



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 PM GMT

PDB ID : 4FM5  
Title : X-ray structure of des-methylflurbiprofen bound to murine COX-2  
Authors : Xu, S.; Banerjee, S.; Windsor, M.A.; Marnett, L.J.  
Deposited on : 2012-06-15  
Resolution : 2.81 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

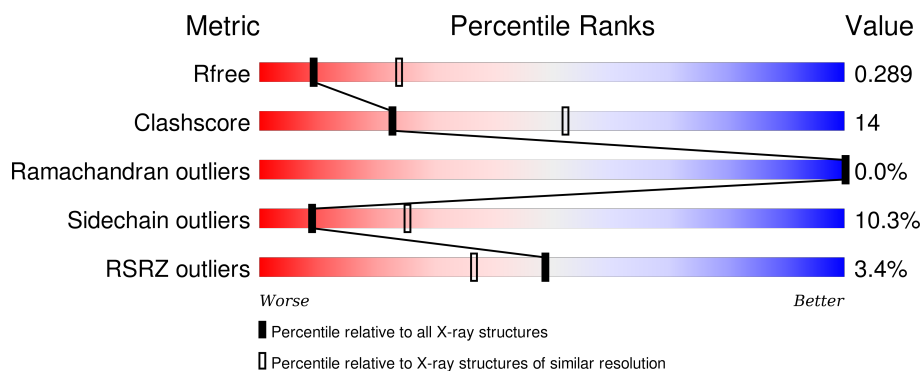
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	604	<div> <div>3%</div> <div>68% 20% • 9%</div> </div>
1	B	604	<div> <div>4%</div> <div>66% 20% • 9%</div> </div>
1	C	604	<div> <div>3%</div> <div>69% 19% • • 9%</div> </div>
1	D	604	<div> <div>2%</div> <div>66% 20% 5% 9%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	703	-	-	X	-
5	DF0	C	706	-	-	-	X

## 2 Entry composition [i](#)

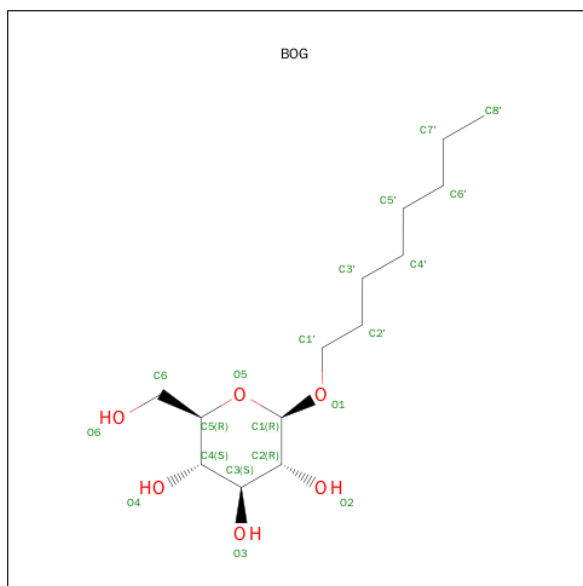
There are 6 unique types of molecules in this entry. The entry contains 18554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

- Molecule 2 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C<sub>14</sub>H<sub>28</sub>O<sub>6</sub>).



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

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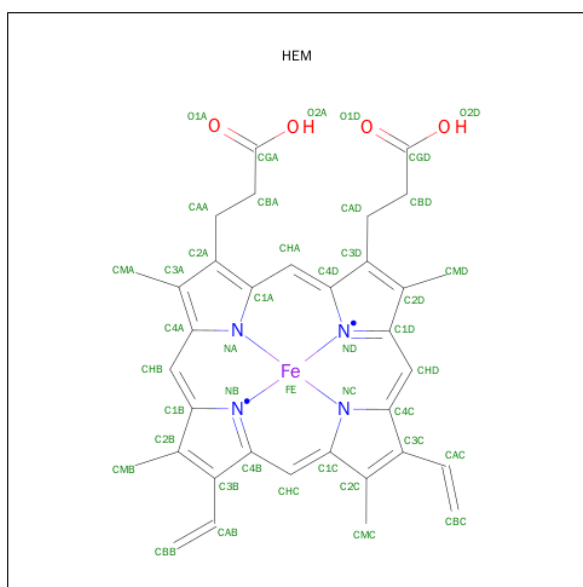
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			20	14	6		
2	D	1	Total	C	O	0	0
			20	14	6		

- 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		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

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



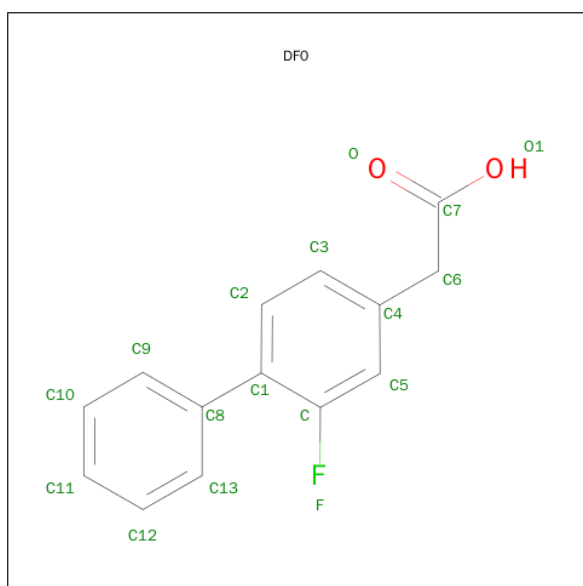
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 5 is (2-FLUOROBIPHENYL-4-YL)ACETIC ACID (three-letter code: DF0) (formula: C<sub>14</sub>H<sub>11</sub>FO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	F	O		
			17	14	1	2		
5	B	1	Total	C	F	O		
			17	14	1	2		
5	C	1	Total	C	F	O		
			17	14	1	2		
5	D	1	Total	C	F	O		
			17	14	1	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	63	Total	O		
			63	63	0	0
6	B	39	Total	O		
			39	39	0	0

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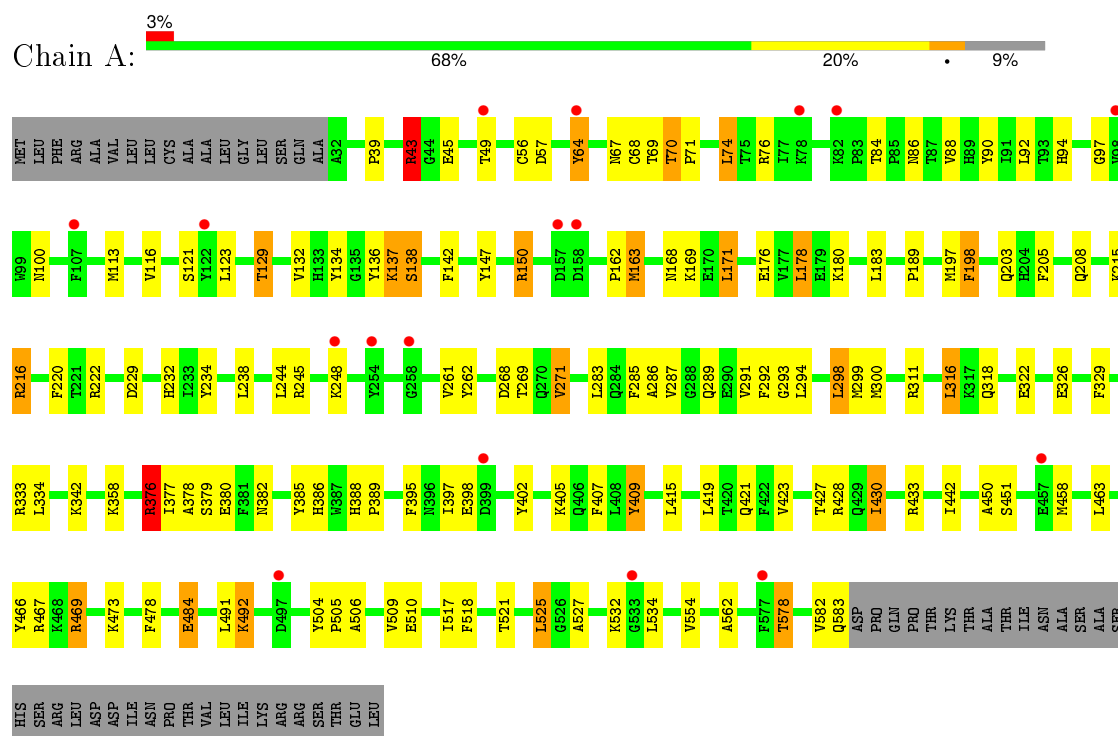
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	37	Total	O	0	0
			37	37		
6	D	47	Total	O	0	0
			47	47		

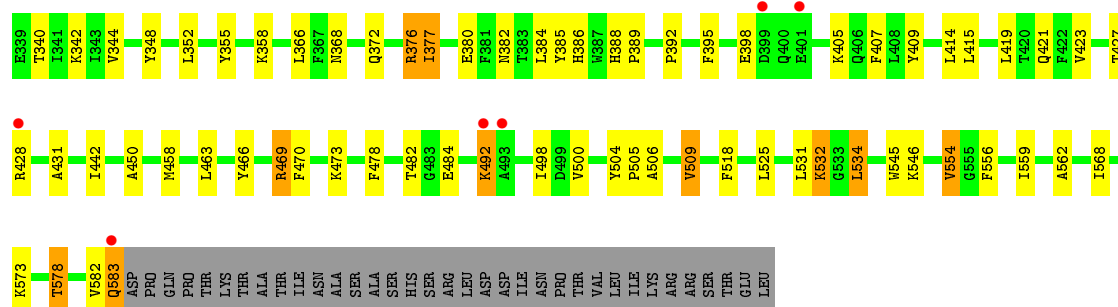
### 3 Residue-property plots

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.

