEU:HD13	1.88	0.73
1:A:352:LEU:HD11	1:A:387:TRP:HH2	1.51	0.73
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.70	0.73
1:B:102:PHE:O	1:B:106:THR:HG23	1.89	0.73
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.70	0.72
1:A:294:LEU:HD22	1:A:409:PHE:HD1	1.54	0.72
1:B:152:LEU:HD21	1:B:469:ARG:HG2	1.70	0.72
1:A:152:LEU:HD21	1:A:469:ARG:HG2	1.70	0.71
1:B:294:LEU:HD22	1:B:409:PHE:HD1	1.54	0.71
5:A:1:IMM:C16	5:A:1:IMM:H172	2.21	0.71
1:A:102:PHE:O	1:A:106:THR:HG23	1.89	0.71
1:B:359:LEU:HD22	5:B:1:IMM:C20	2.21	0.70
1:B:294:LEU:O	1:B:295:LEU:HG	1.91	0.70
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.22	0.70
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.26	0.70
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:O	1:A:295:LEU:HG	1.91	0.69
1:A:359:LEU:HD22	5:A:1:IMM:C20	2.21	0.69
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.22	0.69
5:B:1:IMM:H172	5:B:1:IMM:C16	2.21	0.69
1:B:530:SER:HB3	5:B:1:IMM:H12	1.75	0.68
1:B:91:PHE:CD1	1:B:92:LEU:HD12	2.26	0.68
1:A:530:SER:HB3	5:A:1:IMM:H12	1.75	0.68
1:A:91:PHE:CD1	1:A:92:LEU:HD12	2.26	0.67
1:A:79:ARG:O	1:A:83:ARG:HG3	1.94	0.67
1:B:79:ARG:O	1:B:83:ARG:HG3	1.94	0.66
1:A:187:PHE:HE1	1:A:189:PRO:HB3	1.60	0.66
1:B:187:PHE:HE1	1:B:189:PRO:HB3	1.60	0.66
1:B:386:HIS:HD2	1:B:388:HIS:HE1	1.43	0.66
1:A:386:HIS:HD2	1:A:388:HIS:HE1	1.43	0.66
1:A:88:PHE:CD2	1:A:89:ILE:HD13	2.33	0.63
1:B:88:PHE:HD2	1:B:89:ILE:HD13	1.64	0.63
1:B:88:PHE:CD2	1:B:89:ILE:HD13	2.33	0.63
1:A:88:PHE:HD2	1:A:89:ILE:HD13	1.64	0.63
1:B:116:VAL:O	1:B:120:ARG:HB2	1.98	0.62
1:B:359:LEU:HD22	5:B:1:IMM:H203	1.82	0.62
1:B:123:LEU:O	1:B:469:ARG:NH2	2.32	0.62
1:A:116:VAL:O	1:A:120:ARG:HB2	1.98	0.62
1:A:123:LEU:O	1:A:469:ARG:NH2	2.32	0.62
1:A:470:PHE:CZ	1:A:529:PHE:CE2	2.87	0.62
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.39	0.62
1:B:553:GLU:HG3	1:B:557:ASN:HD21	1.65	0.62
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.35	0.62
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.35	0.61
1:B:470:PHE:CZ	1:B:529:PHE:CE2	2.87	0.61
1:B:126:SER:HA	1:B:127:PRO:C	2.20	0.61
5:A:1:IMM:H16	5:A:1:IMM:C17	2.26	0.61
1:A:359:LEU:HD22	5:A:1:IMM:H203	1.82	0.61
5:B:1:IMM:C17	5:B:1:IMM:H16	2.26	0.61
1:A:553:GLU:HG3	1:A:557:ASN:HD21	1.65	0.61
5:B:1:IMM:C19	5:B:1:IMM:H5	2.31	0.60
1:A:126:SER:HA	1:A:127:PRO:C	2.20	0.60
1:B:85:SER:O	1:B:89:ILE:HG12	2.01	0.60
1:A:85:SER:O	1:A:89:ILE:HG12	2.01	0.60
1:A:49:ARG:O	1:B:320:HIS:HD2	1.85	0.60
1:B:117:LEU:HD12	1:B:531:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LEU:HD12	1:A:531:LEU:HD13	1.84	0.59
1:B:208:GLN:NE2	1:B:230:LEU:H	2.00	0.59
5:A:1:IMM:C19	5:A:1:IMM:H5	2.31	0.59
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.38	0.59
1:B:337:ILE:O	1:B:341:ILE:HG13	2.02	0.59
1:A:290:GLU:H	1:A:290:GLU:CD	2.06	0.59
1:A:531:LEU:HD21	5:A:1:IMM:H7	1.85	0.58
