



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:35 AM GMT

PDB ID : 3PGH  
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-  
PLEXED WITH A NON-SELECTIVE INHIBITOR, FLURBIPROFEN  
Authors : Kurumbail, R.; Stallings, W.  
Deposited on : 1996-12-18  
Resolution : 2.50 Å(reported)

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

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

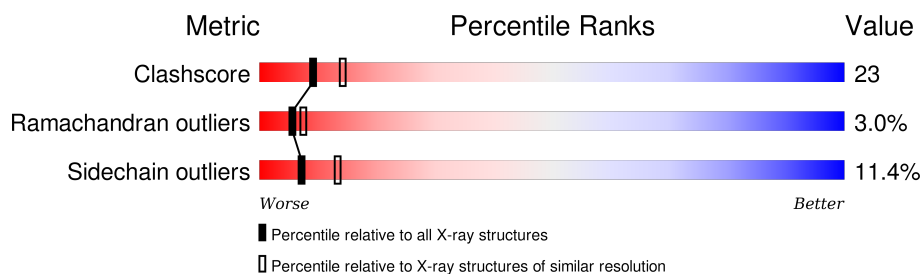
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 Å.





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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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

Note EDS was not executed.

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

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18304 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 CYCLOOXYGENASE-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4473	2886	748	814	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769
C	310	GLN	ASN	CONFLICT	UNP Q05769
C	333	LYS	ARG	CONFLICT	UNP Q05769
D	310	GLN	ASN	CONFLICT	UNP Q05769
D	333	LYS	ARG	CONFLICT	UNP Q05769

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



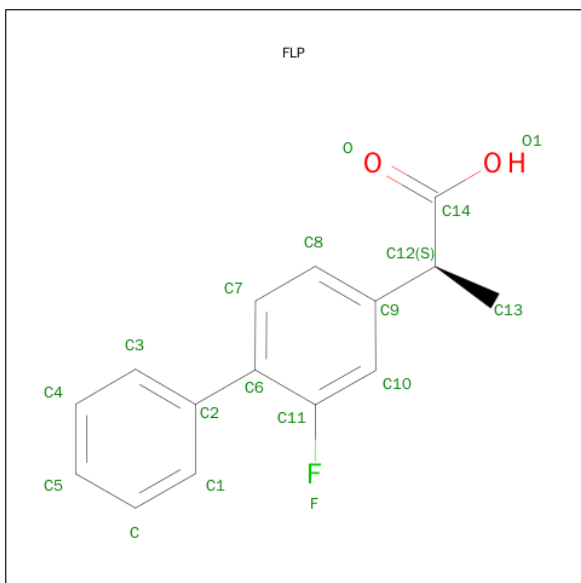
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1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

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



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
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is FLURBIPROFEN (three-letter code: FLP) (formula:  $C_{15}H_{13}FO_2$ ).



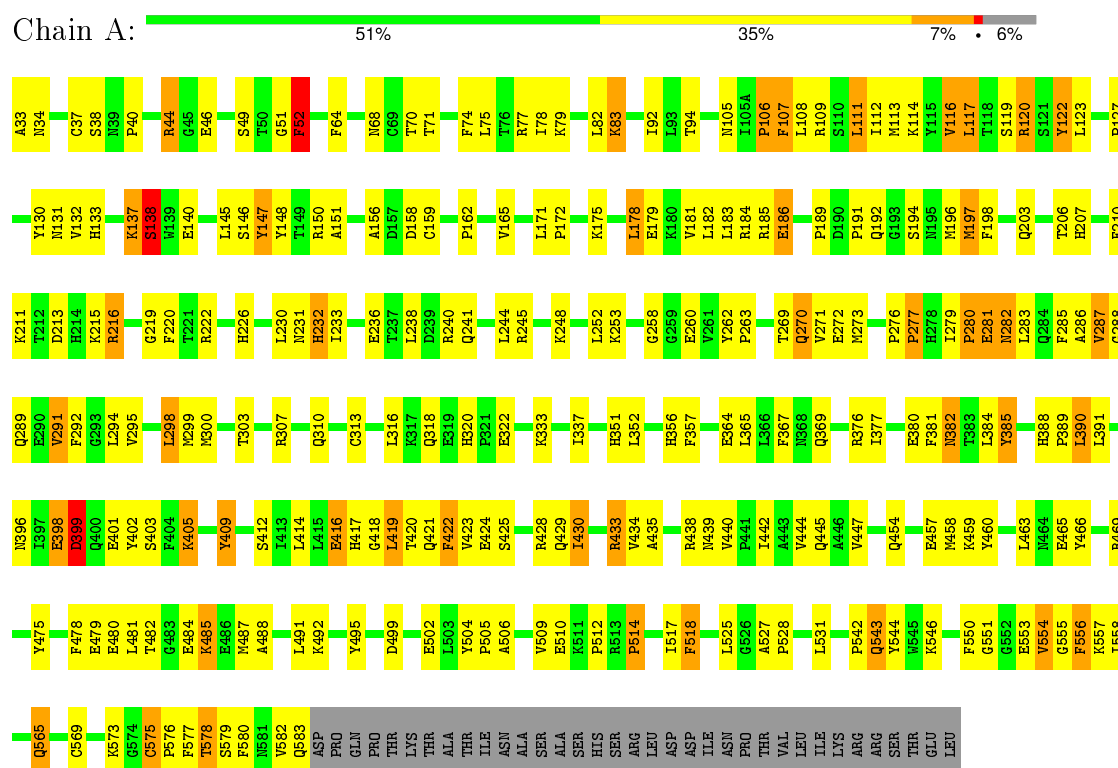
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	F	O	0	0
			18	15	1	2		
4	B	1	Total	C	F	O	0	0
			18	15	1	2		
4	C	1	Total	C	F	O	0	0
			18	15	1	2		
4	D	1	Total	C	F	O	0	0
			18	15	1	2		

### 3 Residue-property plots

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

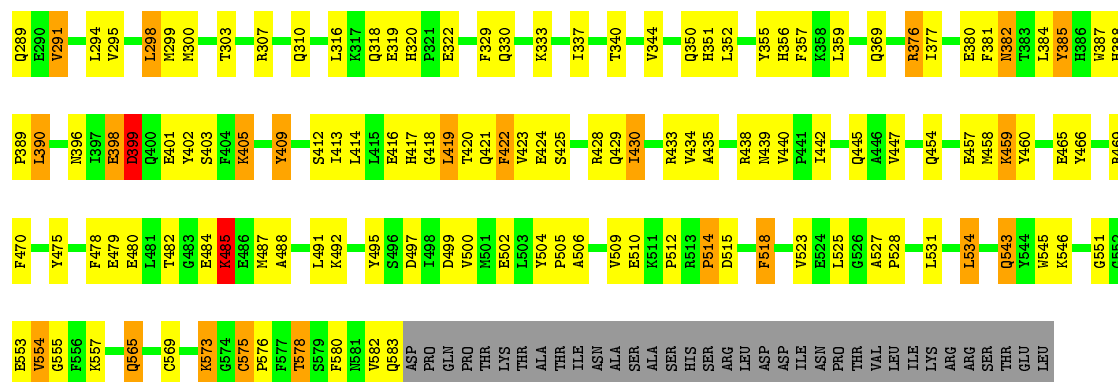
Note EDS was not executed.