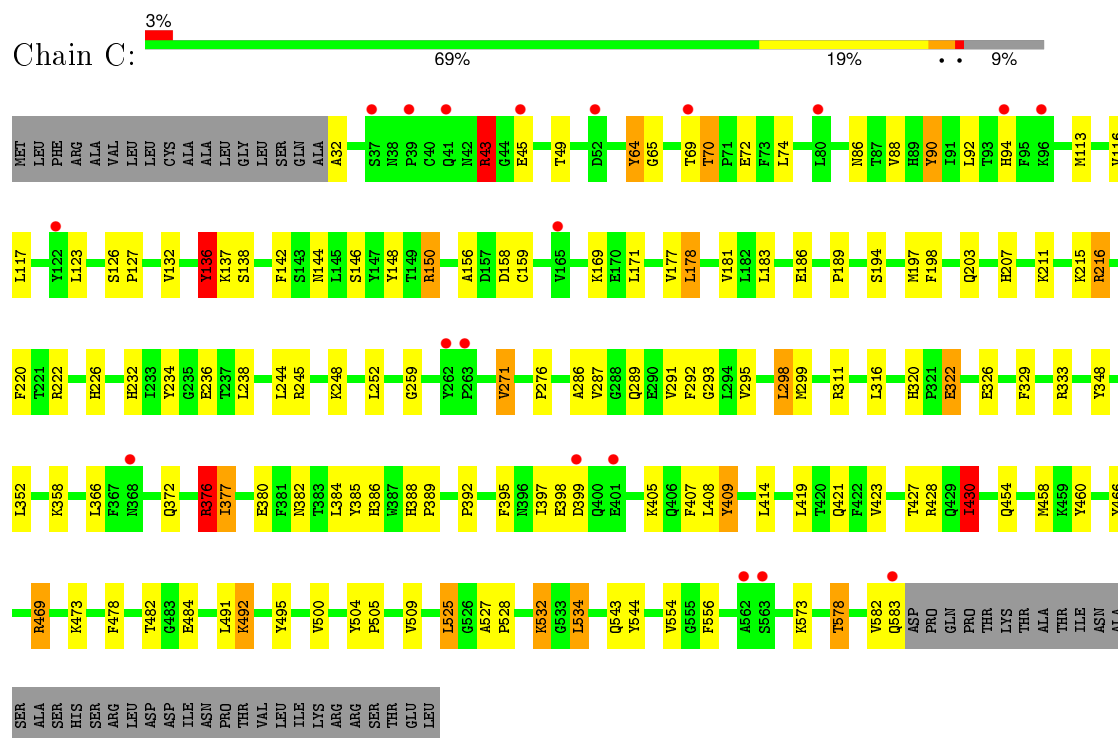
#### • Molecule 1: Prostaglandin G/H synthase 2



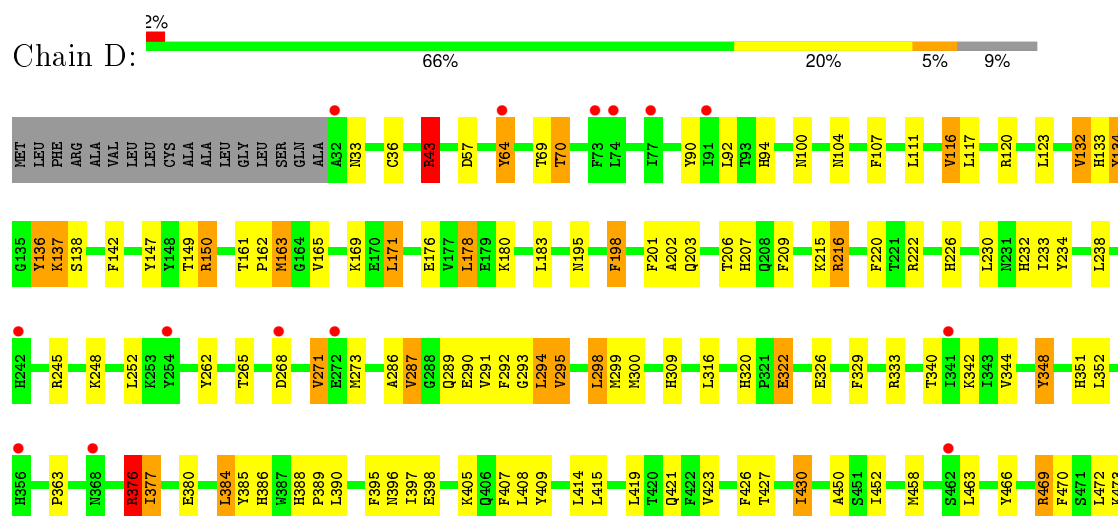


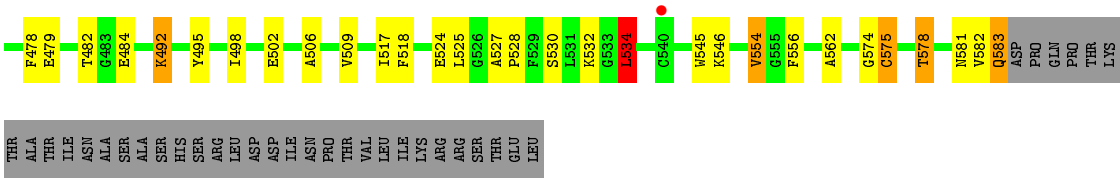


• Molecule 1: Prostaglandin G/H synthase 2



• Molecule 1: Prostaglandin G/H synthase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.63Å 135.70Å 125.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.86 – 2.81 49.86 – 2.81	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.86-2.81) 98.5 (49.86-2.81)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.240 , 0.290 0.240 , 0.289	Depositor DCC
$R_{free}$ test set	3808 reflections (5.38%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.0	Xtriage
Anisotropy	0.282	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 28.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	4 of 74531 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	18554	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.74 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6881e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, DF0, 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	0.74	3/4601 (0.1%)	0.82	7/6239 (0.1%)
1	B	0.76	5/4601 (0.1%)	0.81	4/6239 (0.1%)
1	C	0.74	3/4601 (0.1%)	0.82	4/6239 (0.1%)
1	D	0.85	16/4601 (0.3%)	0.83	7/6239 (0.1%)
All	All	0.77	27/18404 (0.1%)	0.82	22/24956 (0.1%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	147	TYR	CE1-CZ	-11.20	1.24	1.38
1	D	348	TYR	CE1-CZ	-10.52	1.24	1.38
1	D	348	TYR	CG-CD2	-9.67	1.26	1.39
1	D	147	TYR	CG-CD2	-9.19	1.27	1.39
1	D	147	TYR	CG-CD1	-9.03	1.27	1.39
1	D	147	TYR	CE2-CZ	-8.29	1.27	1.38
1	D	574	GLY	C-O	-7.58	1.11	1.23
1	D	348	TYR	CG-CD1	-7.42	1.29	1.39
1	D	136	TYR	CE1-CZ	-7.39	1.28	1.38
1	B	134	TYR	CE1-CZ	-7.30	1.29	1.38
1	D	348	TYR	CE2-CZ	-6.89	1.29	1.38
1	B	136	TYR	CE1-CZ	-5.93	1.30	1.38
1	D	136	TYR	CG-CD1	-5.77	1.31	1.39
1	C	573	LYS	C-O	-5.62	1.12	1.23
1	D	134	TYR	CG-CD1	-5.61	1.31	1.39
1	D	134	TYR	CG-CD2	-5.52	1.31	1.39
1	C	136	TYR	CE1-CZ	-5.51	1.31	1.38
1	A	147	TYR	CE1-CZ	-5.46	1.31	1.38
1	C	220	PHE	CG-CD2	-5.36	1.30	1.38
1	D	136	TYR	CG-CD2	-5.33	1.32	1.39
1	B	220	PHE	CG-CD1	-5.32	1.30	1.38
1	D	134	TYR	CE1-CZ	-5.30	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TYR	CE1-CZ	-5.21	1.31	1.38
1	A	136	TYR	CG-CD1	-5.10	1.32	1.39
1	D	198	PHE	CG-CD2	-5.06	1.31	1.38
1	B	90	TYR	CE1-CZ	-5.02	1.32	1.38
1	B	545	TRP	CD2-CE2	5.01	1.47	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	376	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	B	43	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	C	43	ARG	NE-CZ-NH1	6.73	123.66	120.30
1	A	467	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	534	LEU	CA-CB-CG	6.15	129.45	115.30
1	D	575	CYS	N-CA-C	-6.11	94.50	111.00
1	C	430	ILE	CB-CA-C	-5.91	99.79	111.60
1	A	229	ASP	CB-CG-OD1	5.87	123.58	118.30
1	B	43	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	376	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	60	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	A	376	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	376	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	C	534	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	268	ASP	CB-CG-OD1	5.18	122.97	118.30
1	D	132	VAL	CB-CA-C	-5.16	101.60	111.40
1	D	534	LEU	CA-CB-CG	5.13	127.10	115.30
1	D	495	TYR	N-CA-C	-5.09	97.25	111.00
1	A	43	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	D	163	MET	N-CA-C	-5.08	97.29	111.00
1	A	163	MET	N-CA-C	-5.04	97.40	111.00
1	D	43	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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	4474	0	4375	105	0
1	B	4474	0	4375	134	0
1	C	4474	0	4376	114	0
1	D	4474	0	4375	134	0
2	A	40	0	56	2	0
2	B	20	0	28	0	0
2	C	40	0	56	1	0
2	D	20	0	28	0	0
3	A	28	0	25	1	0
3	B	28	0	25	4	0
3	C	28	0	25	11	0
3	D	28	0	25	2	0
4	A	43	0	30	2	0
4	B	43	0	30	2	0
4	C	43	0	30	1	0
4	D	43	0	30	3	0
5	A	17	0	10	1	0
5	B	17	0	10	1	0
5	C	17	0	10	1	0
5	D	17	0	10	1	0
6	A	63	0	0	24	0
6	B	39	0	0	11	0
6	C	37	0	0	9	0
6	D	47	0	0	17	0
All	All	18554	0	17929	493	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 14.