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.38	0.58
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.85	0.58
1:A:208:GLN:NE2	1:A:230:LEU:H	2.00	0.58
1:B:348:TYR:C	1:B:348:TYR:CD1	2.77	0.58
1:A:337:ILE:O	1:A:341:ILE:HG13	2.02	0.58
1:A:320:HIS:HD2	1:B:49:ARG:O	1.86	0.58
1:A:348:TYR:CD1	1:A:348:TYR:C	2.77	0.58
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.39	0.58
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.85	0.57
1:A:203:GLN:HA	4:A:601:HEM:HBC2	1.86	0.57
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.69	0.57
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.39	0.57
1:B:290:GLU:CD	1:B:290:GLU:H	2.06	0.57
1:B:424:ASP:O	1:B:428:ARG:HG3	2.05	0.57
1:B:531:LEU:HD21	5:B:1:IMM:H7	1.85	0.57
1:B:203:GLN:HA	4:B:601:HEM:HBC2	1.86	0.57
1:B:306:LEU:HD23	1:B:306:LEU:C	2.25	0.57
1:A:306:LEU:HD23	1:A:306:LEU:C	2.25	0.57
1:A:424:ASP:O	1:A:428:ARG:HG3	2.05	0.56
1:B:185:ARG:HH21	1:B:438:ARG:HG2	1.69	0.56
1:A:346:GLU:HG2	1:A:359:LEU:O	2.06	0.56
1:A:518:PHE:CE2	1:A:522:MET:HG2	2.40	0.56
1:B:346:GLU:HG2	1:B:359:LEU:O	2.06	0.56
1:B:518:PHE:CE2	1:B:522:MET:HG2	2.40	0.56
1:B:173:ASP:OD2	1:B:175:GLU:HB3	2.06	0.55
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.41	0.55
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.47	0.55
1:A:79:ARG:HH11	1:A:83:ARG:HH21	1.55	0.55
1:B:289:GLN:HG3	1:B:292:PHE:CZ	2.41	0.55
1:A:173:ASP:OD2	1:A:175:GLU:HB3	2.06	0.55
1:B:176:PHE:HE2	1:B:494:LEU:HD11	1.72	0.55
1:B:386:HIS:HD2	1:B:388:HIS:CE1	2.25	0.54
1:B:113:MET:SD	5:B:1:IMM:H201	2.47	0.54
1:A:113:MET:SD	5:A:1:IMM:H201	2.47	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:PHE:HE2	1:A:494:LEU:HD11	1.72	0.54
1:A:180:ARG:NH1	1:A:490:GLU:OE1	2.40	0.54
1:A:503:PHE:CE2	1:A:507:LEU:HD11	2.42	0.54
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.47	0.54
1:B:180:ARG:NH1	1:B:490:GLU:OE1	2.40	0.54
1:B:503:PHE:CE2	1:B:507:LEU:HD11	2.42	0.54
1:B:79:ARG:HH11	1:B:83:ARG:HH21	1.55	0.54
1:A:215:LYS:H	1:A:215:LYS:CD	2.21	0.53
1:B:554:VAL:HG23	1:B:555:GLY:N	2.23	0.53
1:B:513:HIS:HB2	1:B:516:SER:OG	2.08	0.53
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.43	0.53
1:B:151:ILE:HG13	1:B:529:PHE:CZ	2.43	0.53
1:B:215:LYS:H	1:B:215:LYS:CD	2.21	0.53
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.44	0.53
1:A:388:HIS:N	1:A:389:PRO:CD	2.71	0.53
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.91	0.53
1:B:388:HIS:N	1:B:389:PRO:CD	2.71	0.53
1:B:403:SER:OG	1:B:406:GLN:HG3	2.09	0.53
1:A:513:HIS:HB2	1:A:516:SER:OG	2.08	0.53
1:A:554:VAL:HG23	1:A:555:GLY:N	2.23	0.52
1:A:150:ARG:NH2	1:A:458:LEU:O	2.41	0.52
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.44	0.52
1:A:403:SER:OG	1:A:406:GLN:HG3	2.09	0.52
1:B:537:ASN:OD1	1:B:538:PRO:HD2	2.10	0.52
1:A:537:ASN:OD1	1:A:538:PRO:HD2	2.10	0.52
1:B:353:SER:OG	1:B:354:GLY:N	2.42	0.52
1:A:294:LEU:CD2	1:A:409:PHE:HD1	2.23	0.52