#### • Molecule 1: CYCLOOXYGENASE-2



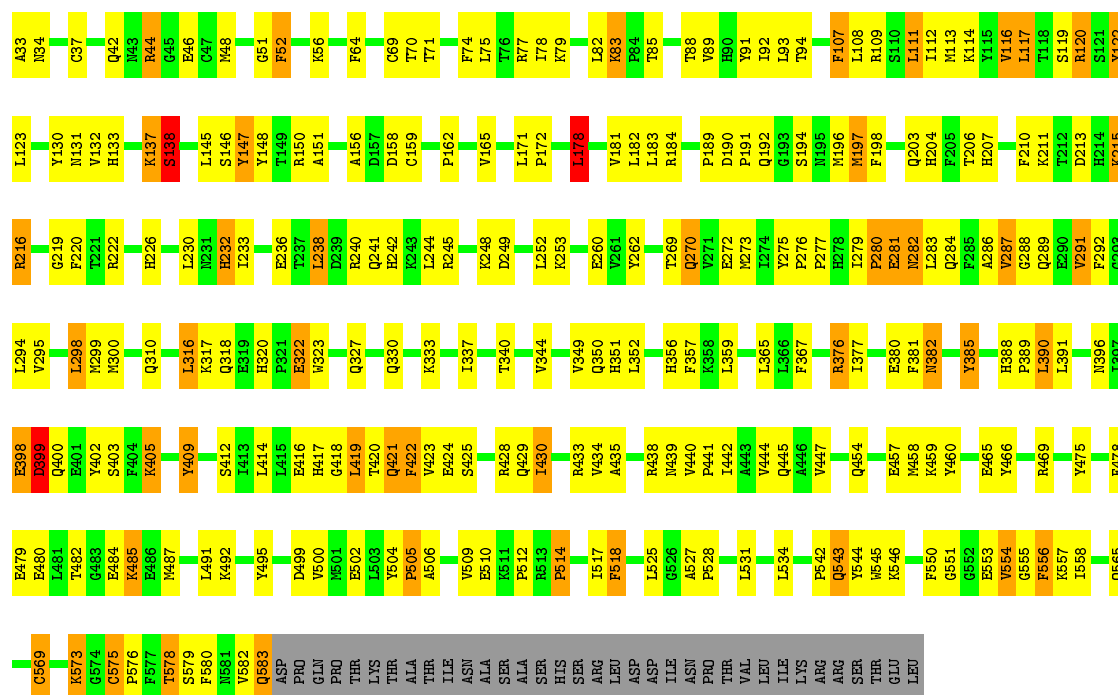
#### • Molecule 1: CYCLOOXYGENASE-2





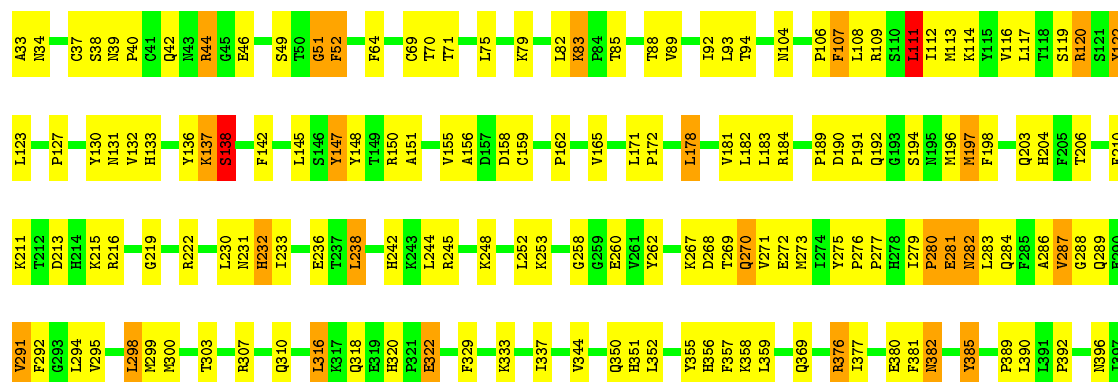
• Molecule 1: CYCLOOXYGENASE-2

Chain C: 51% 34% 8% 6%



• Molecule 1: CYCLOOXYGENASE-2

Chain D: 52% 34% 7% 6%





E398	E399	Q400	E401	Y402	S403	E404	K405	Y409	S412	L413	L414	L415	E416	H417	G418	L419	T420	Q421	F422	Y423	E424	S425	R428	Q429	I430	R433	V434	R438	N439	V440	P441	I442	Q445	A446	V447	Q454	E457	M458	K459	Y460	E465	Y466	R469	Y475	F478	E479	E480
L481	T482	G483	E484	K485	E486	M487	A488	L491	K492	Y495	D499	V500	M501	E502	L503	Y504	P505	A506	V509	E510	K511	P512	R513	P514	I517	F518	L525	G526	A527	P528	L531	L534	Q543	K546	G551	G552	E553	V554	G555	F556	K557	Q565	C569	K573	G574		
C575	P576	F577	T578	S579	F580	N581	V582	Q583	ASP	PRO	GLN	PRO	THR	LYS	THR	ALA	THR	ILE	ASN	ALA	SER	ALA	SER	HIS	SER	ARG	LEU	ASP	ASP	ILE	ASN	PRO	THR	VAL	LEU	ILE	LYS	ARG	ARG	SER	THR	GLU	LEU				

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.50Å 133.80Å 117.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	63.1 (8.00-2.50)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.236 , 0.316	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	0.67	1/4600 (0.0%)	0.85	5/6237 (0.1%)
1	B	0.68	1/4600 (0.0%)	0.86	6/6237 (0.1%)
1	C	0.65	0/4600	0.86	5/6237 (0.1%)
1	D	0.67	1/4600 (0.0%)	0.85	6/6237 (0.1%)
All	All	0.67	3/18400 (0.0%)	0.86	22/24948 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	CYS	CB-SG	-5.72	1.72	1.81
1	B	236	GLU	CG-CD	5.45	1.60	1.51
1	D	479	GLU	CG-CD	5.12	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	390	LEU	CA-CB-CG	6.90	131.17	115.30
1	B	287	VAL	N-CA-C	6.78	129.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	287	VAL	N-CA-C	6.43	128.35	111.00
1	A	390	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	287	VAL	N-CA-C	6.42	128.32	111.00
1	C	287	VAL	N-CA-C	6.33	128.09	111.00
1	B	390	LEU	CA-CB-CG	5.97	129.03	115.30
1	B	258	GLY	N-CA-C	-5.67	98.94	113.10
1	B	111	LEU	CA-CB-CG	5.66	128.31	115.30
1	A	171	LEU	CA-CB-CG	5.65	128.31	115.30
1	C	390	LEU	CA-CB-CG	5.53	128.01	115.30
1	B	485	LYS	N-CA-C	5.52	125.90	111.00
1	D	258	GLY	N-CA-C	-5.48	99.41	113.10
1	B	178	LEU	CA-CB-CG	5.30	127.50	115.30
1	A	281	GLU	N-CA-C	-5.30	96.69	111.00
1	A	258	GLY	N-CA-C	-5.29	99.86	113.10
1	D	111	LEU	CA-CB-CG	5.21	127.29	115.30
1	D	281	GLU	N-CA-C	-5.14	97.12	111.00
1	C	171	LEU	CA-CB-CG	5.12	127.07	115.30
1	D	485	LYS	N-CA-C	5.10	124.78	111.00
1	C	178	LEU	CA-CB-CG	5.06	126.94	115.30
1	C	281	GLU	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	TYR	Sidechain
1	B	147	TYR	Sidechain
1	C	147	TYR	Sidechain
1	C	91	TYR	Sidechain
1	D	147	TYR	Sidechain

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4473	0	4374	207	0
1	B	4473	0	4374	217	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4473	0	4375	215	0
1	D	4473	0	4375	201	0
2	A	42	0	39	4	0
2	B	42	0	39	3	0
2	C	42	0	39	0	0
2	D	42	0	39	0	0
3	A	43	0	30	6	0
3	B	43	0	30	9	0
3	C	43	0	30	6	0
3	D	43	0	30	9	0
4	A	18	0	12	1	0
4	B	18	0	12	6	0
4	C	18	0	12	3	0
4	D	18	0	12	3	0
All	All	18304	0	17822	829	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 23.

