



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:45 AM GMT

PDB ID : 3Q7D  
Title : Structure of (R)-naproxen bound to mCOX-2.  
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Deposited on : 2011-01-04  
Resolution : 2.40 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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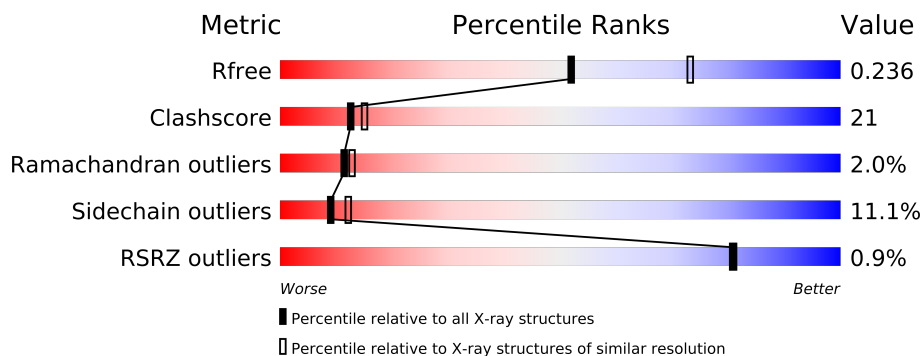
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	587	
1	B	587	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9880 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

Image for chem-comp NAG is not available.

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	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		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).

Image for chem-comp HEM is not available.

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

- Molecule 4 is (2R)-2-(6-METHOXYNAPHTHALEN-2-YL)PROPANOICACID (three-letter code: NPX) (formula: C<sub>14</sub>H<sub>14</sub>O<sub>3</sub>).

Image for chem-comp NPX is not available.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 17	C 14	O 3	0	0
4	B	1	Total 17	C 14	O 3	0	0

- Molecule 5 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).

Image for chem-comp BOG is not available.

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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0
6	A	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

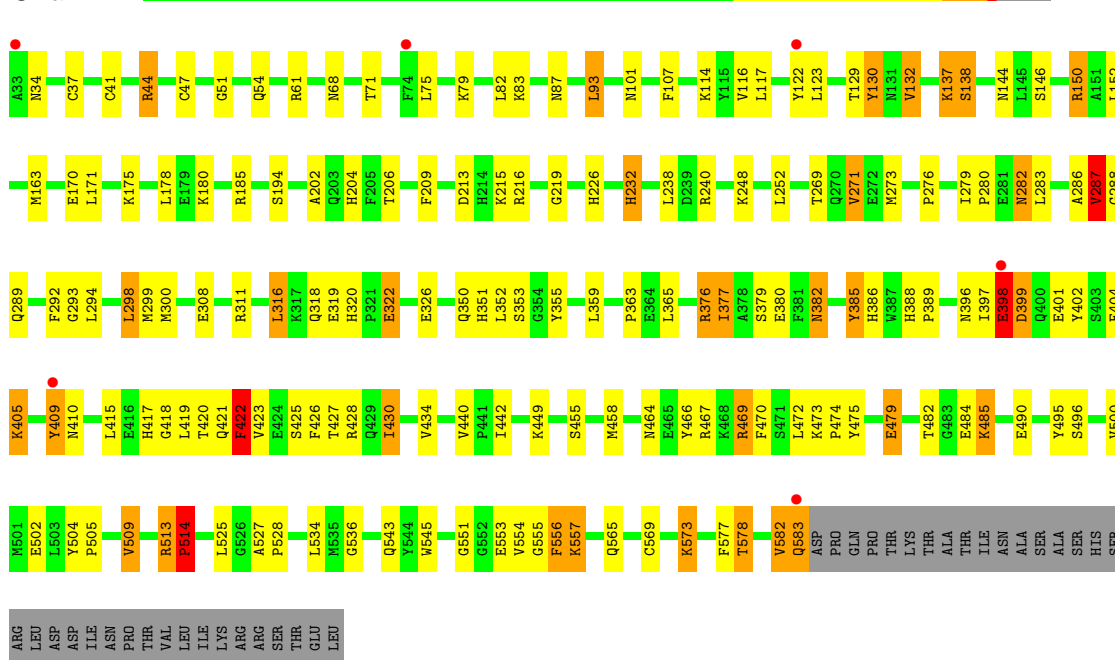
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	309	Total 309	O 309	0	0
7	B	289	Total 289	O 289	0	0

### 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.

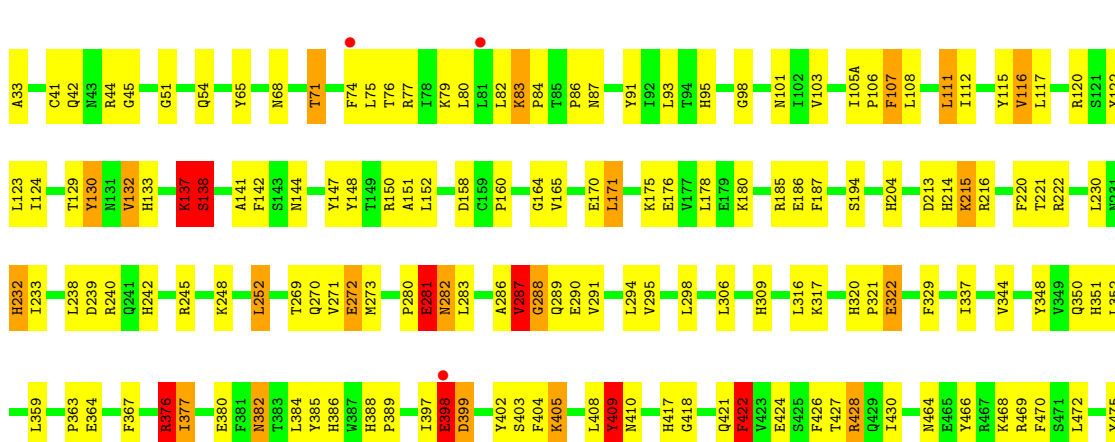
#### • Molecule 1: Prostaglandin G/H synthase 2

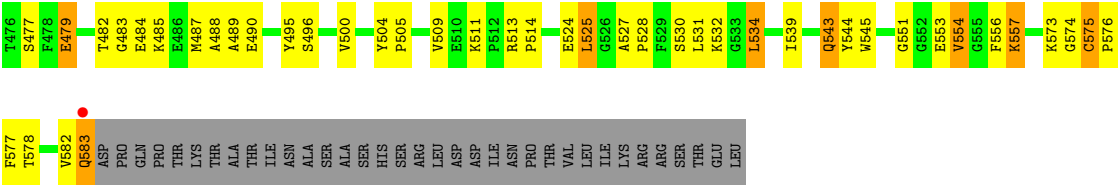
Chain A:



#### • Molecule 1: Prostaglandin G/H synthase 2

Chain B:





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.73Å 133.03Å 181.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.59 – 2.40 29.59 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (29.59-2.40) 99.4 (29.59-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.09 (at 2.31Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.177 , 0.233 0.184 , 0.236	Depositor DCC
$R_{free}$ test set	3311 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.584	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 27.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 65501 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9880	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NPX, HEM, BOG, NAG, CL

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	0.42	0/4601	0.63	3/6239 (0.0%)
1	B	0.42	0/4601	0.62	2/6239 (0.0%)
All	All	0.42	0/9202	0.63	5/12478 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	376	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	B	376	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	287	VAL	N-CA-C	5.23	125.11	111.00
1	B	287	VAL	N-CA-C	5.03	124.59	111.00
1	A	137	LYS	N-CA-C	5.00	124.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	288	GLY	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4474	0	4376	171	0
1	B	4474	0	4376	209	0
2	A	56	0	52	12	0
2	B	56	0	52	10	0
3	A	43	0	30	4	0
3	B	43	0	30	5	0
4	A	17	0	13	1	0
4	B	17	0	13	0	0
5	A	60	0	84	6	0
5	B	40	0	56	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	309	0	0	36	0
7	B	289	0	0	51	0
All	All	9880	0	9082	386	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 21.