1:B:150:ARG:NH2	1:B:458:LEU:O	2.42	0.52
1:A:88:PHE:CZ	1:A:92:LEU:HD21	2.45	0.51
1:A:353:SER:OG	1:A:354:GLY:N	2.42	0.51
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.91	0.51
1:A:386:HIS:HD2	1:A:388:HIS:CE1	2.25	0.51
1:B:391:MET:HG3	4:B:601:HEM:CAB	2.29	0.51
5:A:1:IMM:C19	5:A:1:IMM:C5	2.89	0.51
1:B:464:ASN:ND2	1:B:474:PRO:HB2	2.25	0.51
1:B:187:PHE:CE1	1:B:189:PRO:HB3	2.43	0.51
1:A:42:GLN:HG3	1:A:70:THR:CG2	2.41	0.51
1:B:391:MET:CG	4:B:601:HEM:HAB	2.29	0.51
1:A:58:ASP:HB2	1:B:548:SER:HB3	1.92	0.51
1:A:88:PHE:O	1:A:91:PHE:HB3	2.11	0.51
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:GLN:HG3	1:B:70:THR:CG2	2.41	0.50
1:A:94:THR:O	1:A:95:HIS:ND1	2.44	0.50
1:B:294:LEU:CD2	1:B:409:PHE:HD1	2.23	0.50
1:B:94:THR:O	1:B:95:HIS:ND1	2.44	0.50
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.46	0.50
1:A:187:PHE:CE1	1:A:189:PRO:HB3	2.43	0.50
1:B:175:GLU:O	1:B:179:ARG:HG3	2.11	0.50
1:B:359:LEU:CD1	5:B:1:IMM:H203	2.36	0.50
1:B:88:PHE:O	1:B:91:PHE:HB3	2.11	0.50
1:B:88:PHE:CZ	1:B:92:LEU:HD21	2.45	0.50
1:A:175:GLU:O	1:A:179:ARG:HG3	2.11	0.50
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.46	0.50
1:B:115:LEU:HD23	1:B:119:VAL:HG21	1.94	0.50
5:B:1:IMM:C19	5:B:1:IMM:C5	2.89	0.49
1:A:359:LEU:CD1	5:A:1:IMM:H203	2.36	0.49
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.48	0.49
1:B:184:ARG:HA	1:B:438:ARG:O	2.12	0.49
1:A:522:MET:O	1:A:526:GLY:N	2.46	0.49
1:A:184:ARG:HA	1:A:438:ARG:O	2.12	0.49
1:B:525:MET:O	1:B:529:PHE:HD2	1.95	0.49
1:B:522:MET:O	1:B:526:GLY:N	2.46	0.49
1:A:525:MET:O	1:A:529:PHE:HD2	1.95	0.49
1:A:203:GLN:HG3	4:A:601:HEM:C1C	2.48	0.48
1:A:118:THR:OG1	1:A:119:VAL:N	2.46	0.48
1:B:445:LEU:O	1:B:445:LEU:HG	2.12	0.48
1:A:445:LEU:HG	1:A:445:LEU:O	2.12	0.48
1:A:256:MET:O	1:A:257:LEU:HD23	2.13	0.48
1:A:93:LEU:HD13	1:A:355:TYR:CE2	2.48	0.48
1:A:280:PRO:HG2	1:A:283:SER:OG	2.13	0.48
1:A:528:PRO:O	1:A:529:PHE:C	2.49	0.48
1:B:118:THR:OG1	1:B:119:VAL:N	2.46	0.48
1:B:280:PRO:HG2	1:B:283:SER:OG	2.13	0.48
1:B:203:GLN:HG3	4:B:601:HEM:C1C	2.48	0.48
1:B:528:PRO:O	1:B:529:PHE:C	2.49	0.48
1:B:388:HIS:N	1:B:389:PRO:HD3	2.29	0.48
1:B:93:LEU:HD13	1:B:355:TYR:CE2	2.48	0.48
1:B:304:ILE:HD13	1:B:568:VAL:HG22	1.96	0.48
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.48	0.48
1:A:388:HIS:N	1:A:389:PRO:HD3	2.29	0.47
1:B:348:TYR:HD1	1:B:348:TYR:C	2.17	0.47
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:HIS:CD2	1:B:49:ARG:O	2.68	0.47
1:A:115:LEU:HD23	1:A:119:VAL:HG21	1.94	0.47
1:B:320:HIS:HE1	1:B:551:GLY:O	1.98	0.47
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.49	0.47
1:A:276:PRO:HG2	1:A:279:ILE:HD12	1.97	0.47
1:B:320:HIS:CE1	1:B:551:GLY:O	2.67	0.47
1:A:320:HIS:CE1	1:A:551:GLY:O	2.67	0.47
1:A:254:TYR:HA	1:A:264:PRO:HD3	1.96	0.47
1:B:256:MET:O	1:B:257:LEU:HD23	2.13	0.47
1:B:273:MET:HE2	1:B:287:VAL:HG22	1.96	0.47