All (829) 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:C:424:GLU:HA	1:C:428:ARG:HH21	1.27	0.97
1:A:458:MET:HE2	1:A:460:TYR:HE1	1.27	0.96
1:A:424:GLU:HA	1:A:428:ARG:HH21	1.31	0.96
1:D:424:GLU:HA	1:D:428:ARG:HH21	1.30	0.95
1:B:479:GLU:HG2	1:B:485:LYS:NZ	1.82	0.95
1:C:230:LEU:HG	1:C:337:ILE:HG12	1.50	0.93
1:C:458:MET:HE2	1:C:460:TYR:HE1	1.32	0.93
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.52	0.92
1:D:230:LEU:HG	1:D:337:ILE:HG12	1.52	0.91
1:A:479:GLU:HG2	1:A:485:LYS:NZ	1.85	0.91
1:A:430:ILE:HG23	1:A:582:VAL:HG11	1.53	0.90
1:C:253:LYS:HE3	1:C:269:THR:HG22	1.53	0.89
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.55	0.89
1:D:458:MET:HE2	1:D:460:TYR:HE1	1.39	0.89
1:B:424:GLU:HA	1:B:428:ARG:HH21	1.38	0.88
1:B:458:MET:HE2	1:B:460:TYR:HE1	1.37	0.87
1:A:291:VAL:HG22	1:A:294:LEU:HD12	1.57	0.87
1:B:430:ILE:HG23	1:B:582:VAL:HG11	1.57	0.86
1:D:156:ALA:HB3	1:D:159:CYS:SG	2.15	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:LYS:CE	1:C:269:THR:HG22	2.06	0.86
1:D:405:LYS:HD2	1:D:405:LYS:H	1.42	0.85
1:B:156:ALA:HB3	1:B:159:CYS:SG	2.17	0.85
1:A:458:MET:HE2	1:A:460:TYR:CE1	2.12	0.84
1:B:291:VAL:HG22	1:B:294:LEU:HD12	1.59	0.83
1:C:458:MET:HE2	1:C:460:TYR:CE1	2.15	0.82
1:B:458:MET:HE2	1:B:460:TYR:CE1	2.14	0.82
1:C:479:GLU:HG2	1:C:485:LYS:NZ	1.95	0.81
1:D:430:ILE:HG23	1:D:582:VAL:HG11	1.61	0.80
1:C:291:VAL:HG22	1:C:294:LEU:HD12	1.64	0.80
1:A:253:LYS:HE3	1:A:269:THR:HG22	1.65	0.79
1:D:291:VAL:HG22	1:D:294:LEU:HD12	1.61	0.79
1:D:458:MET:HE2	1:D:460:TYR:CE1	2.18	0.78
1:C:430:ILE:HG23	1:C:582:VAL:HG11	1.63	0.78
1:A:420:THR:HG23	1:A:576:PRO:HG3	1.65	0.78
1:D:380:GLU:HG2	1:D:466:TYR:CE1	2.18	0.78
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.63	0.78
1:C:156:ALA:HB3	1:C:159:CYS:SG	2.24	0.78
1:B:454:GLN:HA	1:B:457:GLU:HG2	1.65	0.78
1:D:398:GLU:HG2	1:D:425:SER:OG	1.83	0.78
1:A:479:GLU:HG2	1:A:485:LYS:HZ2	1.48	0.77
1:A:398:GLU:HG2	1:A:425:SER:OG	1.84	0.77
1:A:184:ARG:HA	1:A:438:ARG:O	1.84	0.77
1:B:184:ARG:HA	1:B:438:ARG:O	1.84	0.77
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.25	0.76
1:D:447:VAL:HG13	3:D:682:HEM:HBA2	1.67	0.76
1:D:527:ALA:HB3	1:D:528:PRO:HD3	1.68	0.76
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.21	0.75
1:B:405:LYS:H	1:B:405:LYS:HD2	1.52	0.75
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.22	0.74
1:B:120:ARG:HG2	1:B:531:LEU:HD12	1.69	0.74
1:C:479:GLU:HG2	1:C:485:LYS:HZ2	1.53	0.74
1:C:83:LYS:NZ	1:C:83:LYS:HB2	2.02	0.74
1:B:420:THR:HG23	1:B:576:PRO:HG3	1.69	0.74
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.22	0.74
1:B:398:GLU:HG2	1:B:425:SER:OG	1.85	0.74
1:C:382:ASN:HD21	3:C:682:HEM:HAD2	1.52	0.73
1:C:184:ARG:HA	1:C:438:ARG:O	1.89	0.73
1:C:120:ARG:HG2	1:C:531:LEU:HD12	1.70	0.73
1:C:398:GLU:HG2	1:C:425:SER:OG	1.88	0.73
1:D:382:ASN:HD21	3:D:682:HEM:HAD2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:LEU:O	1:A:469:ARG:NH2	2.22	0.73
1:C:197:MET:HA	1:C:197:MET:HE2	1.71	0.73
1:C:197:MET:HA	1:C:197:MET:CE	2.18	0.72
1:B:333:LYS:O	1:B:337:ILE:HG13	1.90	0.72
1:C:123:LEU:O	1:C:469:ARG:NH2	2.22	0.72
1:D:280:PRO:CG	1:D:283:LEU:HD12	2.20	0.71
1:C:405:LYS:HD2	1:C:405:LYS:H	1.55	0.71
1:D:420:THR:HG23	1:D:576:PRO:HG3	1.71	0.71
1:D:553:GLU:HG3	1:D:557:LYS:NZ	2.06	0.71
1:D:196:MET:HG2	1:D:429:GLN:HG2	1.73	0.71
1:A:280:PRO:CG	1:A:283:LEU:HD12	2.20	0.70
1:C:420:THR:OG1	1:C:573:LYS:HB3	1.91	0.70
1:D:333:LYS:O	1:D:337:ILE:HG13	1.91	0.70
1:B:281:GLU:O	1:B:283:LEU:N	2.25	0.70
1:B:108:LEU:O	1:B:112:ILE:HG12	1.92	0.70
1:D:253:LYS:HE3	1:D:269:THR:HG22	1.72	0.70
1:A:120:ARG:HG2	1:A:531:LEU:HD12	1.72	0.70
1:A:333:LYS:O	1:A:337:ILE:HG13	1.91	0.69
1:A:295:VAL:CG1	1:A:298:LEU:HD22	2.22	0.69
1:D:479:GLU:HG2	1:D:485:LYS:NZ	2.07	0.69
1:A:382:ASN:HD21	3:A:682:HEM:HAD2	1.56	0.69
1:C:398:GLU:HG3	1:C:421:GLN:NE2	2.06	0.69
1:B:291:VAL:CG2	1:B:294:LEU:HD12	2.21	0.69
1:C:286:ALA:O	1:C:287:VAL:HG22	1.93	0.69
1:B:382:ASN:HD21	3:B:682:HEM:HAD2	1.56	0.68
1:B:83:LYS:NZ	1:B:83:LYS:HB2	2.08	0.68
1:D:120:ARG:HG2	1:D:531:LEU:HD12	1.76	0.68
1:C:295:VAL:CG1	1:C:298:LEU:HD22	2.23	0.68
1:B:479:GLU:HG2	1:B:485:LYS:HZ1	1.59	0.68
1:C:403:SER:HB2	1:C:405:LYS:HD2	1.76	0.68
1:C:295:VAL:HG12	1:C:298:LEU:HD22	1.76	0.68
1:A:253:LYS:CE	1:A:269:THR:HG22	2.24	0.67
1:D:295:VAL:CG1	1:D:298:LEU:HD22	2.25	0.67
1:B:287:VAL:HG11	1:B:299:MET:SD	2.34	0.67
1:B:458:MET:CE	1:B:460:TYR:HE1	2.08	0.67
1:C:454:GLN:HA	1:C:457:GLU:HG2	1.74	0.67
1:D:291:VAL:CG2	1:D:294:LEU:HD12	2.23	0.67
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.76	0.67
1:D:454:GLN:HA	1:D:457:GLU:HG2	1.75	0.67
1:C:291:VAL:CG2	1:C:294:LEU:HD12	2.25	0.67