All (386) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:144:ASN:HD21	2:B:671:NAG:C1	1.31	1.44
1:B:150:ARG:HB2	7:B:829:HOH:O	1.40	1.19
1:A:144:ASN:HD21	2:A:671:NAG:C1	1.57	1.16
1:B:294:LEU:HD22	1:B:409:TYR:HB3	1.26	1.11
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.12	1.11
1:A:185:ARG:HH12	5:A:3:BOG:H5'2	1.17	1.10
1:A:377:ILE:HB	7:A:677:HOH:O	1.48	1.09
1:B:144:ASN:ND2	2:B:671:NAG:C1	2.16	1.07
1:A:68:ASN:HD21	2:A:661:NAG:C1	1.68	1.06
1:B:421:GLN:O	1:B:422:PHE:HB2	1.53	1.06
1:B:322:GLU:HG3	7:B:722:HOH:O	1.52	1.06
1:A:150:ARG:HG2	1:A:150:ARG:HH11	1.20	1.05
1:A:185:ARG:NH1	5:A:3:BOG:H5'2	1.71	1.04

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:421:GLN:O	1:A:422:PHE:HB2	1.61	0.98
1:A:319:GLU:HG3	1:A:554:VAL:HG11	1.48	0.95
1:A:144:ASN:ND2	2:A:671:NAG:C1	2.30	0.94
1:A:150:ARG:HH11	1:A:150:ARG:CG	1.82	0.93
1:B:68:ASN:HD21	2:B:661:NAG:C1	1.84	0.91
1:A:350:GLN:HE22	1:A:359:LEU:H	1.18	0.91
1:B:294:LEU:CD2	1:B:409:TYR:HB3	2.01	0.90
1:B:410:ASN:HD21	2:B:681:NAG:C1	1.85	0.89
1:B:41:CYS:HB3	7:B:832:HOH:O	1.71	0.88
1:A:440:VAL:HG13	7:A:747:HOH:O	1.73	0.88
1:B:281:GLU:O	1:B:283:LEU:N	2.07	0.88
1:B:130:TYR:N	7:B:869:HOH:O	2.07	0.86
1:A:130:TYR:N	7:A:751:HOH:O	2.09	0.86
1:B:398:GLU:O	1:B:399:ASP:HB2	1.74	0.85
1:A:138:SER:N	7:A:908:HOH:O	2.10	0.84
1:B:138:SER:N	7:B:756:HOH:O	2.03	0.84
1:A:68:ASN:ND2	2:A:661:NAG:C1	2.42	0.83
1:A:294:LEU:HD22	1:A:409:TYR:HD2	1.43	0.82
1:A:185:ARG:CZ	7:A:801:HOH:O	2.27	0.82
1:B:350:GLN:HE22	1:B:359:LEU:H	1.28	0.82
1:B:87:ASN:HD22	5:B:620:BOG:H62	1.45	0.81
1:A:150:ARG:HG2	1:A:150:ARG:NH1	1.80	0.80
1:B:150:ARG:CG	1:B:152:LEU:O	2.30	0.80
1:A:479:GLU:HB3	1:A:485:LYS:HZ2	1.47	0.78
1:B:294:LEU:HD22	1:B:409:TYR:CB	2.08	0.78
3:B:682:HEM:HBB2	3:B:682:HEM:HMB2	1.66	0.78
1:A:144:ASN:HD21	2:A:671:NAG:C2	1.97	0.77
1:A:553:GLU:HG3	1:A:557:LYS:NZ	1.99	0.77
1:B:215:LYS:NZ	1:B:222:ARG:HH21	1.83	0.76
1:A:44:ARG:HG2	1:A:44:ARG:NH1	1.89	0.76
1:B:410:ASN:ND2	2:B:681:NAG:C1	2.48	0.75
1:A:557:LYS:HE2	7:A:713:HOH:O	1.85	0.75
1:B:306:LEU:HD23	1:B:306:LEU:C	2.07	0.75
1:A:194:SER:OG	1:A:351:HIS:HE1	1.69	0.75
1:B:294:LEU:HD22	1:B:409:TYR:CD2	2.23	0.74
1:A:554:VAL:HG12	7:A:849:HOH:O	1.87	0.74
1:B:245:ARG:HD2	7:B:4:HOH:O	1.87	0.74
1:A:226:HIS:HA	1:A:377:ILE:CD1	2.18	0.74
1:B:215:LYS:HD3	1:B:215:LYS:N	2.03	0.73
1:B:214:HIS:HD2	7:B:809:HOH:O	1.72	0.73
1:A:410:ASN:HD21	2:A:681:NAG:C1	2.03	0.72
1:B:554:VAL:HG13	7:B:713:HOH:O	1.89	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:ASN:HD21	1:A:475:TYR:H	1.38	0.72
1:A:180:LYS:HD3	1:A:490:GLU:HG3	1.71	0.70
1:B:83:LYS:HE3	1:B:83:LYS:HA	1.72	0.70
1:B:269:THR:OG1	1:B:271:VAL:HG13	1.90	0.70
1:B:112:ILE:HG13	7:B:833:HOH:O	1.90	0.70
1:B:288:GLY:HA3	7:B:825:HOH:O	1.90	0.70
1:A:129:THR:C	7:A:751:HOH:O	2.30	0.69
1:A:405:LYS:HE3	1:A:405:LYS:H	1.55	0.69
3:B:682:HEM:HBC2	3:B:682:HEM:HHD	1.74	0.69
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.75	0.69
1:B:215:LYS:H	1:B:215:LYS:HD3	1.58	0.68
1:A:213:ASP:OD1	1:A:215:LYS:HE2	1.92	0.68
1:A:209:PHE:HB2	1:A:377:ILE:HD12	1.75	0.68
1:B:213:ASP:OD1	1:B:215:LYS:HE2	1.93	0.68
1:A:556:PHE:HB3	1:A:557:LYS:HE3	1.76	0.68
1:B:150:ARG:HG3	1:B:152:LEU:O	1.91	0.68
1:A:479:GLU:HB3	1:A:485:LYS:NZ	2.09	0.68
1:B:294:LEU:HD22	1:B:409:TYR:HD2	1.59	0.68
1:B:294:LEU:HG	7:B:782:HOH:O	1.93	0.68
1:B:150:ARG:NE	7:B:829:HOH:O	2.26	0.68
1:B:240:ARG:HH21	1:B:288:GLY:HA2	1.59	0.68
1:A:150:ARG:NH2	1:A:458:MET:O	2.26	0.67
1:B:91:TYR:O	1:B:95:HIS:HD2	1.77	0.67
1:A:276:PRO:HD2	1:A:279:ILE:HD12	1.76	0.67
1:B:317:LYS:HD2	7:B:24:HOH:O	1.93	0.67
1:B:479:GLU:HB3	1:B:485:LYS:HZ3	1.59	0.67
3:A:682:HEM:HMB2	3:A:682:HEM:HBB2	1.77	0.67
1:B:479:GLU:HB3	1:B:485:LYS:NZ	2.10	0.66
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	1.78	0.66
1:B:288:GLY:C	7:B:825:HOH:O	2.34	0.66
1:A:382:ASN:HD21	3:A:682:HEM:HAD2	1.61	0.65
1:B:215:LYS:H	1:B:215:LYS:CD	2.10	0.65
1:B:115:TYR:HE2	5:B:3:BOG:H3'1	1.61	0.65
1:B:194:SER:OG	1:B:351:HIS:HE1	1.78	0.65
1:A:51:GLY:O	1:B:322:GLU:HG2	1.96	0.65
1:B:129:THR:C	7:B:869:HOH:O	2.34	0.65
1:B:320:HIS:HE1	1:B:551:GLY:O	1.79	0.65
1:B:150:ARG:HG2	1:B:152:LEU:O	1.97	0.65
1:A:226:HIS:HA	1:A:377:ILE:HD13	1.77	0.65
1:A:583:GLN:HB3	7:A:876:HOH:O	1.96	0.65
1:B:273:MET:SD	1:B:286:ALA:O	2.54	0.64
1:A:101:ASN:HB2	7:A:810:HOH:O	1.96	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:ARG:HG2	1:B:220:PHE:CD1	2.32	0.64
1:A:536:GLY:C	7:A:809:HOH:O	2.35	0.64
1:B:240:ARG:NH2	1:B:288:GLY:HA2	2.12	0.64
1:B:288:GLY:CA	7:B:825:HOH:O	2.46	0.64
1:B:75:LEU:HD22	1:B:79:LYS:HE2	1.79	0.64
1:B:83:LYS:HG2	7:B:878:HOH:O	1.98	0.63
1:B:418:GLY:O	1:B:421:GLN:O	2.16	0.63
1:A:287:VAL:HA	7:A:673:HOH:O	1.98	0.63
1:B:295:VAL:HG13	7:B:811:HOH:O	1.98	0.62
1:B:204:HIS:HD2	7:B:2:HOH:O	1.82	0.62
1:A:269:THR:OG1	1:A:271:VAL:HG13	1.99	0.62
1:A:388:HIS:HB2	7:A:747:HOH:O	2.00	0.62
1:A:410:ASN:ND2	2:A:681:NAG:C1	2.63	0.62
1:B:583:GLN:HB2	7:B:859:HOH:O	1.97	0.62
1:A:219:GLY:HA2	7:A:840:HOH:O	2.00	0.62
1:B:216:ARG:HG2	1:B:220:PHE:CG	2.34	0.62
1:B:120:ARG:HG3	1:B:531:LEU:HD12	1.81	0.62
1:B:294:LEU:HD13	1:B:409:TYR:CD2	2.35	0.61
1:A:427:THR:OG1	1:A:578:THR:HG22	1.99	0.61
1:B:294:LEU:HD13	1:B:409:TYR:HD2	1.66	0.61
1:A:51:GLY:C	1:B:322:GLU:HG2	2.21	0.61
1:A:382:ASN:ND2	1:A:386:HIS:HE1	1.99	0.61
2:B:671:NAG:HO4	2:B:9:NAG:C5	2.13	0.60
1:B:306:LEU:O	1:B:306:LEU:HD23	1.99	0.60
1:A:226:HIS:HA	1:A:377:ILE:HD11	1.83	0.60
1:B:215:LYS:HZ1	1:B:222:ARG:HH21	1.48	0.60
1:B:295:VAL:HG22	7:B:811:HOH:O	2.02	0.60
1:B:204:HIS:HE1	7:B:635:HOH:O	1.83	0.60
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.83	0.60
1:B:106:PRO:HD2	1:B:107:PHE:CE2	2.37	0.60
3:A:682:HEM:HBC2	3:A:682:HEM:HHD	1.84	0.59
1:B:487:MET:HE3	7:B:844:HOH:O	2.01	0.59
3:B:682:HEM:CMB	3:B:682:HEM:HBB2	2.33	0.59
1:A:132:VAL:HG22	7:A:14:HOH:O	2.02	0.59
1:B:272:GLU:HG3	7:B:842:HOH:O	2.03	0.59
1:B:402:TYR:OH	1:B:417:HIS:HE1	1.85	0.59
1:B:322:GLU:CG	7:B:722:HOH:O	2.30	0.59