1:A:90:HIS:O	1:A:90:HIS:CD2	2.68	0.47
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.49	0.47
1:A:475:TYR:CE2	1:A:481:LEU:HD12	2.50	0.47
1:B:90:HIS:CD2	1:B:90:HIS:O	2.68	0.47
1:A:348:TYR:C	1:A:348:TYR:HD1	2.17	0.47
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.96	0.47
1:A:130:TYR:HB3	1:A:134:HIS:O	2.15	0.47
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.79	0.46
1:B:179:ARG:HH11	1:B:179:ARG:HB3	1.80	0.46
1:A:548:SER:HB3	1:B:58:ASP:HB2	1.96	0.46
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.51	0.46
1:B:205:PHE:O	1:B:208:GLN:HG2	2.14	0.46
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.97	0.46
1:B:254:TYR:HA	1:B:264:PRO:HD3	1.96	0.46
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.79	0.46
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.97	0.46
1:B:276:PRO:HG2	1:B:279:ILE:CD1	2.46	0.46
1:B:130:TYR:HB3	1:B:134:HIS:O	2.15	0.46
1:A:179:ARG:HB3	1:A:179:ARG:HH11	1.80	0.46
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.46	0.46
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.50	0.46
1:A:205:PHE:O	1:A:208:GLN:HG2	2.14	0.46
1:A:304:ILE:HD13	1:A:568:VAL:HG22	1.96	0.46
1:B:470:PHE:HZ	1:B:529:PHE:CE2	2.32	0.46
1:B:275:TYR:CE2	1:B:284:GLN:HB3	2.51	0.46
1:A:214:GLY:N	1:A:215:LYS:HE2	2.31	0.45
1:A:553:GLU:HG3	1:A:557:ASN:ND2	2.30	0.45
1:B:276:PRO:HG2	1:B:279:ILE:HD12	1.97	0.45
1:A:320:HIS:HE1	1:A:551:GLY:O	1.98	0.45
1:A:388:HIS:CD2	4:A:601:HEM:NB	2.85	0.45
1:A:185:ARG:NE	1:A:438:ARG:HH11	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.87	0.45
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.52	0.45
1:A:61:ARG:NH1	1:B:542:PRO:O	2.50	0.45
1:B:185:ARG:NE	1:B:438:ARG:HH11	2.14	0.45
1:B:256:MET:HA	1:B:260:GLU:O	2.16	0.45
1:B:214:GLY:N	1:B:215:LYS:HE2	2.31	0.45
1:A:389:PRO:HG3	1:A:440:ILE:CG1	2.47	0.45
1:B:289:GLN:HG3	1:B:292:PHE:CE1	2.52	0.45
1:B:470:PHE:HZ	1:B:529:PHE:CZ	2.35	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.76	0.44
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.52	0.44
1:A:470:PHE:HZ	1:A:529:PHE:CE2	2.32	0.44
1:A:49:ARG:O	1:B:320:HIS:CD2	2.67	0.44
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.72	0.44
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.82	0.44
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.52	0.44
1:A:115:LEU:O	1:A:119:VAL:HG23	2.18	0.44
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.53	0.44
1:B:315:LEU:HD12	1:B:558:LEU:HD11	1.99	0.44
1:A:256:MET:HA	1:A:260:GLU:O	2.17	0.44
1:A:216:MET:HG2	3:A:672:NAG:H83	1.99	0.44
1:B:387:TRP:NE1	1:B:522:MET:HE3	2.33	0.44
1:A:387:TRP:HZ2	5:A:1:IMM:I1	2.71	0.44
1:A:315:LEU:HD12	1:A:558:LEU:HD11	1.99	0.44
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.99	0.44
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.53	0.44
1:B:216:MET:HG2	3:B:672:NAG:H83	1.99	0.44