1:C:420:THR:HG23	1:C:576:PRO:HG3	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ALA:O	1:A:287:VAL:HG22	1.95	0.67
1:B:196:MET:HG2	1:B:429:GLN:HG2	1.77	0.67
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.25	0.67
1:B:495:TYR:HE2	1:B:502:GLU:HG3	1.60	0.66
1:A:295:VAL:HG12	1:A:298:LEU:HD22	1.76	0.66
1:A:213:ASP:OD1	1:A:215:LYS:HE2	1.96	0.66
1:A:194:SER:OG	1:A:351:HIS:HE1	1.78	0.66
1:D:458:MET:CE	1:D:460:TYR:HE1	2.08	0.66
1:D:108:LEU:O	1:D:112:ILE:HG12	1.95	0.66
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.75	0.66
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.77	0.66
1:D:123:LEU:O	1:D:469:ARG:NH2	2.29	0.66
1:D:276:PRO:HG2	1:D:409:TYR:CD2	2.29	0.66
1:A:83:LYS:NZ	1:A:83:LYS:HB2	2.11	0.66
1:B:280:PRO:CG	1:B:283:LEU:HD12	2.26	0.65
1:D:148:TYR:HD1	1:D:377:ILE:HG13	1.61	0.65
1:A:276:PRO:HG2	1:A:409:TYR:CD2	2.31	0.65
1:B:183:LEU:HD21	1:B:445:GLN:HB3	1.77	0.65
1:A:458:MET:CE	1:A:460:TYR:HE1	2.08	0.65
1:A:546:LYS:HD2	1:B:46:GLU:OE2	1.97	0.65
1:B:381:PHE:O	1:B:385:TYR:HB2	1.96	0.65
1:C:527:ALA:HB3	1:C:528:PRO:HD3	1.78	0.65
1:B:475:TYR:HA	1:B:480:GLU:OE2	1.97	0.65
1:A:381:PHE:O	1:A:385:TYR:HB2	1.97	0.65
1:D:280:PRO:HG3	1:D:283:LEU:HD12	1.79	0.64
1:D:83:LYS:HB2	1:D:83:LYS:NZ	2.12	0.64
1:D:295:VAL:HG12	1:D:298:LEU:HD22	1.79	0.64
1:C:132:VAL:HG21	1:C:219:GLY:HA3	1.80	0.64
1:D:184:ARG:HA	1:D:438:ARG:O	1.98	0.64
1:B:197:MET:CE	1:B:197:MET:HA	2.28	0.64
1:B:132:VAL:HG21	1:B:219:GLY:HA3	1.80	0.64
1:D:276:PRO:O	1:D:279:ILE:HG12	1.97	0.64
1:A:197:MET:CE	1:A:197:MET:HA	2.29	0.63
1:A:454:GLN:HA	1:A:457:GLU:HG2	1.80	0.63
1:D:120:ARG:HD3	4:D:701:FLP:O	1.99	0.63
1:C:46:GLU:OE2	1:D:546:LYS:HD2	1.99	0.63
1:B:215:LYS:NZ	1:B:222:ARG:HH21	1.96	0.63
1:D:420:THR:OG1	1:D:573:LYS:HB3	1.99	0.63
1:B:148:TYR:HD1	1:B:377:ILE:HG13	1.63	0.63
1:C:196:MET:HG2	1:C:429:GLN:HG2	1.80	0.62
1:B:123:LEU:O	1:B:469:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:PRO:HG2	1:C:409:TYR:CD2	2.34	0.62
1:D:114:LYS:HD3	1:D:369:GLN:NE2	2.14	0.62
1:C:333:LYS:O	1:C:337:ILE:HG13	1.98	0.62
1:A:506:ALA:O	1:A:510:GLU:HB2	1.99	0.62
1:C:85:THR:O	1:C:89:VAL:HG23	2.00	0.62
1:B:398:GLU:HG3	1:B:421:GLN:NE2	2.15	0.62
1:C:504:TYR:HB3	1:C:505:PRO:HD3	1.80	0.62
1:C:506:ALA:O	1:C:510:GLU:HB2	1.99	0.62
1:C:131:ASN:HA	1:C:150:ARG:HG2	1.82	0.62
1:D:475:TYR:HA	1:D:480:GLU:OE2	1.99	0.62
1:A:38:SER:OG	1:A:40:PRO:HD3	1.99	0.62
1:D:211:LYS:HZ1	1:D:236:GLU:HG2	1.64	0.62
1:C:191:PRO:HD2	1:C:433:ARG:HG3	1.80	0.62
1:D:506:ALA:O	1:D:510:GLU:HB2	1.99	0.62
1:C:491:LEU:HD11	1:C:509:VAL:HG11	1.82	0.62
1:A:287:VAL:HG11	1:A:299:MET:SD	2.40	0.61
1:B:253:LYS:HE3	1:B:269:THR:HG22	1.81	0.61
1:C:150:ARG:NH2	1:C:458:MET:O	2.33	0.61
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.82	0.61
1:C:108:LEU:O	1:C:112:ILE:HG12	2.00	0.61
1:A:398:GLU:HG3	1:A:421:GLN:NE2	2.16	0.61
1:A:475:TYR:HA	1:A:480:GLU:OE2	2.00	0.61
1:B:145:LEU:HD23	1:B:376:ARG:CZ	2.31	0.61
1:B:276:PRO:HG2	1:B:409:TYR:CD2	2.35	0.61
1:D:183:LEU:HD21	1:D:445:GLN:HB3	1.81	0.61
1:C:381:PHE:O	1:C:385:TYR:HB2	2.00	0.61
1:B:405:LYS:H	1:B:405:LYS:CD	2.14	0.61
1:D:281:GLU:O	1:D:283:LEU:N	2.34	0.60
1:A:116:VAL:O	1:A:120:ARG:HB2	2.00	0.60
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.82	0.60
1:D:145:LEU:HD23	1:D:376:ARG:CZ	2.31	0.60
1:D:381:PHE:O	1:D:385:TYR:HB2	2.00	0.60
1:A:46:GLU:OE2	1:B:546:LYS:HD2	2.01	0.60
1:A:575:CYS:N	1:A:576:PRO:HD3	2.17	0.60
1:D:197:MET:HA	1:D:197:MET:CE	2.31	0.60
1:A:281:GLU:O	1:A:283:LEU:N	2.34	0.60
1:A:132:VAL:HG21	1:A:219:GLY:HA3	1.82	0.60
1:B:211:LYS:NZ	1:B:236:GLU:CG	2.65	0.60
1:A:147:TYR:OH	2:A:671:NAG:H62	2.01	0.60
1:C:148:TYR:HD1	1:C:377:ILE:HG13	1.64	0.60
1:C:183:LEU:HD21	1:C:445:GLN:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:215:LYS:NZ	1:D:222:ARG:HH21	2.00	0.60
1:B:475:TYR:CD1	1:B:480:GLU:HG2	2.37	0.59
1:A:148:TYR:HD1	1:A:377:ILE:HG13	1.66	0.59
1:D:211:LYS:NZ	1:D:236:GLU:CG	2.66	0.59
1:D:132:VAL:HG21	1:D:219:GLY:HA3	1.83	0.59
1:D:398:GLU:O	1:D:399:ASP:HB2	2.02	0.59
1:B:420:THR:OG1	1:B:573:LYS:HB3	2.03	0.59
1:B:215:LYS:N	1:B:215:LYS:HD3	2.18	0.59
1:C:75:LEU:HG	1:C:79:LYS:HE2	1.83	0.59
1:B:506:ALA:O	1:B:510:GLU:HB2	2.01	0.59
1:C:281:GLU:O	1:C:283:LEU:N	2.35	0.59
1:C:133:HIS:CD2	1:C:147:TYR:HE2	2.21	0.59
1:B:479:GLU:HG2	1:B:485:LYS:HZ2	1.65	0.59
1:C:546:LYS:HD2	1:D:46:GLU:OE2	2.03	0.59
1:A:495:TYR:HE2	1:A:502:GLU:HG3	1.68	0.59
1:A:131:ASN:HA	1:A:150:ARG:HG2	1.85	0.59
1:C:213:ASP:OD1	1:C:215:LYS:HE2	2.02	0.59
1:A:412:SER:O	1:A:416:GLU:HB2	2.02	0.59
1:A:424:GLU:HA	1:A:428:ARG:NH2	2.11	0.58
1:D:504:TYR:HB3	1:D:505:PRO:HD3	1.85	0.58
1:C:475:TYR:HA	1:C:480:GLU:OE2	2.03	0.58
1:D:287:VAL:HG11	1:D:299:MET:SD	2.44	0.58