2:A:671:NAG:O4	2:A:9:NAG:C1	2.51	0.58
1:B:382:ASN:HD21	3:B:682:HEM:HAD2	1.66	0.58
1:B:148:TYR:CD1	1:B:377:ILE:HD11	2.38	0.58
1:A:569:CYS:HB2	7:A:723:HOH:O	2.03	0.58
1:B:124:ILE:HD11	1:B:528:PRO:HB2	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:240:ARG:HH21	1:B:288:GLY:CA	2.16	0.58
1:B:91:TYR:O	1:B:95:HIS:CD2	2.57	0.58
1:A:320:HIS:HE1	1:A:551:GLY:O	1.87	0.58
1:A:554:VAL:HG13	1:A:555:GLY:N	2.19	0.57
1:B:321:PRO:HD2	7:B:722:HOH:O	2.04	0.57
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.04	0.57
1:A:470:PHE:CG	1:A:525:LEU:HD22	2.40	0.57
1:A:107:PHE:HB3	7:A:785:HOH:O	2.04	0.57
1:B:350:GLN:HE22	1:B:359:LEU:N	2.01	0.57
1:A:240:ARG:HE	1:A:288:GLY:HA2	1.69	0.57
1:B:479:GLU:CB	1:B:485:LYS:NZ	2.67	0.57
1:B:144:ASN:HD21	2:B:671:NAG:C2	2.13	0.56
1:A:273:MET:SD	1:A:286:ALA:O	2.63	0.56
1:A:282:ASN:HB3	7:A:763:HOH:O	2.04	0.56
1:A:557:LYS:N	1:A:557:LYS:HE3	2.20	0.56
1:B:116:VAL:O	1:B:120:ARG:HG2	2.06	0.56
1:A:398:GLU:O	1:A:399:ASP:HB2	2.04	0.56
1:B:115:TYR:CD2	5:B:3:BOG:H4'2	2.41	0.56
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.41	0.56
1:B:352:LEU:HD12	1:B:352:LEU:C	2.26	0.56
1:B:543:GLN:H	1:B:543:GLN:CD	2.08	0.56
1:A:129:THR:CA	7:A:751:HOH:O	2.53	0.56
1:A:226:HIS:ND1	1:A:377:ILE:HG12	2.20	0.55
1:B:148:TYR:CE1	1:B:377:ILE:HD11	2.40	0.55
1:B:175:LYS:HD2	7:B:730:HOH:O	2.06	0.55
1:B:150:ARG:CD	1:B:380:GLU:OE2	2.54	0.55
1:B:124:ILE:HD11	1:B:528:PRO:CB	2.36	0.55
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.89	0.55
1:B:142:PHE:O	1:B:376:ARG:NH2	2.29	0.55
1:A:350:GLN:NE2	1:A:359:LEU:H	1.97	0.55
1:B:382:ASN:ND2	1:B:386:HIS:HE1	2.05	0.54
1:B:483:GLY:HA3	1:B:511:LYS:HD3	1.88	0.54
2:B:671:NAG:O4	2:B:9:NAG:O5	2.19	0.54
1:A:283:LEU:HD21	1:A:415:LEU:HD12	1.90	0.54
1:B:553:GLU:HG3	1:B:557:LYS:NZ	2.21	0.54
1:B:123:LEU:O	1:B:469:ARG:NH2	2.41	0.54
1:A:185:ARG:HH11	5:A:3:BOG:H8'3	1.73	0.54
1:A:398:GLU:O	1:A:399:ASP:CB	2.56	0.54
1:B:151:ALA:O	1:B:469:ARG:NH1	2.41	0.54
1:A:87:ASN:CB	5:A:620:BOG:H62	2.38	0.54
1:A:398:GLU:HA	1:A:398:GLU:OE1	2.08	0.53
1:B:290:GLU:HG2	7:B:684:HOH:O	2.07	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:103:VAL:HG11	7:B:833:HOH:O	2.08	0.53
1:B:405:LYS:H	1:B:405:LYS:CD	2.21	0.53
1:B:107:PHE:HB3	7:B:678:HOH:O	2.08	0.53
1:B:464:ASN:HD21	1:B:475:TYR:H	1.56	0.53
1:A:352:LEU:C	1:A:352:LEU:HD12	2.28	0.53
1:B:150:ARG:HD3	1:B:380:GLU:OE2	2.08	0.53
1:A:350:GLN:HE22	1:A:359:LEU:N	1.95	0.53
2:A:671:NAG:O4	2:A:9:NAG:C2	2.57	0.53
1:B:68:ASN:ND2	2:B:661:NAG:C1	2.66	0.53
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.89	0.53
1:A:554:VAL:HG13	1:A:555:GLY:H	1.74	0.52
1:B:245:ARG:HD3	1:B:329:PHE:CD1	2.43	0.52
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.48	0.52
1:A:418:GLY:O	1:A:421:GLN:O	2.27	0.52
1:B:240:ARG:HE	1:B:288:GLY:HA2	1.74	0.52
1:A:405:LYS:CE	1:A:405:LYS:H	2.22	0.52
1:B:575:CYS:H	1:B:576:PRO:CD	2.22	0.52
1:B:479:GLU:OE1	1:B:488:ALA:HB1	2.09	0.52
1:B:388:HIS:N	1:B:389:PRO:CD	2.73	0.51
1:A:294:LEU:HD22	1:A:409:TYR:CD2	2.35	0.51
1:A:404:PHE:HB2	1:A:405:LYS:HE3	1.91	0.51
1:A:405:LYS:HE3	1:A:405:LYS:N	2.24	0.51
1:B:482:THR:HB	7:B:844:HOH:O	2.11	0.51
1:A:300:MET:HG3	1:A:419:LEU:CD1	2.41	0.51
1:A:479:GLU:OE1	1:A:485:LYS:HE3	2.10	0.51
1:B:306:LEU:CD2	1:B:306:LEU:C	2.79	0.51
1:B:176:GLU:HG3	1:B:180:LYS:HE3	1.93	0.51
2:A:671:NAG:O4	2:A:9:NAG:H2	2.11	0.51
1:B:428:ARG:HD2	7:B:766:HOH:O	2.10	0.51
1:B:45:GLY:HA3	7:B:832:HOH:O	2.11	0.51
1:B:180:LYS:HD3	1:B:490:GLU:HG3	1.92	0.51
1:B:86:PRO:HG2	1:B:472:LEU:CD2	2.41	0.51
1:B:421:GLN:O	1:B:422:PHE:CB	2.37	0.51
1:B:280:PRO:O	1:B:281:GLU:C	2.48	0.51
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.92	0.51
1:A:396:ASN:ND2	1:A:401:GLU:HG2	2.25	0.51
1:B:238:LEU:HD11	1:B:242:HIS:NE2	2.25	0.51
1:B:132:VAL:HG22	7:B:25:HOH:O	2.11	0.51
1:B:187:PHE:HE2	1:B:430:ILE:HD13	1.75	0.51
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.93	0.50
1:B:322:GLU:OE2	7:B:722:HOH:O	2.19	0.50
1:B:294:LEU:HD22	1:B:409:TYR:CG	2.46	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:536:GLY:HA3	7:A:809:HOH:O	2.11	0.50
1:A:565:GLN:NE2	7:A:723:HOH:O	2.45	0.50
1:A:204:HIS:HD2	7:A:11:HOH:O	1.95	0.50
1:B:294:LEU:CD2	1:B:409:TYR:HD2	2.25	0.50
1:A:150:ARG:HD2	1:A:379:SER:HB3	1.94	0.50
1:B:574:GLY:O	7:B:758:HOH:O	2.19	0.50
1:B:479:GLU:CB	1:B:485:LYS:HZ1	2.24	0.49
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.94	0.49
1:B:65:TYR:O	1:B:71:THR:HG23	2.11	0.49
1:A:553:GLU:CG	1:A:557:LYS:NZ	2.74	0.49
1:A:276:PRO:HD2	1:A:279:ILE:CD1	2.41	0.49
1:A:286:ALA:O	1:A:288:GLY:N	2.43	0.49
1:A:322:GLU:HG2	1:B:51:GLY:O	2.12	0.49
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.94	0.49
1:B:180:LYS:HB3	1:B:490:GLU:HG2	1.94	0.49
1:A:293:GLY:HA2	1:A:299:MET:CE	2.42	0.49
1:A:137:LYS:C	7:A:908:HOH:O	2.48	0.49
1:B:133:HIS:HD2	1:B:147:TYR:OH	1.95	0.49
1:B:240:ARG:NE	1:B:288:GLY:HA2	2.26	0.49
1:A:556:PHE:HB3	1:A:557:LYS:CE	2.43	0.48
1:A:396:ASN:HB3	7:A:860:HOH:O	2.13	0.48
1:B:363:PRO:HG2	1:B:545:TRP:CD2	2.48	0.48
1:A:68:ASN:HD21	2:A:661:NAG:C2	2.25	0.48
1:B:248:LYS:HB2	1:B:248:LYS:NZ	2.29	0.48
1:A:423:VAL:CG1	1:A:578:THR:HG23	2.43	0.48
1:A:397:ILE:O	1:A:398:GLU:C	2.50	0.48
1:B:472:LEU:HD11	1:B:524:GLU:HB2	1.96	0.48
1:B:384:LEU:C	1:B:384:LEU:HD12	2.33	0.48
1:A:61:ARG:NH2	1:B:367:PHE:HE2	2.10	0.48
1:A:232:HIS:HB2	1:A:292:PHE:CE2	2.49	0.48
1:B:160:PRO:HD2	1:B:164:GLY:O	2.14	0.48
1:A:553:GLU:HG3	1:A:557:LYS:HZ3	1.77	0.47
1:B:42:GLN:HE22	1:B:468:LYS:HE2	1.79	0.47
1:A:294:LEU:HD22	7:A:878:HOH:O	2.14	0.47
3:B:682:HEM:HBC2	3:B:682:HEM:CHD	2.41	0.47
1:B:477:SER:HB2	1:B:479:GLU:HG2	1.95	0.47
1:A:123:LEU:O	1:A:469:ARG:NH2	2.35	0.47
1:A:388:HIS:CB	7:A:747:HOH:O	2.61	0.47
1:B:115:TYR:HD2	5:B:3:BOG:H4'2	1.79	0.47
1:A:175:LYS:NZ	1:A:449:LYS:HD2	2.30	0.47
1:B:150:ARG:HD3	1:B:380:GLU:CD	2.35	0.47
1:B:137:LYS:O	7:B:870:HOH:O	2.20	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:322:GLU:HG3	1:B:51:GLY:C	2.35	0.47
1:A:226:HIS:CA	1:A:377:ILE:HD13	2.43	0.47