All (493) 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:D:294:LEU:CD2	1:D:295:VAL:CG2	1.79	1.57
1:D:294:LEU:HD23	1:D:295:VAL:CG2	1.15	1.55
1:C:144:ASN:HD21	3:C:704:NAG:C1	0.90	1.55
1:D:294:LEU:CD2	1:D:295:VAL:HG22	1.39	1.47
2:A:701:BOG:H8'1	6:A:831:HOH:O	1.27	1.32
1:C:216:ARG:HG3	3:C:703:NAG:C8	1.62	1.29
1:D:430:ILE:HG23	6:D:838:HOH:O	1.27	1.27
1:B:398:GLU:HG3	1:B:421:GLN:NE2	1.60	1.17
1:A:39:PRO:HD3	6:A:823:HOH:O	1.42	1.16
1:A:262:TYR:HE2	1:A:415:LEU:HD23	1.10	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:PHE:HB3	6:B:826:HOH:O	1.45	1.13
1:D:294:LEU:HD23	1:D:295:VAL:HG23	1.12	1.11
1:C:216:ARG:CG	3:C:703:NAG:H81	1.81	1.10
1:B:398:GLU:CG	1:B:421:GLN:NE2	2.18	1.07
1:C:276:PRO:HG3	1:C:409:TYR:HD2	1.18	1.05
1:C:276:PRO:HG3	1:C:409:TYR:CD2	1.91	1.04
1:D:527:ALA:HB3	6:D:833:HOH:O	1.58	1.01
1:D:528:PRO:HD3	6:D:833:HOH:O	1.60	1.01
1:D:294:LEU:CD2	1:D:295:VAL:HG23	1.68	1.01
1:C:216:ARG:HG3	3:C:703:NAG:H81	1.01	1.00
1:A:262:TYR:CE2	1:A:415:LEU:HD23	1.96	0.98
4:D:704:HEM:C1D	6:D:814:HOH:O	2.16	0.97
1:D:554:VAL:HG13	6:D:828:HOH:O	1.64	0.97
1:D:294:LEU:HD21	1:D:295:VAL:CG2	1.91	0.97
1:A:262:TYR:HE2	1:A:415:LEU:CD2	1.78	0.96
1:D:397:ILE:HD11	1:D:426:PHE:CE1	2.01	0.95
1:A:71:PRO:HB2	6:A:838:HOH:O	1.63	0.95
1:B:294:LEU:HD23	1:B:295:VAL:HG23	1.49	0.94
1:C:408:LEU:C	1:C:409:TYR:HD1	1.71	0.93
3:B:702:NAG:C1	3:B:703:NAG:H61	1.98	0.93
1:C:216:ARG:NH1	3:C:703:NAG:H83	1.82	0.93
1:D:107:PHE:HB3	6:D:839:HOH:O	1.68	0.93
1:C:123:LEU:O	1:C:469:ARG:NH2	2.02	0.93
1:C:216:ARG:HH11	3:C:703:NAG:C8	1.83	0.91
1:B:398:GLU:HG3	1:B:421:GLN:HE22	1.25	0.91
1:D:294:LEU:HD21	1:D:295:VAL:HG22	1.44	0.91
1:C:276:PRO:CG	1:C:409:TYR:HD2	1.85	0.89
1:B:123:LEU:O	1:B:469:ARG:NH2	2.06	0.89
1:B:583:GLN:HB3	6:B:833:HOH:O	1.74	0.88
1:D:294:LEU:HA	1:D:409:TYR:CE1	2.09	0.88
1:A:398:GLU:HG3	1:A:421:GLN:NE2	1.89	0.87
1:A:123:LEU:O	1:A:469:ARG:NH2	2.06	0.87
1:B:478:PHE:HD1	1:B:498:ILE:HD13	1.37	0.86
1:D:123:LEU:O	1:D:469:ARG:NH2	2.08	0.86
1:B:392:PRO:HD2	1:B:395:PHE:HE1	1.41	0.85
1:B:478:PHE:CD1	1:B:498:ILE:HD13	2.10	0.85
1:B:64:TYR:HE1	1:B:70:THR:OG1	1.58	0.85
1:A:262:TYR:CE2	1:A:415:LEU:CD2	2.58	0.85
1:D:294:LEU:HD23	1:D:295:VAL:HG22	0.86	0.84
1:B:554:VAL:HG13	6:B:837:HOH:O	1.79	0.83
1:D:142:PHE:O	1:D:376:ARG:NH2	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:ARG:HH11	1:A:43:ARG:HG2	1.43	0.82
1:B:398:GLU:CG	1:B:421:GLN:HE21	1.88	0.81
1:C:43:ARG:HG2	1:C:43:ARG:HH11	1.44	0.81
1:A:168:ASN:HB3	6:A:853:HOH:O	1.80	0.81
1:B:478:PHE:HE1	1:B:498:ILE:HA	1.45	0.81
1:B:355:TYR:OH	5:B:705:DF0:O1	1.96	0.81
1:C:216:ARG:HG3	3:C:703:NAG:H82	1.63	0.81
1:A:245:ARG:NH2	1:A:326:GLU:OE2	2.14	0.80
1:B:43:ARG:HH11	1:B:43:ARG:HG2	1.47	0.80
1:D:43:ARG:HH11	1:D:43:ARG:HG2	1.45	0.80
1:B:113:MET:O	1:B:116:VAL:HG22	1.81	0.80
1:B:294:LEU:CD2	1:B:295:VAL:HG23	2.12	0.80
1:C:544:TYR:HA	1:D:137:LYS:NZ	1.97	0.80
1:A:484:GLU:HB3	6:A:851:HOH:O	1.81	0.80
1:C:392:PRO:HD2	1:C:395:PHE:HE1	1.47	0.79
1:C:216:ARG:NH1	3:C:703:NAG:C8	2.45	0.79
1:D:294:LEU:HA	1:D:409:TYR:CD1	2.18	0.79
1:B:216:ARG:NH1	3:B:702:NAG:O7	2.15	0.79
1:C:245:ARG:NH2	1:C:326:GLU:OE2	2.16	0.79
1:B:64:TYR:CE1	1:B:70:THR:OG1	2.38	0.77
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.65	0.77
1:C:454:GLN:HB3	6:C:821:HOH:O	1.84	0.77
1:D:245:ARG:NH2	1:D:326:GLU:OE2	2.18	0.77
1:D:294:LEU:HB2	1:D:409:TYR:CZ	2.20	0.77
1:B:531:LEU:HB2	6:B:816:HOH:O	1.86	0.75
1:C:216:ARG:CG	3:C:703:NAG:C8	2.51	0.75
1:D:294:LEU:HD22	1:D:295:VAL:HG23	1.68	0.75
1:B:245:ARG:NH2	1:B:326:GLU:OE2	2.20	0.74
1:D:470:PHE:CD1	1:D:525:LEU:HD22	2.22	0.74
1:B:117:LEU:HD23	1:B:366:LEU:HD11	1.69	0.74
1:B:142:PHE:O	1:B:376:ARG:NH2	2.16	0.73
1:D:150:ARG:NH2	1:D:458:MET:O	2.22	0.73
1:B:398:GLU:CD	1:B:421:GLN:HE21	1.93	0.72
1:B:150:ARG:NH2	1:B:458:MET:O	2.23	0.72
1:C:398:GLU:HG3	1:C:421:GLN:NE2	2.04	0.72
1:D:234:TYR:CE2	1:D:333:ARG:HG3	2.25	0.71
1:C:216:ARG:HH11	3:C:703:NAG:H82	1.55	0.70
3:C:703:NAG:C1	3:C:704:NAG:H61	2.22	0.70
1:D:216:ARG:HG3	3:D:702:NAG:O7	1.91	0.70
1:A:113:MET:O	1:A:116:VAL:HG22	1.91	0.70
1:C:408:LEU:C	1:C:409:TYR:CD1	2.62	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:142:PHE:O	1:C:376:ARG:NH2	2.18	0.69
1:A:216:ARG:HG3	3:A:703:NAG:O7	1.93	0.69
1:D:203:GLN:HG2	1:D:298:LEU:HD11	1.75	0.69
1:B:294:LEU:HG	1:B:295:VAL:HG22	1.75	0.68
1:A:285:PHE:CE1	6:A:854:HOH:O	2.45	0.68
1:C:189:PRO:HB3	1:C:430:ILE:HD13	1.76	0.68
1:B:271:VAL:HG22	1:B:286:ALA:HB1	1.76	0.68
1:B:294:LEU:CD2	1:B:295:VAL:CG2	2.71	0.68
1:C:276:PRO:CG	1:C:409:TYR:CD2	2.66	0.68
1:D:64:TYR:HE1	1:D:70:THR:OG1	1.76	0.68
1:C:544:TYR:HA	1:D:137:LYS:HZ1	1.59	0.67
1:B:398:GLU:CB	1:B:421:GLN:NE2	2.57	0.67
1:B:395:PHE:CD2	1:B:407:PHE:CD2	2.83	0.67
1:B:294:LEU:HA	1:B:409:TYR:CD1	2.30	0.67
1:A:68:CYS:SG	6:A:828:HOH:O	2.52	0.67
1:D:427:THR:HG22	1:D:583:GLN:HE22	1.59	0.67
1:B:478:PHE:CE1	1:B:498:ILE:HA	2.27	0.67
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.76	0.67
1:B:478:PHE:CE2	1:B:492:LYS:HA	2.31	0.66
1:D:203:GLN:CG	1:D:298:LEU:HD11	2.26	0.65
1:C:392:PRO:HD2	1:C:395:PHE:CE1	2.31	0.65
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.31	0.65
1:B:92:LEU:HD23	1:B:355:TYR:CZ	2.31	0.65
1:B:117:LEU:HB3	1:B:366:LEU:HD21	1.79	0.65
1:C:458:MET:HE2	6:C:821:HOH:O	1.96	0.65
1:B:392:PRO:HD2	1:B:395:PHE:CE1	2.28	0.64
1:D:294:LEU:CD2	1:D:295:VAL:HG21	2.17	0.64
1:B:271:VAL:CG2	1:B:286:ALA:HB1	2.26	0.64
1:D:479:GLU:HG3	6:D:809:HOH:O	1.98	0.64
1:C:409:TYR:CD1	1:C:409:TYR:N	2.65	0.64
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.78	0.64
1:A:216:ARG:HB3	1:A:220:PHE:CD2	2.32	0.64
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.33	0.64
1:D:195:ASN:HB3	1:D:582:VAL:HG23	1.80	0.64
1:D:64:TYR:CE1	1:D:70:THR:OG1	2.51	0.63
1:D:395:PHE:HD2	1:D:407:PHE:CE2	2.17	0.63
1:A:71:PRO:HG2	6:A:838:HOH:O	1.97	0.63
1:B:398:GLU:CG	1:B:421:GLN:HE22	1.95	0.62
1:D:395:PHE:CD2	1:D:407:PHE:CD2	2.87	0.62
1:D:216:ARG:HB3	1:D:220:PHE:CD2	2.34	0.62
1:C:408:LEU:HB3	1:C:409:TYR:CD1	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:THR:OG1	1:B:578:THR:HG22	1.99	0.62
1:D:395:PHE:CD2	1:D:407:PHE:CE2	2.87	0.62
1:C:146:SER:CB	6:C:815:HOH:O	2.46	0.62
1:B:423:VAL:HG13	1:B:578:THR:HG23	1.81	0.62
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.82	0.62
1:D:450:ALA:HA	6:D:845:HOH:O	2.00	0.62
1:B:423:VAL:CG1	1:B:578:THR:HG23	2.29	0.62
1:C:64:TYR:CE1	1:C:70:THR:OG1	2.52	0.62
1:D:398:GLU:HG3	1:D:421:GLN:NE2	2.14	0.61
1:D:273:MET:CE	1:D:287:VAL:HG22	2.30	0.61
1:B:423:VAL:HG13	1:B:578:THR:CG2	2.30	0.61
1:A:189:PRO:HB3	1:A:430:ILE:HD13	1.83	0.61
1:A:203:GLN:CG	1:A:298:LEU:HD11	2.31	0.61
1:C:150:ARG:NH2	1:C:458:MET:O	2.34	0.60
1:A:285:PHE:CZ	6:A:854:HOH:O	2.53	0.60
1:B:294:LEU:HB2	1:B:409:TYR:CZ	2.36	0.60
1:B:463:LEU:HD22	1:B:506:ALA:HB1	1.82	0.60
1:D:294:LEU:CA	1:D:409:TYR:CE1	2.84	0.60
1:D:427:THR:OG1	1:D:578:THR:HG22	2.00	0.60
1:C:245:ARG:HD3	1:C:329:PHE:CD1	2.37	0.59
1:B:463:LEU:HD22	1:B:506:ALA:CB	2.30	0.59
1:D:463:LEU:HD22	1:D:506:ALA:HB1	1.84	0.59
1:A:245:ARG:HD3	1:A:329:PHE:CD1	2.38	0.59
1:D:344:VAL:HG11	1:D:534:LEU:HD11	1.85	0.59
1:A:451:SER:HB3	6:A:852:HOH:O	2.03	0.59
1:B:245:ARG:HD3	1:B:329:PHE:CE1	2.39	0.58
1:D:463:LEU:HD22	1:D:506:ALA:CB	2.33	0.58
1:A:398:GLU:HG3	1:A:421:GLN:HE22	1.68	0.58
1:B:262:TYR:CE2	1:B:415:LEU:CD2	2.87	0.58
1:B:395:PHE:HD2	1:B:407:PHE:CG	2.22	0.58
1:A:427:THR:OG1	1:A:578:THR:HG22	2.03	0.58
1:A:150:ARG:NH2	1:A:458:MET:O	2.36	0.58
1:C:245:ARG:HD3	1:C:329:PHE:CE1	2.39	0.58