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.31	0.58
1:B:447:VAL:HG13	3:B:682:HEM:HBA2	1.85	0.58
1:B:180:LYS:O	1:B:438:ARG:NH2	2.36	0.58
1:D:398:GLU:HG3	1:D:421:GLN:NE2	2.19	0.57
1:C:398:GLU:O	1:C:399:ASP:HB2	2.04	0.57
1:D:253:LYS:CE	1:D:269:THR:HG22	2.34	0.57
1:D:211:LYS:NZ	1:D:236:GLU:HG2	2.18	0.57
1:D:197:MET:HE2	1:D:197:MET:HA	1.87	0.57
1:A:553:GLU:O	1:A:557:LYS:HE3	2.05	0.57
1:A:150:ARG:NH2	1:A:458:MET:O	2.38	0.57
1:B:253:LYS:CE	1:B:269:THR:HG22	2.34	0.57
1:A:108:LEU:O	1:A:112:ILE:HG12	2.04	0.57
1:C:495:TYR:HE2	1:C:502:GLU:HG3	1.70	0.57
1:A:196:MET:HG2	1:A:429:GLN:HG2	1.86	0.57
1:D:575:CYS:N	1:D:576:PRO:HD3	2.20	0.57
1:C:525:LEU:O	1:C:528:PRO:HD2	2.04	0.57
1:A:276:PRO:O	1:A:279:ILE:HG12	2.05	0.57
1:A:398:GLU:O	1:A:399:ASP:HB2	2.05	0.57
1:B:211:LYS:HZ1	1:B:236:GLU:HG2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:VAL:O	1:B:93:LEU:HD23	2.04	0.57
1:A:475:TYR:CD1	1:A:480:GLU:HG2	2.40	0.56
1:A:133:HIS:HD2	1:A:147:TYR:OH	1.87	0.56
1:C:116:VAL:O	1:C:120:ARG:HB2	2.05	0.56
1:C:287:VAL:HG11	1:C:299:MET:SD	2.44	0.56
1:D:403:SER:HB2	1:D:405:LYS:HD2	1.87	0.56
1:A:420:THR:OG1	1:A:573:LYS:HB3	2.04	0.56
1:B:83:LYS:HB2	1:B:83:LYS:HZ3	1.69	0.56
1:B:211:LYS:NZ	1:B:236:GLU:HG2	2.20	0.56
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.88	0.56
1:C:107:PHE:CD1	1:C:107:PHE:N	2.72	0.56
1:C:475:TYR:CD1	1:C:480:GLU:HG2	2.41	0.56
1:D:402:TYR:OH	1:D:417:HIS:HE1	1.89	0.56
1:D:131:ASN:HA	1:D:150:ARG:HG2	1.87	0.56
1:B:442:ILE:O	1:B:445:GLN:HG2	2.06	0.56
1:B:75:LEU:HG	1:B:79:LYS:HE2	1.87	0.55
1:D:405:LYS:CD	1:D:405:LYS:H	2.15	0.55
1:B:295:VAL:CG1	1:B:298:LEU:HD22	2.37	0.55
1:D:286:ALA:O	1:D:287:VAL:HG22	2.07	0.55
1:C:458:MET:CE	1:C:460:TYR:HE1	2.12	0.55
1:C:405:LYS:H	1:C:405:LYS:CD	2.14	0.55
1:A:203:GLN:HB3	1:A:298:LEU:HD11	1.89	0.55
1:D:211:LYS:HZ1	1:D:236:GLU:CG	2.19	0.55
1:D:553:GLU:HG3	1:D:557:LYS:HZ1	1.72	0.55
1:B:280:PRO:HG3	1:B:283:LEU:HD12	1.87	0.55
1:C:211:LYS:NZ	1:C:236:GLU:CG	2.70	0.55
1:A:543:GLN:NE2	1:B:127:PRO:O	2.40	0.55
1:D:133:HIS:CD2	1:D:147:TYR:HE2	2.25	0.55
1:D:495:TYR:HE2	1:D:502:GLU:HG3	1.72	0.55
1:A:525:LEU:O	1:A:528:PRO:HD2	2.07	0.54
1:C:276:PRO:O	1:C:279:ILE:HG12	2.07	0.54
1:A:183:LEU:HD21	1:A:445:GLN:HB3	1.89	0.54
1:A:211:LYS:NZ	1:A:236:GLU:CG	2.71	0.54
1:A:211:LYS:HZ1	1:A:236:GLU:CG	2.21	0.54
1:B:419:LEU:H	1:B:419:LEU:HD23	1.72	0.54
1:C:553:GLU:HG3	1:C:557:LYS:HE3	1.90	0.54
1:B:181:VAL:HG12	1:B:487:MET:HG2	1.90	0.54
1:D:203:GLN:HB3	1:D:298:LEU:HD11	1.89	0.54
3:B:682:HEM:HBC2	3:B:682:HEM:HHD	1.90	0.54
1:C:215:LYS:N	1:C:215:LYS:HD3	2.22	0.54
1:C:318:GLN:HA	1:C:318:GLN:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:575:CYS:N	1:C:576:PRO:HD3	2.23	0.54
3:A:682:HEM:HBC2	3:A:682:HEM:HHD	1.89	0.54
1:A:509:VAL:O	1:A:509:VAL:HG12	2.08	0.54
1:C:478:PHE:CZ	1:C:495:TYR:HB2	2.43	0.54
1:B:107:PHE:N	1:B:107:PHE:CD1	2.74	0.54
1:A:107:PHE:N	1:A:107:PHE:CD1	2.73	0.54
1:B:478:PHE:CZ	1:B:495:TYR:HB2	2.43	0.54
1:C:253:LYS:HE2	1:C:269:THR:HG22	1.90	0.54
1:B:116:VAL:O	1:B:120:ARG:HB2	2.08	0.54
1:D:479:GLU:HG2	1:D:485:LYS:HZ2	1.73	0.54
1:A:215:LYS:HD3	1:A:215:LYS:N	2.23	0.53
1:B:211:LYS:HZ1	1:B:236:GLU:CG	2.20	0.53
1:B:133:HIS:CD2	1:B:147:TYR:HE2	2.26	0.53
1:A:433:ARG:HD3	1:A:435:ALA:O	2.09	0.53
1:D:215:LYS:HZ1	1:D:222:ARG:HH21	1.56	0.53
1:B:553:GLU:HG3	1:B:557:LYS:HE3	1.91	0.53
1:B:286:ALA:O	1:B:287:VAL:HG22	2.08	0.53
1:C:215:LYS:NZ	1:C:222:ARG:HH21	2.06	0.53
1:C:137:LYS:O	1:C:138:SER:O	2.27	0.53
1:C:145:LEU:HD23	1:C:376:ARG:CZ	2.39	0.53
1:D:181:VAL:HG12	1:D:487:MET:HG2	1.90	0.53
1:B:131:ASN:HA	1:B:150:ARG:HG2	1.90	0.53
1:C:83:LYS:HZ2	1:C:83:LYS:HB2	1.74	0.53
1:D:238:LEU:HD22	1:D:242:HIS:CD2	2.44	0.53
1:C:114:LYS:HE2	1:C:365:LEU:O	2.08	0.53
1:B:418:GLY:O	1:B:420:THR:N	2.41	0.53
1:A:215:LYS:NZ	1:A:222:ARG:HH21	2.07	0.53
1:C:320:HIS:HE1	1:C:551:GLY:O	1.92	0.53
1:B:64:PHE:HD2	1:B:70:THR:O	1.91	0.53
1:B:355:TYR:HE2	4:B:701:FLP:O1	1.91	0.53
1:D:418:GLY:O	1:D:420:THR:N	2.42	0.53
1:B:206:THR:HB	1:B:210:PHE:CD2	2.44	0.53
1:C:478:PHE:CE2	1:C:492:LYS:HA	2.43	0.53
1:A:183:LEU:HD22	1:A:442:ILE:HG12	1.90	0.53
1:A:479:GLU:HG2	1:A:485:LYS:HZ1	1.70	0.53
1:B:398:GLU:O	1:B:399:ASP:HB2	2.09	0.53
1:D:206:THR:HB	1:D:210:PHE:CD2	2.44	0.53
1:B:523:VAL:HA	4:B:701:FLP:H3	1.91	0.53
1:D:475:TYR:CD1	1:D:480:GLU:HG2	2.43	0.53
1:D:273:MET:SD	1:D:286:ALA:O	2.67	0.53
1:B:402:TYR:OH	1:B:417:HIS:HE1	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:CYS:N	1:B:576:PRO:HD3	2.24	0.52
1:B:238:LEU:HD22	1:B:242:HIS:NE2	2.24	0.52
1:A:478:PHE:CZ	1:A:495:TYR:HB2	2.45	0.52
1:B:433:ARG:H	1:B:439:ASN:ND2	2.07	0.52
1:A:137:LYS:HB2	1:A:137:LYS:HZ2	1.73	0.52