1:B:68:ASN:HD21	2:B:661:NAG:C2	2.28	0.47
1:B:215:LYS:HZ2	1:B:222:ARG:HH21	1.60	0.47
1:A:379:SER:CB	7:A:840:HOH:O	2.63	0.47
1:A:388:HIS:N	1:A:389:PRO:CD	2.78	0.47
1:B:291:VAL:O	1:B:291:VAL:HG13	2.14	0.47
1:A:129:THR:HA	7:A:751:HOH:O	2.14	0.47
1:B:485:LYS:HD3	7:B:687:HOH:O	2.15	0.47
1:A:152:LEU:HG	1:A:469:ARG:HG2	1.97	0.47
1:B:215:LYS:CD	1:B:215:LYS:N	2.71	0.47
1:A:87:ASN:HB3	5:A:620:BOG:H62	1.96	0.47
1:A:382:ASN:C	1:A:382:ASN:HD22	2.18	0.46
1:A:75:LEU:HD22	1:A:79:LYS:HE2	1.97	0.46
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.98	0.46
1:B:574:GLY:O	1:B:575:CYS:CB	2.63	0.46
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.79	0.46
1:A:485:LYS:HD3	1:A:485:LYS:HA	1.62	0.46
1:B:151:ALA:HA	7:B:701:HOH:O	2.16	0.46
1:B:575:CYS:H	1:B:576:PRO:HD3	1.80	0.46
1:B:214:HIS:CD2	7:B:809:HOH:O	2.57	0.46
1:B:98:GLY:O	1:B:101:ASN:HB3	2.16	0.46
1:B:129:THR:CA	7:B:869:HOH:O	2.62	0.45
1:A:479:GLU:CB	1:A:485:LYS:NZ	2.79	0.45
1:B:495:TYR:O	1:B:496:SER:HB3	2.16	0.45
1:A:464:ASN:ND2	1:A:475:TYR:H	2.10	0.45
1:A:283:LEU:HD13	7:A:726:HOH:O	2.17	0.45
1:A:513:ARG:O	1:A:514:PRO:C	2.54	0.45
1:B:350:GLN:NE2	1:B:359:LEU:H	2.05	0.45
1:B:105(A):ILE:CD1	1:B:108:LEU:HD12	2.45	0.45
1:B:148:TYR:CZ	1:B:221:THR:HB	2.51	0.45
1:B:111:LEU:HD12	1:B:111:LEU:C	2.37	0.45
1:B:240:ARG:CZ	1:B:288:GLY:HA2	2.46	0.45
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.98	0.45
1:B:74:PHE:O	1:B:77:ARG:HB2	2.16	0.45
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.56	0.45
1:A:93:LEU:HB3	1:A:355:TYR:CD1	2.51	0.45
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.52	0.45
1:B:83:LYS:HA	1:B:84:PRO:HD2	1.83	0.45
1:B:230:LEU:HA	1:B:232:HIS:CD2	2.51	0.45
1:A:322:GLU:CG	1:B:51:GLY:C	2.85	0.45
1:B:294:LEU:CD1	1:B:409:TYR:HD2	2.29	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:430:ILE:HD12	7:A:663:HOH:O	2.17	0.45
1:A:399:ASP:HB3	7:A:797:HOH:O	2.17	0.44
1:B:252:LEU:HD22	1:B:309:HIS:CG	2.52	0.44
1:B:322:GLU:CD	7:B:722:HOH:O	2.53	0.44
1:B:530:SER:O	1:B:534:LEU:HD22	2.18	0.44
1:A:426:PHE:CD1	7:A:636:HOH:O	2.69	0.44
1:A:351:HIS:HD2	7:A:760:HOH:O	2.00	0.44
1:B:272:GLU:HG2	7:B:677:HOH:O	2.16	0.44
1:B:42:GLN:NE2	1:B:468:LYS:HE2	2.33	0.44
1:A:137:LYS:N	7:A:908:HOH:O	2.51	0.44
1:A:398:GLU:HB2	1:A:425:SER:OG	2.18	0.44
1:B:500:VAL:CG1	1:B:500:VAL:O	2.65	0.44
1:A:479:GLU:H	1:A:479:GLU:CD	2.21	0.43
1:B:525:LEU:O	1:B:528:PRO:HD2	2.17	0.43
1:B:187:PHE:CE2	1:B:430:ILE:HD13	2.53	0.43
1:B:364:GLU:HG3	7:B:654:HOH:O	2.19	0.43
1:A:420:THR:OG1	1:A:573:LYS:HB3	2.18	0.43
1:A:377:ILE:HD11	7:A:635:HOH:O	2.18	0.43
3:A:682:HEM:CMB	3:A:682:HEM:HBB2	2.45	0.43
1:A:423:VAL:HG13	1:A:578:THR:CG2	2.49	0.43
1:A:175:LYS:HE2	1:A:175:LYS:HB2	1.82	0.43
1:B:105(A):ILE:CG2	1:B:107:PHE:HD2	2.31	0.43
1:A:467:ARG:HB3	1:A:472:LEU:HB2	2.01	0.43
1:B:351:HIS:HD2	7:B:810:HOH:O	2.02	0.43
1:B:252:LEU:HD22	1:B:309:HIS:CD2	2.54	0.43
1:B:408:LEU:HB2	7:B:792:HOH:O	2.19	0.43
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.54	0.43
1:B:405:LYS:H	1:B:405:LYS:HD2	1.83	0.43
1:B:397:ILE:HD13	1:B:422:PHE:CE2	2.53	0.43
1:A:163:MET:CE	1:A:502:GLU:HG2	2.49	0.43
1:B:539:ILE:HA	1:B:544:TYR:HB3	2.01	0.43
1:A:479:GLU:CG	1:A:485:LYS:HZ1	2.32	0.42
1:B:382:ASN:HD22	1:B:382:ASN:C	2.22	0.42
1:A:282:ASN:HA	7:A:619:HOH:O	2.20	0.42
1:A:202:ALA:O	1:A:206:THR:HG23	2.19	0.42
1:A:405:LYS:H	1:A:405:LYS:CD	2.32	0.42
1:B:230:LEU:HG	1:B:337:ILE:HG12	2.02	0.42
1:B:137:LYS:O	1:B:141:ALA:HB3	2.19	0.42
1:A:150:ARG:HG3	1:A:380:GLU:OE2	2.19	0.42
1:B:75:LEU:O	1:B:79:LYS:HG3	2.20	0.42
1:A:308:GLU:OE2	1:A:311:ARG:NH1	2.52	0.42
1:A:482:THR:HG22	1:A:509:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:61:ARG:HD2	7:B:805:HOH:O	2.20	0.42
1:A:185:ARG:HH12	5:A:3:BOG:C5'	2.07	0.42
1:B:112:ILE:CG1	7:B:833:HOH:O	2.58	0.42
1:B:115:TYR:CE2	5:B:3:BOG:H3'1	2.46	0.42
1:A:352:LEU:HD12	1:A:353:SER:N	2.35	0.42
1:A:114:LYS:HE2	1:A:365:LEU:O	2.20	0.41
1:A:582:VAL:O	1:A:583:GLN:CG	2.68	0.41
1:A:215:LYS:N	1:A:215:LYS:HD3	2.35	0.41
1:A:144:ASN:OD1	1:A:146:SER:HB2	2.19	0.41
1:A:495:TYR:O	1:A:496:SER:HB3	2.20	0.41
1:A:582:VAL:O	1:A:583:GLN:HG2	2.20	0.41
1:B:124:ILE:HD12	1:B:124:ILE:N	2.35	0.41
1:B:430:ILE:O	1:B:430:ILE:HD12	2.20	0.41
1:A:430:ILE:HG13	1:A:430:ILE:H	1.54	0.41
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.55	0.41
1:A:557:LYS:HD3	1:A:557:LYS:HA	1.89	0.41
1:B:575:CYS:O	1:B:575:CYS:SG	2.79	0.41
1:B:427:THR:HB	1:B:428:ARG:NH2	2.35	0.41
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.55	0.41
1:B:403:SER:HB2	1:B:405:LYS:NZ	2.36	0.41
1:B:404:PHE:HB2	1:B:405:LYS:HE3	2.03	0.41
1:B:111:LEU:HD12	1:B:111:LEU:O	2.19	0.41
1:A:385:TYR:CE2	4:A:1591:NPX:H121	2.56	0.41
1:B:215:LYS:CE	1:B:215:LYS:H	2.33	0.41
1:A:543:GLN:HB2	7:B:871:HOH:O	2.20	0.41
1:A:144:ASN:CG	2:A:671:NAG:C1	2.89	0.41
1:B:422:PHE:O	1:B:426:PHE:HB2	2.21	0.41
1:B:489:ALA:HA	7:B:820:HOH:O	2.19	0.40
1:A:298:LEU:HA	1:A:298:LEU:HD12	1.90	0.40
1:A:415:LEU:HD23	1:A:415:LEU:HA	1.86	0.40
1:A:232:HIS:CD2	1:A:232:HIS:H	2.39	0.40
1:B:287:VAL:HA	7:B:650:HOH:O	2.20	0.40
1:B:76:THR:O	1:B:80:LEU:HG	2.22	0.40
1:B:424:GLU:HA	1:B:428:ARG:HH21	1.87	0.40
1:A:473:LYS:HA	1:A:474:PRO:HD2	1.88	0.40
1:B:344:VAL:O	1:B:348:TYR:HB3	2.22	0.40
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.91	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/587 (94%)	523 (95%)	19 (4%)	8 (2%)	15	20
1	B	550/587 (94%)	516 (94%)	20 (4%)	14 (2%)	9	8
All	All	1100/1174 (94%)	1039 (94%)	39 (4%)	22 (2%)	11	13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	287	VAL
1	A	422	PHE
1	B	138	SER
1	B	282	ASN
1	B	287	VAL
1	B	422	PHE
1	B	514	PRO
1	B	575	CYS
1	A	130	TYR
1	A	399	ASP
1	B	399	ASP
1	B	573	LYS
1	A	398	GLU
1	A	514	PRO
1	B	130	TYR
1	B	281	GLU
1	B	398	GLU
1	A	573	LYS
1	B	137	LYS
1	B	409	TYR
1	B	82	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	493/525 (94%)	439 (89%)	54 (11%)	9	12
1	B	493/525 (94%)	438 (89%)	55 (11%)	9	12
All	All	986/1050 (94%)	877 (89%)	109 (11%)	9	12