1:A:64:TYR:CE1	1:A:70:THR:OG1	2.57	0.57
1:C:203:GLN:HG2	1:C:298:LEU:HD11	1.86	0.57
1:D:271:VAL:HG22	1:D:286:ALA:HB1	1.85	0.57
1:C:88:VAL:HG11	2:C:702:BOG:H1'1	1.86	0.57
1:C:423:VAL:HG13	1:C:578:THR:HG23	1.86	0.57
1:B:209:PHE:HB2	1:B:377:ILE:HG21	1.87	0.56
1:D:33:ASN:HB3	1:D:36:CYS:SG	2.45	0.56
1:B:245:ARG:HD3	1:B:329:PHE:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:TYR:CE2	1:B:333:ARG:HG3	2.41	0.56
1:A:245:ARG:HD3	1:A:329:PHE:CE1	2.41	0.56
1:B:203:GLN:HG2	1:B:298:LEU:HD11	1.87	0.56
1:C:271:VAL:HG22	1:C:286:ALA:HB1	1.86	0.56
4:B:704:HEM:HBB2	4:B:704:HEM:HMB1	1.87	0.56
1:C:203:GLN:CG	1:C:298:LEU:HD11	2.36	0.55
1:D:352:LEU:HD12	1:D:352:LEU:C	2.26	0.55
1:C:211:LYS:NZ	1:C:236:GLU:OE1	2.38	0.55
1:A:142:PHE:O	1:A:376:ARG:NH2	2.29	0.55
1:B:117:LEU:HD23	1:B:366:LEU:CD1	2.36	0.55
1:D:245:ARG:HD3	1:D:329:PHE:CE1	2.41	0.55
1:D:273:MET:SD	1:D:290:GLU:HA	2.47	0.55
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.42	0.55
1:D:397:ILE:CD1	1:D:426:PHE:CE1	2.85	0.55
1:B:478:PHE:HE2	1:B:492:LYS:HA	1.72	0.55
1:A:178:LEU:HD22	1:A:183:LEU:HG	1.88	0.54
4:D:704:HEM:HHD	4:D:704:HEM:HBC2	1.89	0.54
1:C:395:PHE:CD2	1:C:407:PHE:CD2	2.96	0.54
1:D:90:TYR:CE1	1:D:94:HIS:CE1	2.95	0.54
1:D:386:HIS:HA	6:D:814:HOH:O	2.05	0.54
1:D:163:MET:HE1	1:D:502:GLU:HG2	1.90	0.54
1:D:397:ILE:HD11	1:D:426:PHE:CZ	2.43	0.54
1:A:45:GLU:OE1	1:A:137:LYS:NZ	2.41	0.54
1:A:198:PHE:CD1	1:A:198:PHE:C	2.81	0.54
1:C:408:LEU:CB	1:C:409:TYR:CD1	2.91	0.53
1:C:478:PHE:CE2	1:C:492:LYS:HA	2.42	0.53
1:B:340:THR:O	1:B:344:VAL:HG23	2.08	0.53
1:D:198:PHE:C	1:D:198:PHE:CD1	2.81	0.53
1:D:230:LEU:HB3	1:D:233:ILE:HD12	1.89	0.53
1:B:382:ASN:O	1:B:386:HIS:HD2	1.92	0.53
1:C:207:HIS:CD2	6:C:832:HOH:O	2.62	0.53
1:A:76:ARG:HB2	6:A:838:HOH:O	2.08	0.53
1:B:478:PHE:CD1	1:B:498:ILE:CD1	2.90	0.53
1:D:245:ARG:HD3	1:D:329:PHE:CD1	2.44	0.53
1:C:64:TYR:HB2	6:C:818:HOH:O	2.08	0.53
1:B:216:ARG:HG3	3:B:702:NAG:O7	2.08	0.53
1:C:408:LEU:HB3	1:C:409:TYR:CE1	2.44	0.53
1:D:90:TYR:HE1	1:D:94:HIS:NE2	2.07	0.53
1:B:251:LYS:HE2	6:B:824:HOH:O	2.09	0.53
1:B:179:GLU:HA	1:B:183:LEU:HD12	1.91	0.52
1:B:372:GLN:HB2	1:B:532:LYS:HZ1	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:LEU:HB2	1:D:409:TYR:OH	2.08	0.52
1:A:450:ALA:HA	6:A:850:HOH:O	2.09	0.52
1:A:57:ASP:C	1:A:57:ASP:OD1	2.48	0.52
1:A:423:VAL:HG13	1:A:578:THR:CG2	2.37	0.52
1:D:116:VAL:O	1:D:120:ARG:HG2	2.10	0.52
1:A:525:LEU:N	1:A:525:LEU:HD23	2.25	0.52
1:D:342:LYS:HG2	1:D:562:ALA:HB3	1.91	0.52
1:C:117:LEU:HD23	1:C:366:LEU:HD11	1.92	0.52
1:A:64:TYR:HD1	1:A:70:THR:O	1.93	0.52
1:D:478:PHE:CE2	1:D:492:LYS:HA	2.45	0.52
1:A:176:GLU:HG2	1:A:180:LYS:HD2	1.92	0.52
1:D:262:TYR:CE2	1:D:415:LEU:CD2	2.93	0.52
1:C:113:MET:O	1:C:116:VAL:HG22	2.10	0.51
1:A:138:SER:HA	1:B:334:LEU:HD11	1.92	0.51
1:D:427:THR:CG2	1:D:583:GLN:HE22	2.23	0.51
1:D:398:GLU:OE2	1:D:421:GLN:HG3	2.10	0.51
1:A:342:LYS:HG2	1:A:562:ALA:HB3	1.91	0.51
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.45	0.51
1:B:178:LEU:HD22	1:B:183:LEU:HG	1.91	0.51
1:D:273:MET:HE2	1:D:287:VAL:HG22	1.93	0.51
1:C:458:MET:HE3	1:C:460:TYR:CE1	2.45	0.51
1:B:265:THR:OG1	1:B:268:ASP:HB3	2.10	0.51
1:A:510:GLU:OE2	1:A:521:THR:OG1	2.27	0.51
1:D:120:ARG:HD2	6:D:833:HOH:O	2.11	0.51
1:B:43:ARG:HG2	1:B:43:ARG:NH1	2.21	0.51
1:D:291:VAL:O	1:D:294:LEU:HB3	2.11	0.51
1:C:197:MET:CE	1:C:578:THR:HG21	2.41	0.51
1:D:386:HIS:CG	6:D:814:HOH:O	2.64	0.51
1:D:384:LEU:C	1:D:384:LEU:HD12	2.30	0.50
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.93	0.50
1:C:382:ASN:O	1:C:386:HIS:HD2	1.93	0.50
1:A:261:VAL:O	1:A:262:TYR:HD1	1.94	0.50
1:A:292:PHE:O	1:A:299:MET:HE1	2.12	0.50
1:B:294:LEU:HG	1:B:295:VAL:CG2	2.40	0.50
1:C:244:LEU:CD2	1:C:271:VAL:HG11	2.42	0.50
1:B:33:ASN:HB3	1:B:36:CYS:SG	2.52	0.50
1:B:388:HIS:N	1:B:389:PRO:HD2	2.27	0.50
1:B:427:THR:HG22	1:B:583:GLN:HE22	1.77	0.50
1:B:32:ALA:HB3	1:B:158:ASP:OD2	2.12	0.50
1:A:395:PHE:HD2	1:A:407:PHE:CE2	2.30	0.49
1:C:259:GLY:HA3	6:C:819:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:295:VAL:HG23	1:D:298:LEU:HD22	1.94	0.49
1:C:352:LEU:HD12	1:C:352:LEU:C	2.33	0.49
1:B:478:PHE:CE1	1:B:498:ILE:CD1	2.95	0.49
1:A:398:GLU:CG	1:A:421:GLN:NE2	2.70	0.49
1:D:252:LEU:HD13	1:D:309:HIS:CD2	2.48	0.49
1:A:433:ARG:HD3	6:A:834:HOH:O	2.13	0.49
1:C:427:THR:OG1	1:C:578:THR:HG22	2.13	0.49
1:B:293:GLY:HA2	1:B:299:MET:HE2	1.95	0.49
1:B:482:THR:HG22	1:B:509:VAL:HG13	1.94	0.49
1:B:352:LEU:HD13	1:B:518:PHE:HE2	1.78	0.49
1:C:177:VAL:O	1:C:181:VAL:HG22	2.13	0.49
1:C:43:ARG:HG2	1:C:43:ARG:NH1	2.21	0.49
1:B:183:LEU:HD22	1:B:442:ILE:HD13	1.95	0.49
1:D:201:PHE:CD1	1:D:348:TYR:CD2	3.01	0.48
1:B:320:HIS:HA	1:B:322:GLU:OE2	2.13	0.48
1:D:472:LEU:HD11	1:D:524:GLU:HB2	1.94	0.48
1:C:395:PHE:HD2	1:C:407:PHE:CG	2.31	0.48
1:C:65:GLY:N	6:C:818:HOH:O	2.32	0.48
1:D:90:TYR:CD1	1:D:94:HIS:CE1	3.02	0.48
1:B:216:ARG:HG3	3:B:702:NAG:H81	1.96	0.48
1:A:76:ARG:HG2	6:A:859:HOH:O	2.13	0.48
1:D:149:THR:OG1	1:D:150:ARG:N	2.46	0.48
1:D:271:VAL:CG2	1:D:286:ALA:HB1	2.44	0.48
1:C:234:TYR:CE2	1:C:333:ARG:HG3	2.48	0.48
1:C:116:VAL:CG2	1:C:117:LEU:N	2.77	0.47
1:D:201:PHE:CD1	1:D:348:TYR:HD2	2.32	0.47
1:C:194:SER:HB3	1:C:198:PHE:HD2	1.79	0.47
4:A:705:HEM:HBC2	4:A:705:HEM:HHD	1.96	0.47
1:B:384:LEU:C	1:B:384:LEU:HD12	2.35	0.47
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.49	0.47
1:D:396:ASN:C	1:D:397:ILE:HD13	2.35	0.47
1:A:395:PHE:CD2	1:A:407:PHE:CE2	3.02	0.47
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.44	0.47
1:C:197:MET:HG3	1:C:578:THR:HG22	1.96	0.47
1:D:202:ALA:O	1:D:206:THR:HG23	2.15	0.47
1:D:388:HIS:N	1:D:389:PRO:HD2	2.30	0.47
1:C:408:LEU:CB	1:C:409:TYR:CE1	2.98	0.47
1:C:276:PRO:HG3	1:C:409:TYR:CE2	2.46	0.47
1:B:398:GLU:CB	1:B:421:GLN:HE22	2.22	0.47
1:A:423:VAL:CG1	1:A:578:THR:HG23	2.40	0.47
1:C:178:LEU:HD22	1:C:183:LEU:HG	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:GLY:HA3	1:B:559:ILE:HD13	1.96	0.47
1:D:265:THR:OG1	1:D:268:ASP:HB3	2.15	0.47
1:B:427:THR:OG1	1:B:578:THR:CG2	2.62	0.47
1:A:388:HIS:N	1:A:389:PRO:HD2	2.29	0.47
1:D:178:LEU:HD22	1:D:183:LEU:HG	1.96	0.47
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.96	0.47
1:A:76:ARG:CB	6:A:838:HOH:O	2.61	0.47
1:C:295:VAL:CG2	1:C:298:LEU:HD22	2.44	0.47
1:D:90:TYR:HE1	1:D:94:HIS:CE1	2.33	0.47
1:C:544:TYR:HA	1:D:137:LYS:HZ3	1.77	0.46
1:D:294:LEU:HD21	1:D:295:VAL:HG21	1.90	0.46
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.50	0.46
1:B:395:PHE:CD2	1:B:407:PHE:CG	3.04	0.46
1:C:293:GLY:HA2	1:C:299:MET:HE2	1.98	0.46
1:C:500:VAL:HG12	1:C:500:VAL:O	2.14	0.46
1:A:261:VAL:C	1:A:262:TYR:HD1	2.18	0.46
1:B:226:HIS:HB3	1:B:376:ARG:HA	1.97	0.46
1:D:582:VAL:HB	6:D:838:HOH:O	2.15	0.46
1:B:382:ASN:O	1:B:386:HIS:CD2	2.69	0.46
1:C:527:ALA:HA	5:C:706:DF0:C2	2.45	0.46
1:B:398:GLU:HB2	1:B:421:GLN:NE2	2.31	0.46
1:A:395:PHE:N	1:A:395:PHE:HD1	2.14	0.46
1:A:205:PHE:O	1:A:208:GLN:HG2	2.16	0.46
1:D:287:VAL:CG2	1:D:289:GLN:O	2.64	0.46
1:A:395:PHE:N	1:A:395:PHE:CD1	2.83	0.46
1:A:269:THR:OG1	1:A:271:VAL:HG13	2.16	0.46
1:D:390:LEU:HD21	1:D:517:ILE:HD11	1.98	0.46
1:D:209:PHE:HB2	1:D:377:ILE:HG21	1.97	0.46
1:A:517:ILE:HG23	1:A:518:PHE:CG	2.51	0.46
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.98	0.45
1:D:320:HIS:HA	1:D:322:GLU:OE2	2.16	0.45
1:A:84:THR:O	1:A:88:VAL:HG23	2.17	0.45
1:D:120:ARG:CZ	6:D:833:HOH:O	2.64	0.45
1:C:136:TYR:N	1:C:136:TYR:CD1	2.84	0.45
1:D:161:THR:O	1:D:163:MET:O	2.34	0.45
1:A:162:PRO:HB2	1:A:171:LEU:HD22	1.97	0.45