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.45	0.52
1:C:433:ARG:H	1:C:439:ASN:ND2	2.08	0.52
1:B:33:ALA:N	1:B:158:ASP:O	2.42	0.52
1:D:389:PRO:HG3	1:D:440:VAL:HG22	1.92	0.52
1:C:423:VAL:HG13	1:C:578:THR:HG23	1.92	0.52
1:A:280:PRO:HG2	1:A:283:LEU:HD12	1.92	0.52
1:A:127:PRO:O	1:B:543:GLN:NE2	2.43	0.52
1:A:64:PHE:HD2	1:A:70:THR:O	1.93	0.52
1:A:418:GLY:O	1:A:420:THR:N	2.43	0.52
1:C:203:GLN:HB3	1:C:298:LEU:HD11	1.91	0.52
1:B:94:THR:O	1:B:356:HIS:CE1	2.63	0.52
1:C:402:TYR:OH	1:C:417:HIS:HE1	1.93	0.52
1:D:318:GLN:HA	1:D:318:GLN:NE2	2.25	0.52
1:B:203:GLN:HG3	3:B:682:HEM:C2C	2.45	0.52
1:A:178:LEU:O	1:A:182:LEU:HB2	2.10	0.52
1:A:145:LEU:HD23	1:A:376:ARG:CZ	2.38	0.52
1:B:44:ARG:HD2	1:B:469:ARG:HD2	1.92	0.52
1:D:419:LEU:HD23	1:D:419:LEU:H	1.75	0.52
1:B:119:SER:O	1:B:122:TYR:HD1	1.93	0.52
1:B:203:GLN:HB3	1:B:298:LEU:HD11	1.92	0.52
1:D:215:LYS:N	1:D:215:LYS:HD3	2.24	0.52
1:C:194:SER:OG	1:C:351:HIS:HE1	1.93	0.52
1:A:402:TYR:OH	1:A:417:HIS:HE1	1.93	0.52
1:D:382:ASN:ND2	3:D:682:HEM:HAD2	2.22	0.51
1:C:509:VAL:HG12	1:C:509:VAL:O	2.10	0.51
1:B:423:VAL:HG13	1:B:578:THR:HG23	1.90	0.51
1:D:150:ARG:NH2	1:D:458:MET:O	2.43	0.51
1:C:382:ASN:ND2	3:C:682:HEM:HAD2	2.24	0.51
1:C:553:GLU:O	1:C:557:LYS:HG2	2.10	0.51
1:C:192:GLN:OE1	1:C:517:ILE:HG22	2.10	0.51
1:D:107:PHE:N	1:D:107:PHE:CD1	2.74	0.51
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.92	0.51
1:C:83:LYS:HZ3	1:C:83:LYS:HB2	1.73	0.51
1:B:238:LEU:HD22	1:B:242:HIS:CD2	2.45	0.51
1:B:38:SER:OG	1:B:40:PRO:HD3	2.09	0.51
1:D:276:PRO:HG2	1:D:409:TYR:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:THR:HB	1:C:210:PHE:CD2	2.45	0.51
1:B:470:PHE:CG	1:B:525:LEU:HD22	2.46	0.51
3:C:682:HEM:HBC2	3:C:682:HEM:HHD	1.92	0.51
1:D:260:GLU:HB2	1:D:262:TYR:CE2	2.45	0.51
1:B:509:VAL:HG12	1:B:509:VAL:O	2.11	0.51
1:C:133:HIS:CD2	1:C:147:TYR:CE2	2.99	0.51
1:A:389:PRO:HG3	1:A:440:VAL:HG22	1.92	0.51
1:A:74:PHE:O	1:A:77:ARG:HB2	2.11	0.51
1:D:553:GLU:O	1:D:557:LYS:HG2	2.11	0.51
1:D:232:HIS:CD2	1:D:233:ILE:HG13	2.46	0.51
1:A:419:LEU:HD23	1:A:419:LEU:H	1.75	0.51
1:C:113:MET:HA	1:C:116:VAL:HG13	1.94	0.50
1:B:281:GLU:C	1:B:283:LEU:H	2.15	0.50
1:C:412:SER:O	1:C:416:GLU:HB2	2.11	0.50
1:D:42:GLN:O	1:D:69:CYS:HB2	2.10	0.50
1:B:525:LEU:O	1:B:528:PRO:HD2	2.11	0.50
1:D:447:VAL:HG13	3:D:682:HEM:CBA	2.39	0.50
1:A:211:LYS:NZ	1:A:236:GLU:HG2	2.26	0.50
1:C:119:SER:O	1:C:122:TYR:HD1	1.94	0.50
1:A:211:LYS:HZ1	1:A:236:GLU:HG2	1.76	0.50
1:A:150:ARG:HD2	1:A:380:GLU:OE2	2.10	0.50
3:D:682:HEM:HHD	3:D:682:HEM:HBC2	1.94	0.50
1:B:276:PRO:O	1:B:279:ILE:HG12	2.11	0.50
1:D:491:LEU:HD11	1:D:509:VAL:HG11	1.94	0.50
1:C:424:GLU:HA	1:C:428:ARG:NH2	2.11	0.50
1:D:38:SER:OG	1:D:40:PRO:HD3	2.11	0.50
1:A:553:GLU:O	1:A:557:LYS:HG2	2.11	0.50
1:C:211:LYS:HZ1	1:C:236:GLU:CG	2.25	0.50
1:C:232:HIS:CD2	1:C:233:ILE:HG13	2.47	0.50
1:D:275:TYR:CD2	1:D:284:GLN:HG2	2.46	0.50
1:A:414:LEU:HD11	1:A:419:LEU:CD2	2.42	0.50
1:D:75:LEU:HG	1:D:79:LYS:HE2	1.92	0.50
1:D:119:SER:O	1:D:122:TYR:HD1	1.95	0.50
1:A:181:VAL:HG12	1:A:487:MET:HG2	1.92	0.50
1:C:198:PHE:HB2	1:C:580:PHE:HB3	1.94	0.50
1:C:211:LYS:NZ	1:C:236:GLU:HG2	2.26	0.50
1:B:478:PHE:CE2	1:B:492:LYS:HA	2.47	0.50
1:A:433:ARG:H	1:A:439:ASN:ND2	2.09	0.50
1:B:197:MET:HE2	1:B:197:MET:HA	1.93	0.50
1:D:509:VAL:HG12	1:D:509:VAL:O	2.12	0.50
1:B:260:GLU:HB2	1:B:262:TYR:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:HG12	1:B:298:LEU:HD22	1.92	0.49
1:C:553:GLU:O	1:C:557:LYS:HE3	2.12	0.49
1:B:527:ALA:HA	4:B:701:FLP:C7	2.41	0.49
1:A:260:GLU:HB2	1:A:262:TYR:CE2	2.47	0.49
1:A:175:LYS:HD2	1:A:179:GLU:OE2	2.12	0.49
1:B:389:PRO:HB2	1:B:434:VAL:HA	1.94	0.49
1:C:414:LEU:HD11	1:C:419:LEU:CD2	2.41	0.49
1:C:269:THR:O	1:C:270:GLN:HB2	2.13	0.49
1:C:398:GLU:HG3	1:C:421:GLN:HE22	1.75	0.49
1:A:273:MET:SD	1:A:286:ALA:O	2.70	0.49
1:B:183:LEU:HD22	1:B:442:ILE:HG12	1.94	0.49
1:D:122:TYR:O	1:D:122:TYR:CD2	2.66	0.49
1:D:33:ALA:N	1:D:158:ASP:O	2.46	0.49
1:C:275:TYR:CD2	1:C:284:GLN:HG2	2.48	0.49
1:B:203:GLN:HG3	3:B:682:HEM:C1C	2.48	0.49
1:C:112:ILE:HB	1:C:357:PHE:CZ	2.47	0.49
1:D:33:ALA:HB3	1:D:158:ASP:OD2	2.12	0.49
1:B:382:ASN:ND2	3:B:682:HEM:HAD2	2.24	0.49
1:C:389:PRO:HG3	1:C:440:VAL:HG22	1.94	0.49
1:D:94:THR:O	1:D:356:HIS:CE1	2.65	0.49
1:A:206:THR:HB	1:A:210:PHE:CD2	2.47	0.49
1:C:414:LEU:HD11	1:C:419:LEU:HD23	1.93	0.49
1:D:423:VAL:HG13	1:D:578:THR:HG23	1.95	0.49
1:D:64:PHE:HD2	1:D:70:THR:O	1.95	0.49
1:C:33:ALA:N	1:C:158:ASP:O	2.46	0.49
1:B:303:THR:O	1:B:307:ARG:HD3	2.13	0.49
1:B:273:MET:SD	1:B:286:ALA:O	2.71	0.49
1:B:423:VAL:CG1	1:B:578:THR:HG23	2.43	0.49
1:D:89:VAL:O	1:D:93:LEU:HD23	2.13	0.49
1:C:350:GLN:HE22	1:C:359:LEU:H	1.61	0.49