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	54	GLN
1	A	71	THR
1	A	82	LEU
1	A	83	LYS
1	A	93	LEU
1	A	116	VAL
1	A	117	LEU
1	A	122	TYR
1	A	132	VAL
1	A	150	ARG
1	A	170	GLU
1	A	171	LEU
1	A	178	LEU
1	A	216	ARG
1	A	232	HIS
1	A	238	LEU
1	A	248	LYS
1	A	252	LEU
1	A	271	VAL
1	A	282	ASN
1	A	289	GLN
1	A	298	LEU
1	A	316	LEU
1	A	318	GLN
1	A	322	GLU
1	A	326	GLU
1	A	376	ARG
1	A	377	ILE

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Mol	Chain	Res	Type
1	A	382	ASN
1	A	385	TYR
1	A	398	GLU
1	A	405	LYS
1	A	409	TYR
1	A	422	PHE
1	A	428	ARG
1	A	430	ILE
1	A	442	ILE
1	A	455	SER
1	A	469	ARG
1	A	479	GLU
1	A	484	GLU
1	A	485	LYS
1	A	500	VAL
1	A	509	VAL
1	A	513	ARG
1	A	514	PRO
1	A	534	LEU
1	A	556	PHE
1	A	557	LYS
1	A	577	PHE
1	A	578	THR
1	A	582	VAL
1	A	583	GLN
1	B	44	ARG
1	B	54	GLN
1	B	71	THR
1	B	83	LYS
1	B	93	LEU
1	B	107	PHE
1	B	111	LEU
1	B	116	VAL
1	B	117	LEU
1	B	122	TYR
1	B	132	VAL
1	B	137	LYS
1	B	138	SER
1	B	165	VAL
1	B	170	GLU
1	B	171	LEU
1	B	178	LEU