1:B:287:VAL:HG11	1:B:302:ALA:HB1	1.97	0.45
1:A:71:PRO:CB	6:A:838:HOH:O	2.37	0.45
1:B:45:GLU:OE1	1:B:137:LYS:NZ	2.42	0.45
1:D:423:VAL:HG13	1:D:578:THR:CG2	2.47	0.45
1:A:86:ASN:HD22	1:A:86:ASN:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:LEU:HD23	1:B:355:TYR:CE1	2.51	0.45
1:C:398:GLU:CG	1:C:421:GLN:NE2	2.76	0.45
1:C:64:TYR:HD1	1:C:70:THR:O	1.99	0.45
1:A:382:ASN:O	1:A:386:HIS:HD2	1.99	0.45
1:B:194:SER:HB3	1:B:198:PHE:HD2	1.82	0.45
1:B:117:LEU:HD23	1:B:366:LEU:CG	2.47	0.45
1:B:273:MET:SD	1:B:290:GLU:HA	2.57	0.45
1:D:295:VAL:CG2	1:D:298:LEU:HD22	2.46	0.44
1:A:395:PHE:CD2	1:A:407:PHE:CD2	3.06	0.44
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.80	0.44
1:C:482:THR:HG22	1:C:509:VAL:CG1	2.46	0.44
1:C:126:SER:HA	1:C:127:PRO:C	2.37	0.44
2:A:701:BOG:C8'	6:A:831:HOH:O	2.11	0.44
1:D:479:GLU:CG	6:D:809:HOH:O	2.62	0.44
1:C:500:VAL:CG1	1:C:500:VAL:O	2.65	0.44
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.98	0.44
1:C:388:HIS:N	1:C:389:PRO:HD2	2.32	0.44
1:C:491:LEU:HD11	1:C:509:VAL:HG11	2.00	0.44
1:C:384:LEU:C	1:C:384:LEU:HD12	2.38	0.44
1:C:198:PHE:HE1	1:C:348:TYR:CE1	2.35	0.44
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.53	0.44
1:D:162:PRO:HB2	1:D:171:LEU:HD22	1.98	0.44
1:B:427:THR:CG2	1:B:583:GLN:HE22	2.31	0.44
1:C:320:HIS:HA	1:C:322:GLU:OE2	2.18	0.44
4:C:705:HEM:HMB1	4:C:705:HEM:HBB2	1.99	0.44
1:B:197:MET:HG3	1:B:578:THR:HG22	1.99	0.44
1:A:45:GLU:OE2	1:B:546:LYS:HD2	2.18	0.44
1:B:320:HIS:CA	1:B:322:GLU:OE2	2.66	0.44
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.58	0.44
1:C:504:TYR:HB3	1:C:505:PRO:HD3	2.00	0.44
1:A:504:TYR:HB3	1:A:505:PRO:HD3	2.00	0.44
1:B:176:GLU:HG2	1:B:180:LYS:HD2	2.00	0.43
1:A:163:MET:HB3	6:A:846:HOH:O	2.18	0.43
1:C:414:LEU:HD11	1:C:419:LEU:HD23	2.00	0.43
1:C:382:ASN:HB3	6:C:812:HOH:O	2.17	0.43
1:D:273:MET:CE	1:D:287:VAL:CG2	2.96	0.43
1:A:318:GLN:HG3	6:A:822:HOH:O	2.19	0.43
1:A:90:TYR:HE1	1:A:94:HIS:NE2	2.16	0.43
1:D:198:PHE:CD2	1:D:351:HIS:HD2	2.37	0.43
1:C:525:LEU:N	1:C:525:LEU:HD23	2.33	0.43
1:D:294:LEU:HD23	1:D:295:VAL:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:ARG:NH1	6:D:833:HOH:O	2.52	0.43
1:A:129:THR:HG22	1:A:137:LYS:HD2	1.99	0.43
1:C:482:THR:HG22	1:C:509:VAL:HG12	2.01	0.43
1:A:300:MET:HG3	1:A:419:LEU:HD22	2.00	0.43
1:A:197:MET:HG3	1:A:578:THR:HG22	1.99	0.43
1:B:203:GLN:CG	1:B:298:LEU:HD11	2.49	0.43
1:B:194:SER:HB3	1:B:198:PHE:CD2	2.53	0.43
1:A:378:ALA:O	1:A:379:SER:C	2.55	0.43
1:D:452:ILE:HG23	6:D:823:HOH:O	2.19	0.43
1:D:176:GLU:HG2	1:D:180:LYS:HD2	2.01	0.43
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.54	0.43
1:D:90:TYR:HE1	1:D:94:HIS:CD2	2.37	0.43
1:B:57:ASP:OD1	1:B:57:ASP:C	2.58	0.43
1:A:271:VAL:HG22	1:A:286:ALA:HB1	2.01	0.43
1:C:293:GLY:HA2	1:C:299:MET:CE	2.49	0.43
1:B:450:ALA:HA	6:B:836:HOH:O	2.18	0.43
4:B:704:HEM:HBC2	4:B:704:HEM:HHD	2.01	0.42
1:C:117:LEU:HB3	1:C:366:LEU:HD21	2.02	0.42
1:C:90:TYR:CE1	1:C:94:HIS:CG	3.07	0.42
1:C:32:ALA:HB3	1:C:158:ASP:OD2	2.20	0.42
1:C:197:MET:HE3	1:C:578:THR:HG21	2.00	0.42
1:A:293:GLY:HA2	1:A:299:MET:CE	2.49	0.42
1:B:230:LEU:HB3	1:B:233:ILE:HD12	2.01	0.42
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.54	0.42
1:B:500:VAL:CG1	1:B:500:VAL:O	2.66	0.42
1:D:395:PHE:N	1:D:395:PHE:CD1	2.87	0.42
1:D:395:PHE:HD1	1:D:395:PHE:N	2.16	0.42
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.54	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.83	0.42
1:B:423:VAL:HG13	1:B:578:THR:HG21	2.01	0.42
1:B:205:PHE:CE2	1:B:344:VAL:HG21	2.55	0.42
1:B:132:VAL:HG22	6:B:806:HOH:O	2.19	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE2	2.01	0.42
1:D:530:SER:O	1:D:534:LEU:HD22	2.19	0.42
1:A:64:TYR:CD1	1:A:70:THR:O	2.73	0.42
1:A:388:HIS:N	1:A:389:PRO:CD	2.83	0.42
1:A:478:PHE:CE2	1:A:492:LYS:HA	2.54	0.42
1:D:120:ARG:NE	5:D:705:DF0:O	2.52	0.42
1:C:226:HIS:HB3	1:C:376:ARG:HA	2.01	0.42
1:A:67:ASN:C	6:A:828:HOH:O	2.57	0.42
1:C:148:TYR:CE1	1:C:377:ILE:HD11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.54	0.42
1:C:45:GLU:OE2	1:D:546:LYS:HD2	2.20	0.42
1:B:132:VAL:HG13	6:B:827:HOH:O	2.19	0.42
1:B:90:TYR:CD1	1:B:90:TYR:C	2.93	0.42
1:A:90:TYR:CE1	1:A:94:HIS:CE1	3.08	0.42
1:A:397:ILE:HD13	1:A:402:TYR:CD2	2.55	0.42
1:D:363:PRO:HG2	1:D:545:TRP:CD2	2.54	0.42
1:B:113:MET:O	1:B:117:LEU:HD13	2.20	0.41
1:D:216:ARG:NH1	3:D:702:NAG:O7	2.53	0.41
1:C:189:PRO:HB3	1:C:430:ILE:CD1	2.48	0.41
1:C:287:VAL:HG21	1:C:292:PHE:HB2	2.02	0.41
1:B:296:PRO:HD3	6:B:802:HOH:O	2.20	0.41
1:A:74:LEU:HD22	1:A:74:LEU:O	2.20	0.41
1:A:43:ARG:NH1	1:A:43:ARG:HG2	2.20	0.41
1:D:100:ASN:O	1:D:104:ASN:ND2	2.44	0.41
1:D:525:LEU:O	1:D:528:PRO:HD2	2.21	0.41
1:B:478:PHE:CE1	1:B:498:ILE:HD12	2.55	0.41
1:C:492:LYS:O	1:C:495:TYR:O	2.39	0.41
1:B:90:TYR:CE1	1:B:94:HIS:CG	3.08	0.41
1:A:463:LEU:HD22	1:A:506:ALA:CB	2.50	0.41
1:B:294:LEU:CG	1:B:295:VAL:CG2	2.99	0.41
1:D:226:HIS:HB3	1:D:376:ARG:HA	2.03	0.41
1:D:287:VAL:HG23	1:D:289:GLN:O	2.20	0.41
1:D:287:VAL:HG21	1:D:292:PHE:HB2	2.02	0.41
1:C:423:VAL:CG1	1:C:578:THR:HG23	2.50	0.41
1:D:517:ILE:HG23	1:D:518:PHE:CG	2.55	0.41
1:A:90:TYR:CD1	1:A:94:HIS:CE1	3.08	0.41
1:C:427:THR:OG1	1:C:578:THR:CG2	2.69	0.41
4:A:705:HEM:HMB2	4:A:705:HEM:HBB2	2.02	0.41
1:D:482:THR:HG22	1:D:509:VAL:HG13	2.02	0.41
1:D:423:VAL:HG13	1:D:578:THR:HG21	2.02	0.41
1:D:478:PHE:CD1	1:D:498:ILE:HD13	2.56	0.41
1:C:198:PHE:CE1	1:C:348:TYR:CE1	3.08	0.41
1:B:122:TYR:HB2	6:B:829:HOH:O	2.21	0.41
1:A:527:ALA:HA	5:A:706:DF0:C2	2.50	0.41
1:B:216:ARG:HG2	1:B:220:PHE:CD2	2.55	0.41
1:C:271:VAL:CG2	1:C:286:ALA:HB1	2.48	0.41
1:B:152:LEU:HD12	1:B:466:TYR:CD1	2.56	0.41
1:C:86:ASN:H	1:C:86:ASN:HD22	1.69	0.41
1:A:245:ARG:HD2	6:A:812:HOH:O	2.20	0.41
1:C:189:PRO:CB	1:C:430:ILE:HD13	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:TYR:C	1:C:90:TYR:HD1	2.24	0.41
1:B:368:ASN:HB3	6:B:825:HOH:O	2.20	0.41
1:A:283:LEU:HD21	1:A:415:LEU:HD12	2.03	0.41
1:B:395:PHE:CE2	1:B:407:PHE:CD2	3.09	0.41
1:A:285:PHE:CD1	6:A:854:HOH:O	2.73	0.41
1:A:525:LEU:N	1:A:525:LEU:CD2	2.83	0.41
1:B:162:PRO:HB2	1:B:171:LEU:HD22	2.02	0.41
1:B:196:MET:CE	1:B:431:ALA:HA	2.51	0.41
1:D:293:GLY:HA2	1:D:299:MET:HE2	2.03	0.41
1:C:372:GLN:HB2	1:C:532:LYS:NZ	2.36	0.41
4:D:704:HEM:C2D	6:D:814:HOH:O	2.58	0.41
1:B:388:HIS:N	1:B:389:PRO:CD	2.84	0.41
1:A:334:LEU:HD23	1:A:334:LEU:HA	1.83	0.41
1:C:72:GLU:HG2	6:C:828:HOH:O	2.19	0.41
1:B:197:MET:CE	1:B:578:THR:HG21	2.51	0.40
1:A:292:PHE:O	1:A:299:MET:CE	2.69	0.40
1:A:382:ASN:O	1:A:386:HIS:CD2	2.75	0.40
1:C:372:GLN:HB2	1:C:532:LYS:HZ1	1.86	0.40
1:D:57:ASP:C	1:D:57:ASP:OD1	2.60	0.40
1:B:117:LEU:HD23	1:B:366:LEU:HD21	2.02	0.40
1:A:56:CYS:HB3	6:A:828:HOH:O	2.20	0.40
1:D:340:THR:O	1:D:344:VAL:HG23	2.22	0.40
1:D:201:PHE:HD1	1:D:348:TYR:CD2	2.39	0.40
1:B:198:PHE:HE1	1:B:348:TYR:CE1	2.39	0.40
1:B:198:PHE:CE1	1:B:348:TYR:CE1	3.09	0.40
1:C:525:LEU:O	1:C:528:PRO:HD2	2.22	0.40
1:A:97:GLY:HA2	6:A:845:HOH:O	2.21	0.40
1:B:478:PHE:HE1	1:B:498:ILE:HD12	1.86	0.40
1:C:398:GLU:HG3	1:C:421:GLN:HE22	1.79	0.40
1:D:133:HIS:C	1:D:134:TYR:CD1	2.95	0.40
1:D:423:VAL:CG1	1:D:578:THR:HG23	2.51	0.40
1:D:300:MET:HG3	1:D:419:LEU:HD22	2.03	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	550/604 (91%)	527 (96%)	23 (4%)	0	100	100
1	B	550/604 (91%)	526 (96%)	24 (4%)	0	100	100
1	C	550/604 (91%)	523 (95%)	26 (5%)	1 (0%)	52	83
1	D	550/604 (91%)	524 (95%)	26 (5%)	0	100	100
All	All	2200/2416 (91%)	2100 (96%)	99 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	397	ILE