1:A:357:LEU:HD12	1:A:358:GLN:N	2.33	0.44
1:B:251:LYS:HG3	1:B:310:ASN:CG	2.38	0.44
1:B:115:LEU:O	1:B:119:VAL:HG23	2.18	0.44
1:B:357:LEU:HD12	1:B:358:GLN:N	2.33	0.44
1:A:344:VAL:CG1	1:A:534:LEU:HD21	2.48	0.44
1:B:344:VAL:CG1	1:B:534:LEU:HD21	2.48	0.44
1:B:331:THR:O	1:B:335:ILE:HG13	2.18	0.44
1:A:387:TRP:NE1	1:A:522:MET:CE	2.81	0.43
1:A:88:PHE:CE1	1:A:92:LEU:HD11	2.53	0.43
1:A:331:THR:O	1:A:335:ILE:HG13	2.18	0.43
1:B:388:HIS:CD2	4:B:601:HEM:NB	2.85	0.43
1:B:387:TRP:NE1	1:B:522:MET:CE	2.81	0.43
1:B:553:GLU:HG3	1:B:557:ASN:ND2	2.31	0.43
1:A:341:ILE:HD12	1:A:539:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:MET:HB3	1:B:462:PRO:HG3	1.99	0.43
1:A:391:MET:CG	4:A:601:HEM:HAB	2.30	0.43
1:B:389:PRO:HG3	1:B:440:ILE:CG1	2.47	0.43
1:B:387:TRP:HZ2	5:B:1:IMM:I1	2.71	0.43
1:B:88:PHE:CE1	1:B:92:LEU:HD11	2.53	0.43
1:B:503:PHE:CZ	1:B:507:LEU:HD11	2.53	0.43
1:A:251:LYS:HG3	1:A:310:ASN:CG	2.38	0.43
1:B:345:ILE:HG12	1:B:534:LEU:HD23	2.01	0.43
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.52	0.43
1:A:189:PRO:HA	1:A:432:GLY:HA2	2.00	0.43
1:A:470:PHE:HZ	1:A:529:PHE:CZ	2.35	0.43
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.88	0.43
1:A:273:MET:HE2	1:A:287:VAL:HG22	2.01	0.43
1:A:127:PRO:HG2	1:B:544:TYR:CE1	2.53	0.43
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.87	0.43
1:B:85:SER:HA	1:B:86:PRO:HD3	1.78	0.43
1:B:189:PRO:HA	1:B:432:GLY:HA2	2.00	0.43
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.53	0.43
1:B:215:LYS:HE3	1:B:222:LYS:NZ	2.34	0.43
1:B:43:HIS:O	1:B:44:GLN:HB2	2.19	0.43
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.72	0.43
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.01	0.43
1:B:295:LEU:HD21	4:B:601:HEM:HBB2	2.01	0.43
1:B:384:LEU:HG	5:B:1:IMM:I1	2.89	0.43
1:A:239:GLU:CD	1:A:239:GLU:H	2.22	0.43
1:B:165:THR:HG22	1:B:166:LYS:HG2	2.01	0.43
1:A:391:MET:HG3	4:A:601:HEM:CAB	2.29	0.42
1:B:341:ILE:HD12	1:B:539:ILE:HD11	2.01	0.42
1:A:555:GLY:O	1:A:558:LEU:HB2	2.19	0.42
1:B:366:LEU:HA	1:B:366:LEU:HD23	1.76	0.42
1:B:575:CYS:HA	1:B:576:PRO:HD2	1.93	0.42
1:A:215:LYS:HE3	1:A:222:LYS:NZ	2.34	0.42
1:A:387:TRP:NE1	1:A:522:MET:HE3	2.34	0.42
1:A:372:GLN:HE22	1:B:372:GLN:HA	1.83	0.42
1:A:198:PHE:C	1:A:198:PHE:CD1	2.93	0.42
1:A:345:ILE:HG12	1:A:534:LEU:HD23	2.01	0.42
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.50	0.42
1:B:198:PHE:CD1	1:B:198:PHE:C	2.93	0.42
1:B:252:LEU:HA	1:B:252:LEU:HD12	1.92	0.42
1:A:544:TYR:CE1	1:B:127:PRO:HG2	2.55	0.42
1:B:239:GLU:H	1:B:239:GLU:CD	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:HIS:O	1:A:44:GLN:HB2	2.19	0.42
1:A:384:LEU:HG	5:A:1:IMM:I1	2.89	0.42
1:A:42:GLN:HG3	1:A:70:THR:HG23	2.02	0.42
1:A:355:TYR:CD1	1:A:355:TYR:N	2.88	0.42
1:A:481:LEU:HD22	1:A:501:LEU:CD2	2.50	0.42
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.50	0.42
1:A:339:GLU:HG2	1:A:562:ALA:HB2	2.02	0.42