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Mol	Chain	Res	Type
1	B	185	ARG
1	B	186	GLU
1	B	215	LYS
1	B	232	HIS
1	B	239	ASP
1	B	252	LEU
1	B	270	GLN
1	B	272	GLU
1	B	281	GLU
1	B	282	ASN
1	B	289	GLN
1	B	298	LEU
1	B	316	LEU
1	B	322	GLU
1	B	376	ARG
1	B	377	ILE
1	B	382	ASN
1	B	385	TYR
1	B	398	GLU
1	B	405	LYS
1	B	409	TYR
1	B	422	PHE
1	B	428	ARG
1	B	479	GLU
1	B	484	GLU
1	B	509	VAL
1	B	513	ARG
1	B	525	LEU
1	B	532	LYS
1	B	534	LEU
1	B	543	GLN
1	B	554	VAL
1	B	556	PHE
1	B	557	LYS
1	B	577	PHE
1	B	578	THR
1	B	582	VAL
1	B	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	68	ASN
1	A	95	HIS
1	A	133	HIS
1	A	203	GLN
1	A	204	HIS
1	A	214	HIS
1	A	232	HIS
1	A	242	HIS
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	370	GLN
1	A	382	ASN
1	A	386	HIS
1	A	396	ASN
1	A	417	HIS
1	A	454	GLN
1	A	464	ASN
1	A	583	GLN
1	B	42	GLN
1	B	68	ASN
1	B	95	HIS
1	B	105	ASN
1	B	133	HIS
1	B	144	ASN
1	B	203	GLN
1	B	204	HIS
1	B	214	HIS
1	B	232	HIS
1	B	282	ASN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	382	ASN
1	B	386	HIS
1	B	396	ASN
1	B	411	ASN
1	B	417	HIS
1	B	454	GLN
1	B	464	ASN



### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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$
4	NPX	A	1591	-	18,18,18	1.31	2 (11%)	25,25,25	1.25	4 (16%)
5	BOG	A	3	-	20,20,20	1.32	2 (10%)	25,25,25	1.06	2 (8%)
5	BOG	A	6	-	20,20,20	1.40	3 (15%)	25,25,25	1.34	3 (12%)
5	BOG	A	620	-	20,20,20	1.36	3 (15%)	25,25,25	1.36	3 (12%)
2	NAG	A	661	-	12,14,15	0.76	1 (8%)	15,19,21	0.82	1 (6%)
2	NAG	A	671	-	12,14,15	0.86	1 (8%)	15,19,21	1.45	2 (13%)
2	NAG	A	681	-	12,14,15	0.74	1 (8%)	15,19,21	0.84	1 (6%)
3	HEM	A	682	1,7	49,50,50	2.67	17 (34%)	46,82,82	2.16	10 (21%)
2	NAG	A	9	-	12,14,15	0.65	0	15,19,21	1.08	1 (6%)
4	NPX	B	1591	-	18,18,18	1.29	1 (5%)	25,25,25	1.08	0
5	BOG	B	3	-	20,20,20	1.36	2 (10%)	25,25,25	1.19	4 (16%)
5	BOG	B	620	-	20,20,20	1.34	2 (10%)	25,25,25	1.20	4 (16%)
2	NAG	B	661	-	12,14,15	0.60	0	15,19,21	1.31	2 (13%)
2	NAG	B	671	-	12,14,15	0.80	0	15,19,21	1.08	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	681	-	12,14,15	0.74	1 (8%)	15,19,21	1.85	2 (13%)
3	HEM	B	682	1	49,50,50	2.64	18 (36%)	46,82,82	2.08	9 (19%)
2	NAG	B	9	-	12,14,15	0.67	0	15,19,21	0.80	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
4	NPX	A	1591	-	-	0/10/10/10	0/0/2/2
5	BOG	A	3	-	-	0/11/31/31	0/1/1/1
5	BOG	A	6	-	-	0/11/31/31	0/1/1/1
5	BOG	A	620	-	-	0/11/31/31	0/1/1/1
2	NAG	A	661	-	-	0/6/23/26	0/1/1/1
2	NAG	A	671	-	-	0/6/23/26	0/1/1/1
2	NAG	A	681	-	-	0/6/23/26	0/1/1/1
3	HEM	A	682	1,7	-	0/14/114/114	0/0/8/8
2	NAG	A	9	-	-	0/6/23/26	0/1/1/1
4	NPX	B	1591	-	-	0/10/10/10	0/0/2/2
5	BOG	B	3	-	-	0/11/31/31	0/1/1/1
5	BOG	B	620	-	-	0/11/31/31	0/1/1/1
2	NAG	B	661	-	-	0/6/23/26	0/1/1/1
2	NAG	B	671	-	-	0/6/23/26	0/1/1/1
2	NAG	B	681	-	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/14/114/114	0/0/8/8
2	NAG	B	9	-	-	0/6/23/26	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	682	HEM	C2B-C1B	7.86	1.46	1.44
3	A	682	HEM	C2B-C1B	6.50	1.46	1.44
3	A	682	HEM	C2D-C1D	6.19	1.46	1.44
3	B	682	HEM	C3C-C2C	-5.83	1.33	1.43
3	A	682	HEM	C3D-C2D	5.67	1.53	1.43
3	B	682	HEM	C3B-C2B	-5.40	1.34	1.43
3	B	682	HEM	C2D-C1D	5.29	1.45	1.44
3	B	682	HEM	C3D-C2D	5.17	1.52	1.43
3	A	682	HEM	C3B-C2B	-5.15	1.34	1.43
3	A	682	HEM	C3C-C2C	-5.09	1.34	1.43
3	A	682	HEM	FE-ND	4.83	2.15	1.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3C-CAC	4.79	1.55	1.40
3	A	682	HEM	C3B-CAB	4.75	1.55	1.40
3	B	682	HEM	C3B-CAB	4.69	1.55	1.40
3	A	682	HEM	C4A-C3A	4.65	1.46	1.40
3	B	682	HEM	C3C-CAC	4.43	1.54	1.40
3	B	682	HEM	C4A-C3A	4.38	1.45	1.40
3	A	682	HEM	C3D-C4D	4.19	1.45	1.44
5	A	6	BOG	C4-C3	-4.11	1.41	1.52
5	B	3	BOG	C4-C3	-4.07	1.41	1.52
5	B	620	BOG	C4-C3	-4.05	1.41	1.52
3	B	682	HEM	FE-ND	3.96	2.12	1.97
5	A	620	BOG	C4-C3	-3.95	1.41	1.52
5	A	3	BOG	C4-C3	-3.90	1.42	1.52
3	B	682	HEM	FE-NB	3.42	2.10	1.97
3	A	682	HEM	FE-NA	3.25	2.06	1.92
3	A	682	HEM	FE-NC	3.14	2.09	1.97
3	B	682	HEM	C3D-C4D	2.73	1.45	1.44
3	B	682	HEM	FE-NA	2.72	2.04	1.92
3	B	682	HEM	FE-NC	2.52	2.07	1.97
3	A	682	HEM	CMD-C2D	2.51	1.55	1.47
5	A	620	BOG	O5-C5	2.42	1.50	1.44
3	A	682	HEM	CHB-C1B	2.40	1.39	1.35
3	A	682	HEM	CMB-C2B	2.38	1.54	1.47
3	B	682	HEM	CMD-C2D	2.36	1.54	1.47
3	B	682	HEM	CMB-C2B	2.35	1.54	1.47
2	A	661	NAG	O5-C5	-2.34	1.41	1.45
5	B	3	BOG	O5-C5	2.33	1.50	1.44
3	B	682	HEM	CHB-C1B	2.32	1.39	1.35
3	B	682	HEM	CMC-C2C	2.32	1.54	1.47
5	A	3	BOG	O3-C3	2.26	1.48	1.43
4	B	1591	NPX	C8-C9	-2.21	1.49	1.52
5	B	620	BOG	O5-C5	2.21	1.49	1.44
2	A	671	NAG	O5-C5	-2.20	1.41	1.45
5	A	6	BOG	O4-C4	2.18	1.48	1.43
4	A	1591	NPX	C8-C9	-2.18	1.49	1.52
2	A	681	NAG	O5-C5	-2.15	1.41	1.45
3	B	682	HEM	CHA-C4D	2.14	1.38	1.35
3	A	682	HEM	CMC-C2C	2.14	1.54	1.47
3	A	682	HEM	FE-NB	2.12	2.05	1.97
5	A	6	BOG	C3-C2	-2.10	1.46	1.52
5	A	620	BOG	O3-C3	2.09	1.48	1.43
2	B	681	NAG	O5-C5	-2.04	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1591	NPX	C3-C2	2.02	1.40	1.36