### 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	493/537 (92%)	442 (90%)	51 (10%)	9	25
1	B	493/537 (92%)	443 (90%)	50 (10%)	9	26
1	C	493/537 (92%)	440 (89%)	53 (11%)	8	23
1	D	493/537 (92%)	443 (90%)	50 (10%)	9	26
All	All	1972/2148 (92%)	1768 (90%)	204 (10%)	9	25

All (204) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	49	THR
1	A	64	TYR
1	A	69	THR
1	A	70	THR

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Mol	Chain	Res	Type
1	A	74	LEU
1	A	92	LEU
1	A	100	ASN
1	A	121	SER
1	A	129	THR
1	A	132	VAL
1	A	137	LYS
1	A	138	SER
1	A	150	ARG
1	A	169	LYS
1	A	171	LEU
1	A	178	LEU
1	A	198	PHE
1	A	215	LYS
1	A	216	ARG
1	A	222	ARG
1	A	232	HIS
1	A	238	LEU
1	A	248	LYS
1	A	271	VAL
1	A	289	GLN
1	A	291	VAL
1	A	298	LEU
1	A	311	ARG
1	A	316	LEU
1	A	322	GLU
1	A	358	LYS
1	A	376	ARG
1	A	377	ILE
1	A	385	TYR
1	A	405	LYS
1	A	409	TYR
1	A	428	ARG
1	A	430	ILE
1	A	442	ILE
1	A	469	ARG
1	A	473	LYS
1	A	484	GLU
1	A	492	LYS
1	A	525	LEU
1	A	532	LYS
1	A	534	LEU

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Mol	Chain	Res	Type
1	A	554	VAL
1	A	578	THR
1	A	582	VAL
1	A	583	GLN
1	B	43	ARG
1	B	49	THR
1	B	64	TYR
1	B	69	THR
1	B	70	THR
1	B	90	TYR
1	B	92	LEU
1	B	111	LEU
1	B	132	VAL
1	B	137	LYS
1	B	138	SER
1	B	150	ARG
1	B	165	VAL
1	B	169	LYS
1	B	171	LEU
1	B	178	LEU
1	B	215	LYS
1	B	216	ARG
1	B	222	ARG
1	B	238	LEU
1	B	248	LYS
1	B	287	VAL
1	B	289	GLN
1	B	291	VAL
1	B	294	LEU
1	B	295	VAL
1	B	298	LEU
1	B	316	LEU
1	B	322	GLU
1	B	326	GLU
1	B	358	LYS
1	B	376	ARG
1	B	377	ILE
1	B	385	TYR
1	B	405	LYS
1	B	428	ARG
1	B	469	ARG
1	B	473	LYS

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Mol	Chain	Res	Type
1	B	484	GLU
1	B	492	LYS
1	B	509	VAL
1	B	532	LYS
1	B	534	LEU
1	B	554	VAL
1	B	556	PHE
1	B	568	ILE
1	B	573	LYS
1	B	578	THR
1	B	582	VAL
1	B	583	GLN
1	C	43	ARG
1	C	49	THR
1	C	64	TYR
1	C	69	THR
1	C	70	THR
1	C	74	LEU
1	C	90	TYR
1	C	92	LEU
1	C	132	VAL
1	C	136	TYR
1	C	137	LYS
1	C	138	SER
1	C	150	ARG
1	C	169	LYS
1	C	171	LEU
1	C	178	LEU
1	C	186	GLU
1	C	215	LYS
1	C	216	ARG
1	C	222	ARG
1	C	232	HIS
1	C	238	LEU
1	C	248	LYS
1	C	252	LEU
1	C	271	VAL
1	C	289	GLN
1	C	291	VAL
1	C	298	LEU
1	C	311	ARG
1	C	316	LEU

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Mol	Chain	Res	Type
1	C	322	GLU
1	C	358	LYS
1	C	376	ARG
1	C	377	ILE
1	C	385	TYR
1	C	399	ASP
1	C	405	LYS
1	C	409	TYR
1	C	428	ARG
1	C	430	ILE
1	C	469	ARG
1	C	473	LYS
1	C	484	GLU
1	C	492	LYS
1	C	525	LEU
1	C	532	LYS
1	C	534	LEU
1	C	543	GLN
1	C	554	VAL
1	C	556	PHE
1	C	578	THR
1	C	582	VAL
1	C	583	GLN
1	D	43	ARG
1	D	64	TYR
1	D	69	THR
1	D	70	THR
1	D	92	LEU
1	D	111	LEU
1	D	116	VAL
1	D	117	LEU
1	D	132	VAL
1	D	136	TYR
1	D	137	LYS
1	D	138	SER
1	D	150	ARG
1	D	165	VAL
1	D	169	LYS
1	D	171	LEU
1	D	178	LEU
1	D	207	HIS
1	D	215	LYS