1:A:88:PHE:HD2	1:A:89:ILE:CD1	2.32	0.41
1:A:566:LYS:O	1:A:570:LEU:HB2	2.20	0.41
1:B:513:HIS:HB3	1:B:514:PRO:HD2	2.02	0.41
1:A:513:HIS:HB3	1:A:514:PRO:HD2	2.02	0.41
1:B:88:PHE:HD2	1:B:89:ILE:CD1	2.32	0.41
1:B:339:GLU:HG2	1:B:562:ALA:HB2	2.02	0.41
1:B:294:LEU:HD22	1:B:409:PHE:CE1	2.55	0.41
1:B:566:LYS:O	1:B:570:LEU:HB2	2.20	0.41
1:A:183:LEU:HD23	1:A:184:ARG:N	2.35	0.41
1:B:555:GLY:O	1:B:558:LEU:HB2	2.19	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.76	0.41
1:A:389:PRO:HG3	1:A:440:ILE:HG13	2.02	0.41
1:A:295:LEU:HD21	4:A:601:HEM:HBB2	2.01	0.41
1:A:230:LEU:HG	1:A:233:ILE:HD12	2.03	0.41
1:B:108:ILE:O	1:B:112:LEU:HG	2.21	0.41
1:B:481:LEU:HD22	1:B:501:LEU:CD2	2.50	0.41
1:B:355:TYR:N	1:B:355:TYR:CD1	2.88	0.41
1:A:372:GLN:HA	1:B:372:GLN:HE22	1.85	0.41
1:A:240:ARG:HG3	1:A:271:VAL:HG22	2.03	0.41
1:B:96:GLY:O	1:B:99:LEU:N	2.54	0.41
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.51	0.41
1:B:42:GLN:HG3	1:B:70:THR:HG23	2.02	0.41
1:B:389:PRO:HG3	1:B:440:ILE:HG13	2.02	0.41
1:B:386:HIS:CD2	1:B:388:HIS:HE1	2.32	0.41
1:B:522:MET:O	1:B:526:GLY:HA3	2.21	0.41
1:B:208:GLN:HE22	1:B:230:LEU:HD12	1.86	0.41
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.87	0.41
1:A:108:ILE:O	1:A:112:LEU:HG	2.21	0.41
1:A:96:GLY:O	1:A:99:LEU:N	2.54	0.41
1:A:197:MET:CE	1:A:423:VAL:HG13	2.51	0.41
1:A:294:LEU:HD22	1:A:409:PHE:CE1	2.55	0.40
1:A:85:SER:HA	1:A:86:PRO:HD3	1.78	0.40
1:A:490:GLU:HA	1:A:493:GLU:HG2	2.03	0.40
1:B:195:ASN:ND2	1:B:427:SER:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:GLN:NE2	1:B:358:GLN:HA	2.36	0.40
1:B:269:ALA:O	1:B:271:VAL:N	2.54	0.40
1:B:108:ILE:HG13	1:B:108:ILE:H	1.67	0.40
1:B:197:MET:CE	1:B:423:VAL:HG13	2.51	0.40
1:B:84:PRO:HB2	1:B:88:PHE:CD2	2.57	0.40
1:B:531:LEU:HG	5:B:1:IMM:C7	2.52	0.40
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.40
1:B:183:LEU:HD23	1:B:184:ARG:N	2.35	0.40
1:B:184:ARG:HB2	1:B:439:ASN:C	2.42	0.40
1:A:542:PRO:O	1:B:61:ARG:NH1	2.54	0.40
1:B:230:LEU:HG	1:B:233:ILE:HD12	2.03	0.40
1:B:49:ARG:HH11	1:B:49:ARG:CG	2.35	0.40
1:B:213:SER:OG	1:B:215:LYS:HG2	2.21	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%)	496 (90%)	47 (9%)	6 (1%)	17	64
1	B	549/576 (95%)	496 (90%)	47 (9%)	6 (1%)	17	64
All	All	1098/1152 (95%)	992 (90%)	94 (9%)	12 (1%)	17	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	514	PRO
1	B	514	PRO
1	A	520	GLU
1	A	528	PRO
1	B	520	GLU

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Mol	Chain	Res	Type
1	B	528	PRO
1	A	503	PHE
1	B	503	PHE
1	A	270	PRO
1	A	295	LEU
1	B	270	PRO
1	B	295	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%)	436 (90%)	50 (10%)	9	40
1	B	486/506 (96%)	436 (90%)	50 (10%)	9	40
All	All	972/1012 (96%)	872 (90%)	100 (10%)	9	40

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	70	THR
1	A	111	THR
1	A	115	LEU
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	126	SER