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.27	0.49
1:C:133:HIS:HD2	1:C:147:TYR:OH	1.95	0.48
1:A:423:VAL:HG13	1:A:578:THR:HG23	1.95	0.48
1:D:344:VAL:HG12	1:D:534:LEU:HD21	1.93	0.48
1:A:113:MET:HA	1:A:116:VAL:HG13	1.94	0.48
1:B:85:THR:O	1:B:89:VAL:HG23	2.14	0.48
1:D:133:HIS:HD2	1:D:147:TYR:OH	1.96	0.48
1:C:74:PHE:O	1:C:77:ARG:HB2	2.13	0.48
1:D:320:HIS:HE1	1:D:551:GLY:O	1.95	0.48
3:D:682:HEM:HHH	3:D:682:HEM:CBC	2.44	0.48
1:C:352:LEU:HD11	1:C:518:PHE:CZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:HIS:CD2	1:A:147:TYR:HE1	2.31	0.48
1:A:137:LYS:O	1:A:138:SER:O	2.30	0.48
1:B:244:LEU:HD11	1:B:288:GLY:HA2	1.95	0.48
1:A:147:TYR:OH	2:A:671:NAG:C6	2.61	0.48
1:C:478:PHE:HZ	1:C:495:TYR:HB2	1.78	0.48
1:D:245:ARG:HD3	1:D:329:PHE:CD2	2.48	0.48
1:B:172:PRO:HG3	1:B:495:TYR:CE1	2.49	0.48
1:A:398:GLU:HG2	1:A:425:SER:HG	1.78	0.48
1:C:442:ILE:O	1:C:445:GLN:HG2	2.13	0.48
1:B:210:PHE:HB3	3:B:682:HEM:HBD1	1.95	0.48
1:D:172:PRO:HG3	1:D:495:TYR:CE1	2.48	0.48
1:C:350:GLN:HE22	1:C:359:LEU:N	2.11	0.48
1:A:197:MET:HA	1:A:197:MET:HE2	1.94	0.48
1:C:280:PRO:CG	1:C:283:LEU:HD12	2.44	0.48
1:D:238:LEU:HD22	1:D:242:HIS:NE2	2.29	0.48
1:B:553:GLU:O	1:B:557:LYS:HE3	2.14	0.48
1:D:137:LYS:O	1:D:138:SER:O	2.32	0.48
1:A:320:HIS:HE1	1:A:551:GLY:O	1.96	0.48
1:A:276:PRO:HG2	1:A:409:TYR:CG	2.49	0.47
1:A:75:LEU:HG	1:A:79:LYS:HE2	1.94	0.47
1:A:33:ALA:HB3	1:A:158:ASP:OD2	2.14	0.47
1:D:244:LEU:HD11	1:D:288:GLY:HA2	1.96	0.47
1:A:232:HIS:CD2	1:A:233:ILE:HG13	2.49	0.47
1:A:140:GLU:OE2	2:A:671:NAG:O5	2.32	0.47
1:C:137:LYS:HB2	1:C:137:LYS:HZ2	1.79	0.47
1:B:438:ARG:NH1	1:B:487:MET:HG3	2.29	0.47
1:C:385:TYR:OH	4:C:701:FLP:H	2.15	0.47
1:A:172:PRO:HG3	1:A:495:TYR:CE1	2.50	0.47
1:D:85:THR:O	1:D:89:VAL:HG23	2.14	0.47
1:C:64:PHE:HD2	1:C:70:THR:O	1.97	0.47
1:B:414:LEU:HD11	1:B:419:LEU:CD2	2.44	0.47
1:A:94:THR:O	1:A:356:HIS:CE1	2.68	0.47
1:C:260:GLU:HB2	1:C:262:TYR:CE2	2.49	0.47
1:B:42:GLN:O	1:B:69:CYS:HB2	2.14	0.47
1:D:527:ALA:HA	4:D:701:FLP:C7	2.44	0.47
1:B:213:ASP:OD1	1:B:215:LYS:HE2	2.14	0.47
1:C:181:VAL:HG12	1:C:487:MET:HG2	1.96	0.47
1:A:108:LEU:O	1:A:111:LEU:HB3	2.14	0.47
1:B:119:SER:O	1:B:122:TYR:CD1	2.68	0.47
1:B:320:HIS:HE1	1:B:551:GLY:O	1.98	0.47
1:A:577:PHE:CE1	1:D:267:LYS:NZ	2.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:LEU:O	1:C:182:LEU:HB2	2.15	0.47
1:B:232:HIS:CD2	1:B:233:ILE:HG13	2.49	0.47
1:A:294:LEU:HD22	1:A:409:TYR:CE1	2.50	0.47
1:D:116:VAL:O	1:D:120:ARG:HB2	2.14	0.47
1:C:389:PRO:HB2	1:C:434:VAL:HA	1.96	0.47
1:C:543:GLN:NE2	1:D:127:PRO:O	2.48	0.47
1:D:104:ASN:ND2	1:D:358:LYS:HB2	2.30	0.47
1:B:150:ARG:NH2	1:B:458:MET:O	2.47	0.47
1:B:215:LYS:HZ3	1:B:222:ARG:HH21	1.62	0.47
1:A:280:PRO:HG3	1:A:283:LEU:HD12	1.97	0.47
1:D:137:LYS:HZ2	1:D:137:LYS:HB2	1.80	0.47
1:B:114:LYS:HD3	1:B:369:GLN:NE2	2.29	0.47
1:B:421:GLN:OE1	1:B:421:GLN:HA	2.15	0.47
1:B:113:MET:HA	1:B:116:VAL:HG13	1.97	0.47
3:B:682:HEM:CBC	3:B:682:HEM:HHD	2.44	0.47
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.97	0.47
1:B:352:LEU:HD11	1:B:518:PHE:CZ	2.49	0.47
1:B:137:LYS:HZ2	1:B:137:LYS:HB2	1.80	0.47
1:C:447:VAL:HG13	3:C:682:HEM:HBA2	1.97	0.46
1:C:273:MET:SD	1:C:286:ALA:O	2.73	0.46
1:A:83:LYS:HB2	1:A:83:LYS:HZ3	1.80	0.46
1:D:119:SER:O	1:D:122:TYR:CD1	2.68	0.46
1:B:420:THR:HA	1:B:576:PRO:HG2	1.98	0.46
1:A:482:THR:HG22	1:A:509:VAL:HG12	1.98	0.46
1:D:155:VAL:HG12	1:D:459:LYS:NZ	2.31	0.46
1:D:230:LEU:HD23	1:D:230:LEU:N	2.30	0.46
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.96	0.46
1:D:269:THR:O	1:D:270:GLN:HB2	2.14	0.46
1:C:108:LEU:O	1:C:111:LEU:HB3	2.16	0.46
1:C:183:LEU:HD22	1:C:442:ILE:HG12	1.97	0.46
1:C:419:LEU:H	1:C:419:LEU:HD23	1.78	0.46
1:A:33:ALA:N	1:A:158:ASP:O	2.48	0.46
1:B:387:TRP:HZ2	4:B:701:FLP:H5	1.81	0.46
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.50	0.46
1:D:83:LYS:HB2	1:D:83:LYS:HZ2	1.80	0.46
1:A:244:LEU:HD11	1:A:288:GLY:HA2	1.96	0.46
1:C:203:GLN:O	1:C:207:HIS:ND1	2.48	0.46
1:C:89:VAL:O	1:C:93:LEU:HD23	2.14	0.46
1:C:482:THR:HG22	1:C:509:VAL:HG12	1.96	0.46
1:D:442:ILE:O	1:D:445:GLN:HG2	2.14	0.46
1:B:319:GLU:HG3	1:B:554:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:PHE:HZ	1:B:495:TYR:HB2	1.80	0.46
1:C:119:SER:O	1:C:122:TYR:CD1	2.68	0.46
1:D:112:ILE:HB	1:D:357:PHE:CZ	2.50	0.46
1:C:385:TYR:CZ	4:C:701:FLP:H	2.50	0.46
1:C:553:GLU:HG3	1:C:557:LYS:CE	2.46	0.46
1:B:137:LYS:O	1:B:138:SER:O	2.33	0.46
1:C:34:ASN:HB3	1:C:37:CYS:SG	2.55	0.46
1:C:122:TYR:CD2	1:C:122:TYR:O	2.69	0.46
1:C:109:ARG:HG3	1:C:357:PHE:CE1	2.50	0.46
1:D:198:PHE:HB2	1:D:580:PHE:HB3	1.98	0.46
1:A:114:LYS:HE2	1:A:365:LEU:O	2.16	0.46
1:D:465:GLU:HA	1:D:465:GLU:OE1	2.16	0.46
1:D:178:LEU:O	1:D:182:LEU:HB2	2.16	0.46