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Mol	Chain	Res	Type
1	D	216	ARG
1	D	222	ARG
1	D	232	HIS
1	D	238	LEU
1	D	248	LYS
1	D	271	VAL
1	D	287	VAL
1	D	294	LEU
1	D	295	VAL
1	D	298	LEU
1	D	316	LEU
1	D	322	GLU
1	D	376	ARG
1	D	377	ILE
1	D	384	LEU
1	D	385	TYR
1	D	405	LYS
1	D	408	LEU
1	D	430	ILE
1	D	469	ARG
1	D	473	LYS
1	D	484	GLU
1	D	492	LYS
1	D	532	LYS
1	D	534	LEU
1	D	554	VAL
1	D	556	PHE
1	D	575	CYS
1	D	578	THR
1	D	581	ASN
1	D	583	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	204	HIS
1	A	370	GLN
1	A	421	GLN
1	B	421	GLN
1	B	570	ASN
1	B	583	GLN

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Mol	Chain	Res	Type
1	C	86	ASN
1	C	144	ASN
1	C	204	HIS
1	C	327	GLN
1	C	421	GLN
1	C	445	GLN
1	D	86	ASN
1	D	421	GLN
1	D	583	GLN

### 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 ⓘ

8 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	703	3	14,14,15	0.28	0	15,19,21	0.53	0
3	NAG	A	704	1,3	14,14,15	0.89	1 (7%)	15,19,21	1.52	3 (20%)
3	NAG	B	702	3	14,14,15	0.27	0	15,19,21	0.54	0
3	NAG	B	703	1,3	14,14,15	0.66	0	15,19,21	1.47	2 (13%)
3	NAG	C	703	3	14,14,15	0.28	0	15,19,21	0.53	0
3	NAG	C	704	1,3	14,14,15	0.28	0	15,19,21	0.53	0
3	NAG	D	702	3	14,14,15	0.27	0	15,19,21	0.53	0
3	NAG	D	703	1,3	14,14,15	0.60	0	15,19,21	1.30	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	703	3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	703	3	-	0/6/23/26	0/1/1/1
3	NAG	C	704	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	702	3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	1,3	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	704	NAG	O5-C1	-2.79	1.39	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	704	NAG	C3-C4-C5	-2.18	106.39	110.20
3	B	703	NAG	C4-C3-C2	-2.02	108.08	111.23
3	A	704	NAG	O4-C4-C5	2.29	115.32	109.24
3	B	703	NAG	O5-C5-C6	2.94	113.71	107.35
3	A	704	NAG	C1-O5-C5	3.65	116.88	112.25
3	D	703	NAG	C1-O5-C5	4.12	117.48	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0
3	B	702	NAG	4	0
3	B	703	NAG	1	0
3	C	703	NAG	10	0
3	C	704	NAG	2	0
3	D	702	NAG	2	0

## 5.6 Ligand geometry

14 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
2	BOG	A	701	-	20,20,20	0.39	0	25,25,25	2.29	6 (24%)
2	BOG	A	702	-	20,20,20	0.47	0	25,25,25	1.28	4 (16%)
4	HEM	A	705	1	30,50,50	2.98	14 (46%)	24,82,82	2.79	12 (50%)
5	DF0	A	706	-	15,18,18	1.80	1 (6%)	21,24,24	1.70	4 (19%)
2	BOG	B	701	-	20,20,20	0.57	0	25,25,25	1.58	7 (28%)
4	HEM	B	704	1	30,50,50	3.29	16 (53%)	24,82,82	2.96	15 (62%)
5	DF0	B	705	-	15,18,18	1.97	1 (6%)	21,24,24	1.29	4 (19%)
2	BOG	C	701	-	20,20,20	0.45	0	25,25,25	0.62	0
2	BOG	C	702	-	20,20,20	0.73	1 (5%)	25,25,25	1.64	5 (20%)
4	HEM	C	705	1	30,50,50	3.10	14 (46%)	24,82,82	3.57	13 (54%)
5	DF0	C	706	-	15,18,18	1.64	1 (6%)	21,24,24	1.42	3 (14%)
2	BOG	D	701	-	20,20,20	0.45	0	25,25,25	0.62	0
4	HEM	D	704	1	30,50,50	3.22	14 (46%)	24,82,82	2.65	10 (41%)
5	DF0	D	705	-	15,18,18	1.98	1 (6%)	21,24,24	1.31	4 (19%)

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
2	BOG	A	701	-	-	0/11/31/31	0/1/1/1
2	BOG	A	702	-	-	0/11/31/31	0/1/1/1
4	HEM	A	705	1	-	0/10/54/54	0/0/8/8
5	DF0	A	706	-	-	0/6/8/8	0/2/2/2
2	BOG	B	701	-	-	0/11/31/31	0/1/1/1
4	HEM	B	704	1	-	0/10/54/54	0/0/8/8
5	DF0	B	705	-	-	0/6/8/8	0/2/2/2
2	BOG	C	701	-	-	0/11/31/31	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	C	702	-	-	0/11/31/31	0/1/1/1
4	HEM	C	705	1	-	0/10/54/54	0/0/8/8
5	DF0	C	706	-	-	0/6/8/8	0/2/2/2
2	BOG	D	701	-	-	0/11/31/31	0/1/1/1
4	HEM	D	704	1	-	0/10/54/54	0/0/8/8
5	DF0	D	705	-	-	0/6/8/8	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	HEM	C3B-C4B	-4.58	1.47	1.51
4	A	705	HEM	C3B-C4B	-4.31	1.48	1.51
4	C	705	HEM	C3B-C4B	-4.20	1.48	1.51
4	D	704	HEM	C3B-C4B	-3.12	1.49	1.51
4	B	704	HEM	C3D-C4D	-3.05	1.47	1.51
4	C	705	HEM	C3C-CAC	-2.87	1.45	1.51
4	B	704	HEM	C2D-C3D	-2.83	1.46	1.54
4	A	705	HEM	C2D-C3D	-2.70	1.46	1.54
4	D	704	HEM	C2D-C3D	-2.70	1.46	1.54
4	A	705	HEM	C2C-C1C	-2.67	1.47	1.52
4	C	705	HEM	C2C-C1C	-2.63	1.47	1.52
4	B	704	HEM	C2C-C1C	-2.42	1.48	1.52
4	D	704	HEM	C3D-C4D	-2.41	1.48	1.51
4	B	704	HEM	C3C-CAC	-2.41	1.46	1.51
4	C	705	HEM	C2D-C3D	-2.34	1.47	1.54
4	D	704	HEM	C2C-C1C	-2.07	1.48	1.52
4	A	705	HEM	C4A-CHB	2.01	1.45	1.39
4	C	705	HEM	FE-ND	2.03	2.08	1.97
4	A	705	HEM	C1A-CHA	2.12	1.45	1.39
4	B	704	HEM	C4A-CHB	2.16	1.45	1.39
4	A	705	HEM	CHC-C4B	2.20	1.45	1.38
4	C	705	HEM	C4A-CHB	2.21	1.45	1.39
2	C	702	BOG	O1-C1	2.24	1.44	1.40
4	C	705	HEM	CHD-C1D	2.29	1.45	1.38
4	B	704	HEM	CHC-C4B	2.29	1.45	1.38
4	D	704	HEM	C4A-CHB	2.29	1.46	1.39
4	B	704	HEM	C1A-CHA	2.36	1.46	1.39
4	A	705	HEM	CHD-C1D	2.37	1.45	1.38
4	C	705	HEM	CHC-C4B	2.41	1.45	1.38
4	D	704	HEM	CHD-C1D	2.43	1.45	1.38
4	D	704	HEM	FE-ND	2.54	2.10	1.97
4	C	705	HEM	CHC-C1C	2.62	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	704	HEM	CHD-C1D	2.63	1.46	1.38
4	A	705	HEM	FE-ND	2.64	2.11	1.97
4	B	704	HEM	FE-ND	2.65	2.11	1.97
4	A	705	HEM	FE-NB	2.72	2.11	1.97
4	D	704	HEM	CHC-C4B	2.73	1.46	1.38
4	A	705	HEM	CHC-C1C	2.81	1.43	1.36
4	C	705	HEM	FE-NB	2.95	2.13	1.97
4	B	704	HEM	FE-NB	2.99	2.13	1.97
4	D	704	HEM	C2A-C3A	3.24	1.47	1.37
4	D	704	HEM	FE-NB	3.25	2.14	1.97
4	B	704	HEM	CHC-C1C	3.47	1.44	1.36
4	C	705	HEM	C2A-C3A	3.48	1.48	1.37
4	A	705	HEM	C2A-C3A	3.52	1.48	1.37
4	B	704	HEM	C2A-C3A	3.56	1.48	1.37
4	D	704	HEM	CHC-C1C	3.72	1.45	1.36
4	A	705	HEM	CHD-C4C	3.77	1.45	1.36
4	C	705	HEM	CHD-C4C	4.33	1.46	1.36
4	D	704	HEM	CHD-C4C	4.39	1.46	1.36
4	B	704	HEM	CHD-C4C	4.85	1.47	1.36
5	C	706	DF0	C1-C	5.82	1.46	1.38
5	A	706	DF0	C1-C	6.67	1.47	1.38
5	D	705	DF0	C1-C	7.12	1.48	1.38
5	B	705	DF0	C1-C	7.14	1.48	1.38
4	A	705	HEM	C1C-NC	7.82	1.45	1.36
4	C	705	HEM	C4C-NC	9.00	1.47	1.36
4	B	704	HEM	C1C-NC	9.17	1.47	1.36
4	A	705	HEM	C4C-NC	9.36	1.47	1.36
4	C	705	HEM	C1C-NC	9.38	1.47	1.36
4	B	704	HEM	C4C-NC	9.61	1.47	1.36
4	D	704	HEM	C1C-NC	9.71	1.48	1.36
4	D	704	HEM	C4C-NC	9.90	1.48	1.36