1	A	145	VAL
1	A	165	THR
1	A	170	GLN
1	A	171	LEU
1	A	179	ARG
1	A	183	LEU
1	A	185	ARG
1	A	186	LYS

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Mol	Chain	Res	Type
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	252	LEU
1	A	271	VAL
1	A	291	VAL
1	A	298	LEU
1	A	300	LEU
1	A	316	LEU
1	A	317	LYS
1	A	322	THR
1	A	345	ILE
1	A	348	TYR
1	A	376	ARG
1	A	384	LEU
1	A	385	TYR
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	497	ASP
1	A	514	PRO
1	A	518	PHE
1	A	530	SER
1	A	556	PHE
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	70	THR
1	B	111	THR
1	B	115	LEU
1	B	116	VAL
1	B	117	LEU
1	B	120	ARG
1	B	126	SER

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Mol	Chain	Res	Type
1	B	145	VAL
1	B	165	THR
1	B	170	GLN
1	B	171	LEU
1	B	179	ARG
1	B	183	LEU
1	B	185	ARG
1	B	186	LYS
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	251	LYS
1	B	252	LEU
1	B	271	VAL
1	B	291	VAL
1	B	298	LEU
1	B	300	LEU
1	B	316	LEU
1	B	317	LYS
1	B	322	THR
1	B	345	ILE
1	B	348	TYR
1	B	376	ARG
1	B	384	LEU
1	B	385	TYR
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	497	ASP
1	B	514	PRO
1	B	518	PHE
1	B	530	SER
1	B	556	PHE
1	B	563	THR
1	B	564	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS
1	A	170	GLN
1	A	203	GLN
1	A	207	HIS
1	A	208	GLN
1	A	237	ASN
1	A	241	GLN
1	A	320	HIS
1	A	358	GLN
1	A	372	GLN
1	A	375	ASN
1	A	443	HIS
1	A	513	HIS
1	A	557	ASN
1	B	134	HIS
1	B	170	GLN
1	B	203	GLN
1	B	207	HIS
1	B	208	GLN
1	B	237	ASN
1	B	241	GLN
1	B	320	HIS
1	B	358	GLN
1	B	375	ASN
1	B	443	HIS
1	B	513	HIS
1	B	557	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

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	1.11	2 (13%)
3	NAG	A	672	3	14,14,15	1.10	1 (7%)	15,19,21	1.23	1 (6%)
3	NAG	B	671	1,3	14,14,15	0.54	0	15,19,21	1.11	2 (13%)
3	NAG	B	672	3	14,14,15	1.10	1 (7%)	15,19,21	1.22	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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	672	NAG	C4-C5	2.30	1.58	1.53
3	B	672	NAG	C4-C5	2.31	1.58	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	672	NAG	C4-C3-C2	-3.09	106.42	111.23
3	B	672	NAG	C4-C3-C2	-3.08	106.44	111.23
3	B	671	NAG	C6-C5-C4	-2.34	107.25	113.02
3	A	671	NAG	C6-C5-C4	-2.33	107.26	113.02
3	A	671	NAG	C2-N2-C7	-2.04	120.42	123.04
3	B	671	NAG	C2-N2-C7	-2.03	120.43	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.6 Ligand geometry [i](#)

8 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	IMM	A	1	-	21,27,27	1.16	2 (9%)	26,39,39	1.09	3 (11%)
4	HEM	A	601	1	30,50,50	2.95	10 (33%)	24,82,82	2.75	10 (41%)
2	NAG	A	661	1	14,14,15	0.77	0	15,19,21	1.36	1 (6%)
2	NAG	A	681	1	14,14,15	0.77	0	15,19,21	0.87	1 (6%)
5	IMM	B	1	-	21,27,27	1.17	2 (9%)	26,39,39	1.10	3 (11%)
4	HEM	B	601	1	30,50,50	2.94	10 (33%)	24,82,82	2.75	10 (41%)
2	NAG	B	661	1	14,14,15	0.77	0	15,19,21	1.37	1 (6%)