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	682	HEM	C3B-C4B-NB	-8.25	108.10	114.00
3	B	682	HEM	C3B-C4B-NB	-6.89	109.07	114.00
3	B	682	HEM	C4D-ND-C1D	6.83	112.15	105.16
3	A	682	HEM	C4D-ND-C1D	6.47	111.78	105.16
2	B	681	NAG	O5-C5-C6	5.40	112.64	106.98
3	B	682	HEM	C2D-C1D-ND	-4.08	108.11	112.93
3	B	682	HEM	CBD-CAD-C3D	-3.97	105.70	114.37
2	A	671	NAG	O5-C5-C6	3.94	111.11	106.98
5	A	6	BOG	O5-C5-C4	3.87	116.92	109.76
3	A	682	HEM	C2D-C1D-ND	-3.87	108.36	112.93
2	B	681	NAG	O5-C5-C4	-3.83	105.79	110.65
3	B	682	HEM	CHC-C1C-NC	3.55	127.81	124.73
3	A	682	HEM	CBD-CAD-C3D	-3.32	107.13	114.37
2	B	661	NAG	O5-C5-C4	3.30	114.83	110.65
3	A	682	HEM	C1B-NB-C4B	3.29	108.53	105.16
5	A	620	BOG	C1'-O1-C1	3.26	119.81	113.96
3	A	682	HEM	CHC-C4B-NB	3.17	127.22	124.58
2	B	661	NAG	C3-C4-C5	3.13	115.80	110.20
3	A	682	HEM	C3A-C4A-NA	-3.01	107.14	109.41
5	A	620	BOG	O5-C5-C4	2.98	115.27	109.76
3	A	682	HEM	C4C-NC-C1C	2.91	108.56	105.53
5	A	620	BOG	O6-C6-C5	2.83	121.11	111.36
3	B	682	HEM	C3A-C4A-NA	-2.72	107.36	109.41
5	A	3	BOG	C1'-O1-C1	2.70	118.81	113.96
5	B	620	BOG	C1'-O1-C1	2.65	118.73	113.96
3	B	682	HEM	C1B-NB-C4B	2.65	107.87	105.16
5	B	3	BOG	C1'-O1-C1	2.64	118.70	113.96
5	B	3	BOG	O5-C5-C4	2.63	114.64	109.76
3	A	682	HEM	CHC-C1C-NC	2.56	126.95	124.73
4	A	1591	NPX	C10-C9-C8	-2.55	106.92	112.83
4	A	1591	NPX	C8-C9-C15	2.54	117.03	108.70
5	A	6	BOG	C1'-O1-C1	2.50	118.45	113.96
2	A	671	NAG	O4-C4-C3	-2.49	104.76	110.35
3	B	682	HEM	C4C-NC-C1C	2.49	108.12	105.53
3	B	682	HEM	CBA-CAA-C2A	-2.45	108.37	112.69
5	B	620	BOG	O6-C6-C5	2.44	119.76	111.36
2	A	9	NAG	C3-C4-C5	2.35	114.41	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	3	BOG	O6-C6-C5	2.30	119.27	111.36
2	A	681	NAG	O5-C5-C6	2.27	109.36	106.98
2	A	661	NAG	O5-C5-C4	-2.26	107.78	110.65
4	A	1591	NPX	O-C15-OXT	-2.21	119.07	124.07
2	B	671	NAG	O4-C4-C3	-2.21	105.40	110.35
5	B	620	BOG	O5-C5-C4	2.19	113.82	109.76
5	B	620	BOG	O1-C1'-C2'	2.19	118.42	109.87
5	A	3	BOG	O6-C6-C5	2.15	118.75	111.36
5	A	6	BOG	O1-C1'-C2'	2.14	118.22	109.87
5	B	3	BOG	O1-C1'-C2'	2.12	118.14	109.87
4	A	1591	NPX	O2-C1-C6	-2.10	119.29	124.63
2	B	671	NAG	C2-N2-C7	-2.08	119.60	123.09
2	B	671	NAG	C3-C4-C5	2.01	113.79	110.20
3	A	682	HEM	C4A-CHB-C1B	-2.00	124.83	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	552/587 (94%)	-0.54	6 (1%) 77 77	15, 26, 47, 62	0
1	B	552/587 (94%)	-0.54	4 (0%) 84 84	14, 26, 47, 70	0
All	All	1104/1174 (94%)	-0.54	10 (0%) 81 81	14, 26, 47, 70	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	GLN	3.7
1	B	81	LEU	3.6
1	A	583	GLN	3.6
1	A	122	TYR	2.9
1	A	74	PHE	2.9
1	A	409	TYR	2.9
1	B	398	GLU	2.8
1	B	74	PHE	2.6
1	A	398	GLU	2.2
1	A	33	ALA	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	BOG	A	620	20/20	0.26	-	43,58,65,65	0
6	CL	B	1	1/1	0.06	-	32,32,32,32	0
5	BOG	B	620	20/20	0.26	-	39,63,73,75	0
2	NAG	B	9	14/15	0.33	-	41,54,64,66	0
2	NAG	B	661	14/15	0.25	-	43,54,60,62	0
3	HEM	B	682	43/43	0.12	-	20,25,40,61	0
4	NPX	B	1591	17/17	0.15	-	20,28,43,45	0
5	BOG	A	6	20/20	0.17	-	45,51,58,59	0
3	HEM	A	682	43/43	0.10	-	17,25,44,60	0
2	NAG	B	671	14/15	0.10	-	25,30,35,38	0
2	NAG	A	671	14/15	0.12	-	21,30,36,39	0
2	NAG	B	681	14/15	0.20	-	40,46,50,57	0
2	NAG	A	681	14/15	0.18	-	40,48,54,55	0
2	NAG	A	661	14/15	0.23	-	43,55,64,64	0
6	CL	A	1	1/1	0.09	-	33,33,33,33	0
2	NAG	A	9	14/15	0.24	-	37,54,62,63	0
5	BOG	B	3	20/20	0.16	-	49,55,63,64	0
5	BOG	A	3	20/20	0.10	-	27,33,37,39	0
4	NPX	A	1591	17/17	0.12	-	21,24,34,40	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.