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	705	HEM	C3C-CAC-CBC	-8.44	111.50	124.46
2	A	701	BOG	O1-C1-C2	-7.97	97.97	108.04
4	C	705	HEM	C2C-C1C-CHC	-4.38	117.02	123.68
4	C	705	HEM	C3B-C4B-CHC	-4.11	117.37	123.16
5	A	706	DF0	C5-C-C1	-3.67	119.62	124.24
4	C	705	HEM	CBD-CAD-C3D	-3.44	103.55	113.55
4	A	705	HEM	C2C-C1C-CHC	-3.39	118.53	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	706	DF0	C5-C-C1	-3.37	120.00	124.24
2	A	702	BOG	O1-C1-C2	-3.35	103.80	108.04
5	A	706	DF0	C8-C1-C	-3.33	118.78	123.05
4	D	704	HEM	C2C-C1C-CHC	-3.20	118.81	123.68
4	A	705	HEM	C3B-C4B-CHC	-3.19	118.67	123.16
2	C	702	BOG	O1-C1-C2	-3.02	104.23	108.04
5	C	706	DF0	C7-C6-C4	-2.90	106.99	112.73
4	B	704	HEM	C2C-C1C-CHC	-2.86	119.34	123.68
4	A	705	HEM	C1D-CHD-C4C	-2.73	121.26	125.82
2	A	701	BOG	C4-C3-C2	-2.72	105.71	110.79
2	B	701	BOG	C4-C3-C2	-2.71	105.73	110.79
2	B	701	BOG	O2-C2-C3	-2.70	104.26	110.34
4	B	704	HEM	C3C-CAC-CBC	-2.67	120.36	124.46
4	B	704	HEM	C3B-C4B-CHC	-2.64	119.45	123.16
5	B	705	DF0	C5-C-C1	-2.63	120.93	124.24
5	D	705	DF0	C8-C1-C	-2.53	119.80	123.05
4	C	705	HEM	C4B-CHC-C1C	-2.48	121.68	125.82
4	D	704	HEM	C3B-C4B-CHC	-2.40	119.79	123.16
4	D	704	HEM	C1D-CHD-C4C	-2.39	121.83	125.82
2	B	701	BOG	O5-C1-C2	-2.38	105.39	110.28
5	B	705	DF0	C8-C1-C	-2.33	120.06	123.05
4	B	704	HEM	C4B-CHC-C1C	-2.25	122.07	125.82
2	A	701	BOG	O6-C6-C5	-2.24	103.93	111.33
4	A	705	HEM	CBD-CAD-C3D	-2.15	107.28	113.55
2	A	702	BOG	O5-C1-C2	-2.14	105.88	110.28
4	B	704	HEM	C3B-CAB-CBB	-2.11	121.22	124.46
5	D	705	DF0	C13-C8-C1	-2.08	117.74	120.93
5	D	705	DF0	C7-C6-C4	-2.08	108.62	112.73
4	B	704	HEM	C1D-CHD-C4C	-2.03	122.43	125.82
2	B	701	BOG	C1'-O1-C1	2.02	117.48	113.94
2	B	701	BOG	O2-C2-C1	2.07	114.56	110.02
4	B	704	HEM	CBA-CAA-C2A	2.11	116.31	112.53
2	A	702	BOG	O5-C1-O1	2.15	115.23	110.05
4	B	704	HEM	C3B-C4B-NB	2.30	116.03	111.63
5	D	705	DF0	C2-C1-C8	2.36	123.16	118.78
5	B	705	DF0	F-C-C5	2.43	123.16	118.59
4	A	705	HEM	C3B-C4B-NB	2.44	116.30	111.63
2	A	701	BOG	O3-C3-C4	2.47	115.89	110.34
4	A	705	HEM	CAA-C2A-C1A	2.49	129.71	127.01
2	B	701	BOG	C1-O5-C5	2.58	118.75	113.75
2	C	702	BOG	O5-C1-O1	2.59	116.30	110.05
4	D	704	HEM	C3B-C4B-NB	2.63	116.66	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	702	BOG	C1-O5-C5	2.64	118.88	113.75
5	B	705	DF0	C2-C1-C8	2.67	123.72	118.78
5	C	706	DF0	F-C-C5	2.71	123.68	118.59
2	A	702	BOG	O5-C5-C4	2.84	115.01	109.68
2	C	702	BOG	C3-C4-C5	2.86	115.18	110.20
5	A	706	DF0	F-C-C5	2.87	123.98	118.59
4	C	705	HEM	C3B-C4B-NB	2.95	117.27	111.63
5	A	706	DF0	C2-C1-C	3.02	118.90	115.90
2	B	701	BOG	O5-C5-C4	3.32	115.91	109.68
4	D	704	HEM	CMD-C2D-C3D	3.54	130.02	114.35
4	B	704	HEM	CMD-C2D-C3D	3.56	130.08	114.35
4	B	704	HEM	C2C-C1C-NC	3.70	116.45	110.21
4	C	705	HEM	CMD-C2D-C3D	3.74	130.90	114.35
4	C	705	HEM	CAA-C2A-C1A	3.75	131.08	127.01
4	A	705	HEM	CMD-C2D-C3D	3.76	130.99	114.35
4	C	705	HEM	CMC-C2C-C3C	3.78	125.96	116.53
4	A	705	HEM	C2C-C1C-NC	3.86	116.71	110.21
2	A	701	BOG	C1-O5-C5	3.86	121.23	113.75
2	A	701	BOG	O5-C5-C4	4.06	117.30	109.68
4	C	705	HEM	CAD-C3D-C4D	4.12	127.00	112.47
4	D	704	HEM	C2C-C1C-NC	4.14	117.19	110.21
4	D	704	HEM	CMC-C2C-C3C	4.17	126.94	116.53
4	B	704	HEM	CMC-C2C-C3C	4.21	127.05	116.53
4	B	704	HEM	CAD-C3D-C4D	4.27	127.52	112.47
4	B	704	HEM	CAA-C2A-C1A	4.34	131.72	127.01
4	A	705	HEM	CAD-C3D-C4D	4.43	128.11	112.47
4	D	704	HEM	CAD-C3D-C4D	4.52	128.41	112.47
4	A	705	HEM	CMC-C2C-C3C	4.75	128.40	116.53
2	C	702	BOG	O5-C5-C4	5.10	119.25	109.68
4	A	705	HEM	CAD-C3D-C2D	5.18	128.10	113.22
4	B	704	HEM	CAD-C3D-C2D	5.55	129.16	113.22
4	C	705	HEM	CAD-C3D-C2D	5.65	129.45	113.22
4	D	704	HEM	CMB-C2B-C3B	5.65	130.64	116.53
4	A	705	HEM	CMB-C2B-C3B	5.66	130.66	116.53
4	D	704	HEM	CAD-C3D-C2D	5.73	129.69	113.22
4	C	705	HEM	CMB-C2B-C3B	5.74	130.86	116.53
4	C	705	HEM	C2C-C1C-NC	5.89	120.14	110.21
4	B	704	HEM	CMB-C2B-C3B	6.45	132.63	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	BOG	2	0
4	A	705	HEM	2	0
5	A	706	DF0	1	0
4	B	704	HEM	2	0
5	B	705	DF0	1	0
2	C	702	BOG	1	0
4	C	705	HEM	1	0
5	C	706	DF0	1	0
4	D	704	HEM	3	0
5	D	705	DF0	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	552/604 (91%)	-0.09	17 (3%)	52 40	24, 44, 67, 110	0
1	B	552/604 (91%)	0.01	23 (4%)	40 28	27, 43, 68, 90	0
1	C	552/604 (91%)	-0.14	19 (3%)	49 37	26, 43, 66, 110	0
1	D	552/604 (91%)	-0.12	15 (2%)	58 46	24, 42, 67, 101	0
All	All	2208/2416 (91%)	-0.08	74 (3%)	49 37	24, 43, 67, 110	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	GLN	6.5
1	B	52	ASP	5.3
1	C	583	GLN	5.3
1	D	242	HIS	4.5
1	C	399	ASP	4.4
1	C	563	SER	4.1
1	B	428	ARG	3.7
1	A	122	TYR	3.7
1	B	69	THR	3.6
1	B	401	GLU	3.6
1	B	493	ALA	3.5
1	B	97	GLY	3.3
1	B	96	LYS	3.2
1	C	39	PRO	3.2
1	B	94	HIS	3.2
1	A	157	ASP	3.2
1	B	168	ASN	3.1
1	C	45	GLU	3.1
1	A	533	GLY	3.1
1	B	492	LYS	3.1
1	C	41	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	254	TYR	3.0
1	B	55	LYS	3.0
1	D	74	LEU	2.9
1	C	368	ASN	2.9
1	A	577	PHE	2.9
1	D	64	TYR	2.8
1	B	32	ALA	2.8
1	D	91	ILE	2.7
1	B	399	ASP	2.7
1	B	95	PHE	2.7
1	B	90	TYR	2.7
1	C	37	SER	2.7
1	C	80	LEU	2.7
1	C	122	TYR	2.6
1	A	107	PHE	2.6
1	D	77	ILE	2.6
1	D	462	SER	2.6
1	D	272	GLU	2.6
1	A	49	THR	2.5
1	A	258	GLY	2.5
1	B	38	ASN	2.5
1	C	165	VAL	2.4
1	A	98	VAL	2.4
1	A	254	TYR	2.4
1	C	262	TYR	2.4
1	D	73	PHE	2.3
1	A	82	LYS	2.3
1	D	268	ASP	2.3
1	A	457	GLU	2.3
1	C	96	LYS	2.3
1	C	94	HIS	2.3
1	C	263	PRO	2.3
1	A	497	ASP	2.2
1	D	341	ILE	2.2
1	B	246	LEU	2.2
1	A	158	ASP	2.2
1	B	73	PHE	2.2
1	B	251	LYS	2.2
1	C	69	THR	2.1
1	C	562	ALA	2.1
1	B	126	SER	2.1
1	C	401	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	52	ASP	2.1
1	A	399	ASP	2.1
1	B	239	ASP	2.1
1	D	32	ALA	2.1
1	D	540	CYS	2.0
1	A	64	TYR	2.0
1	D	356	HIS	2.0
1	B	252	LEU	2.0
1	A	78	LYS	2.0
1	A	248	LYS	2.0
1	D	368	ASN	2.0

## 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	D	703	14/15	0.92	0.14	0.64	32,38,41,41	0
3	NAG	C	704	14/15	0.94	0.16	-0.48	28,35,37,39	0
3	NAG	A	704	14/15	0.94	0.15	-0.50	36,39,44,47	0
3	NAG	A	703	14/15	0.90	0.20	-0.68	62,71,78,82	0
3	NAG	B	703	14/15	0.91	0.14	-0.94	34,38,40,43	0
3	NAG	D	702	14/15	0.91	0.14	-	50,59,63,64	0
3	NAG	B	702	14/15	0.85	0.21	-	38,43,47,48	0
3	NAG	C	703	14/15	0.89	0.14	-	47,57,64,65	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( $\text{\AA}^2$ )	Q<0.9
5	DF0	C	706	17/17	0.93	0.27	2.49	41,43,48,48	0
2	BOG	C	702	20/20	0.90	0.30	1.92	54,62,67,69	0
5	DF0	D	705	17/17	0.86	0.26	1.24	34,37,44,45	0
2	BOG	C	701	20/20	0.91	0.23	1.21	47,53,59,62	0
4	HEM	D	704	43/43	0.94	0.21	1.05	35,47,78,93	0
2	BOG	B	701	20/20	0.90	0.20	1.02	55,61,68,69	0
4	HEM	C	705	43/43	0.94	0.20	0.84	37,44,58,60	0
4	HEM	A	705	43/43	0.94	0.20	0.54	30,47,69,92	0
2	BOG	A	702	20/20	0.81	0.26	0.39	58,66,73,74	0
5	DF0	B	705	17/17	0.92	0.19	0.28	37,46,52,53	0
2	BOG	D	701	20/20	0.90	0.21	0.27	40,45,50,50	0
2	BOG	A	701	20/20	0.91	0.19	0.17	53,58,70,70	0
4	HEM	B	704	43/43	0.96	0.16	-0.35	33,44,59,67	0
5	DF0	A	706	17/17	0.94	0.16	-0.50	47,49,54,54	0

## 6.5 Other polymers

There are no such residues in this entry.