2	NAG	B	681	1	14,14,15	0.77	0	15,19,21	0.87	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
5	IMM	A	1	-	-	0/8/14/14	0/3/3/3
4	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
5	IMM	B	1	-	-	0/8/14/14	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	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

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	601	HEM	C3C-CAC	-8.57	1.35	1.51
4	B	601	HEM	C3C-CAC	-8.56	1.35	1.51
4	B	601	HEM	C2D-C3D	-7.15	1.33	1.54
4	A	601	HEM	C2D-C3D	-7.15	1.33	1.54
4	A	601	HEM	C3B-CAB	-5.86	1.40	1.51
4	B	601	HEM	C3B-CAB	-5.83	1.40	1.51
4	B	601	HEM	C2C-C1C	-4.78	1.43	1.52
4	A	601	HEM	C2C-C1C	-4.77	1.43	1.52
4	A	601	HEM	C3D-C4D	-4.24	1.46	1.51
4	B	601	HEM	C3D-C4D	-4.18	1.46	1.51
4	B	601	HEM	C1A-CHA	-2.42	1.33	1.39
4	A	601	HEM	C1A-CHA	-2.41	1.33	1.39
5	A	1	IMM	C2-C3	-2.25	1.35	1.39
5	B	1	IMM	C2-C3	-2.23	1.35	1.39
5	B	1	IMM	C18-C3	-2.19	1.49	1.52
5	A	1	IMM	C18-C3	-2.18	1.49	1.52
4	A	601	HEM	CBC-CAC	2.07	1.41	1.29
4	B	601	HEM	CBC-CAC	2.08	1.41	1.29
4	A	601	HEM	CAA-C2A	2.38	1.56	1.52
4	B	601	HEM	CAA-C2A	2.40	1.56	1.52
4	A	601	HEM	CBB-CAB	3.06	1.47	1.29
4	B	601	HEM	CBB-CAB	3.06	1.47	1.29
4	A	601	HEM	C3B-C4B	4.44	1.55	1.51
4	B	601	HEM	C3B-C4B	4.45	1.55	1.51

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	C3C-CAC-CBC	-5.67	115.75	124.46
4	B	601	HEM	C3C-CAC-CBC	-5.67	115.75	124.46
2	B	661	NAG	C2-N2-C7	-4.88	116.76	123.04
2	A	661	NAG	C2-N2-C7	-4.86	116.80	123.04
4	A	601	HEM	CHC-C4B-NB	-2.97	117.37	124.52
4	B	601	HEM	CHC-C4B-NB	-2.96	117.38	124.52
2	B	681	NAG	C2-N2-C7	-2.30	120.08	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	681	NAG	C2-N2-C7	-2.29	120.10	123.04
5	A	1	IMM	C17-C2-C3	-2.23	124.16	129.08
5	B	1	IMM	C17-C2-C3	-2.21	124.18	129.08
5	B	1	IMM	C19-C18-C3	-2.14	112.22	116.31
5	A	1	IMM	C19-C18-C3	-2.13	112.23	116.31
4	B	601	HEM	C3B-CAB-CBB	2.50	128.29	124.46
4	A	601	HEM	C3B-CAB-CBB	2.52	128.32	124.46
4	B	601	HEM	C2D-C3D-C4D	2.94	106.48	101.50
4	A	601	HEM	C2D-C3D-C4D	2.95	106.49	101.50
4	B	601	HEM	CMB-C2B-C3B	3.10	124.27	116.53
4	A	601	HEM	CMB-C2B-C3B	3.10	124.28	116.53
5	A	1	IMM	C11-C10-N1	3.30	122.26	118.02
5	B	1	IMM	C11-C10-N1	3.30	122.26	118.02
4	A	601	HEM	C3B-C4B-CHC	3.55	128.17	123.16
4	B	601	HEM	C3B-C4B-CHC	3.58	128.20	123.16
4	B	601	HEM	CAD-C3D-C4D	3.95	126.40	112.47
4	A	601	HEM	CAD-C3D-C4D	3.95	126.41	112.47
4	A	601	HEM	CMC-C2C-C3C	4.60	128.01	116.53
4	B	601	HEM	CMC-C2C-C3C	4.61	128.05	116.53
4	A	601	HEM	CAD-C3D-C2D	4.83	127.09	113.22
4	B	601	HEM	CAD-C3D-C2D	4.84	127.12	113.22
4	A	601	HEM	CBA-CAA-C2A	4.85	121.22	112.53
4	B	601	HEM	CBA-CAA-C2A	4.86	121.24	112.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	IMM	15	0
4	A	601	HEM	7	0
5	B	1	IMM	16	0
4	B	601	HEM	7	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](#)

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.