1:C:189:PRO:CB	1:C:430:ILE:HD12	2.46	0.46
1:D:113:MET:HA	1:D:116:VAL:HG13	1.97	0.46
1:D:355:TYR:HE2	4:D:701:FLP:O1	1.99	0.46
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.51	0.46
1:A:544:TYR:OH	1:B:142:PHE:HB2	2.16	0.46
1:C:204:HIS:ND1	1:C:292:PHE:CE2	2.84	0.46
1:D:280:PRO:HG2	1:D:283:LEU:HD12	1.97	0.45
1:C:146:SER:O	1:C:220:PHE:HA	2.16	0.45
1:B:482:THR:HG22	1:B:509:VAL:HG12	1.97	0.45
3:C:682:HEM:HHD	3:C:682:HEM:CBC	2.45	0.45
1:A:151:ALA:O	1:A:469:ARG:NH1	2.50	0.45
1:A:391:LEU:HD21	3:A:682:HEM:HHC	1.98	0.45
1:A:414:LEU:HD11	1:A:419:LEU:HD23	1.97	0.45
1:D:231:ASN:C	1:D:231:ASN:OD1	2.55	0.45
1:C:85:THR:OG1	1:C:88:THR:HG23	2.16	0.45
1:B:276:PRO:HG2	1:B:409:TYR:CG	2.51	0.45
1:B:414:LEU:HD11	1:B:419:LEU:HD23	1.98	0.45
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.98	0.45
1:B:491:LEU:HD11	1:B:509:VAL:HG11	1.96	0.45
1:A:269:THR:O	1:A:270:GLN:HB2	2.17	0.45
1:C:181:VAL:CG2	1:C:509:VAL:HG21	2.47	0.45
1:A:112:ILE:HB	1:A:357:PHE:CZ	2.52	0.45
1:B:147:TYR:OH	2:B:671:NAG:C6	2.64	0.45
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.71	0.45
1:D:414:LEU:HD11	1:D:419:LEU:CD2	2.46	0.45
1:D:412:SER:O	1:D:416:GLU:HB2	2.17	0.45
1:C:510:GLU:O	1:C:512:PRO:HD3	2.17	0.45
1:B:553:GLU:O	1:B:557:LYS:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:THR:O	1:A:307:ARG:HD3	2.17	0.45
1:C:465:GLU:OE1	1:C:465:GLU:HA	2.17	0.45
1:D:34:ASN:HB3	1:D:37:CYS:SG	2.57	0.45
1:A:398:GLU:HG3	1:A:421:GLN:CD	2.37	0.45
1:D:210:PHE:CE1	1:D:382:ASN:HA	2.52	0.45
1:C:398:GLU:HG3	1:C:421:GLN:CD	2.37	0.45
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.51	0.45
1:C:238:LEU:HD22	1:C:242:HIS:NE2	2.32	0.45
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.52	0.45
1:D:203:GLN:HG3	3:D:682:HEM:C1C	2.52	0.45
1:C:418:GLY:O	1:C:420:THR:N	2.49	0.45
1:D:133:HIS:CD2	1:D:147:TYR:CE2	3.04	0.45
1:C:210:PHE:HB3	3:C:682:HEM:HBD1	1.99	0.45
1:D:44:ARG:HD2	1:D:469:ARG:HD2	1.98	0.45
1:B:389:PRO:HG3	1:B:440:VAL:HG22	1.98	0.45
1:B:554:VAL:CG1	1:B:555:GLY:N	2.80	0.45
1:C:500:VAL:HG12	1:C:500:VAL:O	2.17	0.45
1:D:151:ALA:O	1:D:469:ARG:NH1	2.50	0.44
1:A:185:ARG:HB2	1:A:186:GLU:H	1.65	0.44
1:A:575:CYS:N	1:A:576:PRO:CD	2.80	0.44
1:D:83:LYS:HG3	1:D:83:LYS:O	2.17	0.44
1:C:216:ARG:HB3	1:C:220:PHE:CD2	2.53	0.44
1:C:244:LEU:HD11	1:C:288:GLY:HA2	2.00	0.44
1:A:482:THR:OG1	1:A:488:ALA:HB2	2.17	0.44
1:A:553:GLU:HG3	1:A:557:LYS:CE	2.47	0.44
1:B:33:ALA:HB3	1:B:158:ASP:OD2	2.18	0.44
1:D:155:VAL:HG12	1:D:459:LYS:HZ3	1.83	0.44
1:A:105:ASN:O	1:A:106:PRO:HD3	2.18	0.44
1:C:151:ALA:O	1:C:469:ARG:NH1	2.50	0.44
1:D:213:ASP:OD1	1:D:215:LYS:HE2	2.18	0.44
1:D:478:PHE:CZ	1:D:495:TYR:HB2	2.52	0.44
1:A:442:ILE:O	1:A:445:GLN:HG2	2.18	0.44
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.52	0.44
1:A:192:GLN:OE1	1:A:517:ILE:HG22	2.17	0.44
1:D:194:SER:OG	1:D:351:HIS:HE1	2.00	0.44
1:A:525:LEU:HD23	1:A:525:LEU:N	2.32	0.44
1:A:478:PHE:HZ	1:A:495:TYR:HB2	1.81	0.44
1:A:138:SER:HB2	1:B:330:GLN:HB3	2.00	0.44
1:A:51:GLY:O	1:A:52:PHE:CB	2.66	0.44
1:D:316:LEU:HD12	1:D:316:LEU:HA	1.87	0.44
1:B:113:MET:O	1:B:117:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.84	0.44
1:D:389:PRO:HB2	1:D:434:VAL:HA	1.98	0.44
1:B:122:TYR:CD2	1:B:122:TYR:O	2.71	0.44
1:B:240:ARG:O	1:B:241:GLN:C	2.56	0.44
1:B:344:VAL:HG12	1:B:534:LEU:HD21	1.99	0.44
1:A:120:ARG:HD3	4:A:701:FLP:O	2.18	0.44
1:A:382:ASN:ND2	3:A:682:HEM:HAD2	2.29	0.44
1:B:44:ARG:HD2	1:B:469:ARG:CD	2.48	0.44
1:C:276:PRO:HG2	1:C:409:TYR:CG	2.52	0.44
1:A:478:PHE:O	1:A:481:LEU:HB3	2.18	0.44
1:C:33:ALA:HB3	1:C:158:ASP:OD2	2.17	0.44
1:D:433:ARG:H	1:D:439:ASN:ND2	2.15	0.44
1:B:189:PRO:CB	1:B:430:ILE:HD12	2.48	0.44
1:D:482:THR:HG22	1:D:509:VAL:HG12	2.00	0.44
1:B:350:GLN:HE22	1:B:359:LEU:N	2.16	0.44
1:A:230:LEU:N	1:A:230:LEU:HD23	2.31	0.44
1:C:197:MET:CA	1:C:197:MET:CE	2.93	0.44
3:A:682:HEM:CBC	3:A:682:HEM:HHD	2.47	0.44
1:D:109:ARG:HG3	1:D:357:PHE:CE1	2.53	0.44
1:A:133:HIS:CD2	1:A:147:TYR:CE1	3.06	0.44
1:B:388:HIS:N	1:B:389:PRO:CD	2.81	0.44
1:D:500:VAL:O	1:D:500:VAL:HG12	2.17	0.44
1:B:197:MET:HE3	1:B:197:MET:HA	2.00	0.43
1:D:482:THR:OG1	1:D:488:ALA:HB2	2.17	0.43
1:A:352:LEU:HD11	1:A:518:PHE:CZ	2.52	0.43
1:A:565:GLN:HG3	1:D:268:ASP:OD1	2.18	0.43
1:A:147:TYR:OH	2:A:671:NAG:C5	2.66	0.43
1:C:352:LEU:HD11	1:C:518:PHE:HZ	1.81	0.43
1:B:269:THR:O	1:B:270:GLN:HB2	2.17	0.43
1:B:114:LYS:HB2	1:B:114:LYS:HE3	1.86	0.43
1:B:172:PRO:HG3	1:B:495:TYR:CD1	2.53	0.43
1:D:232:HIS:HD2	1:D:233:ILE:HG13	1.82	0.43
1:C:210:PHE:CE1	1:C:382:ASN:HA	2.53	0.43
1:A:119:SER:O	1:A:122:TYR:HD1	2.02	0.43
1:C:122:TYR:CE1	1:C:123:LEU:CD2	3.01	0.43
1:B:133:HIS:CD2	1:B:147:TYR:CE2	3.07	0.43
1:A:114:LYS:HD3	1:A:369:GLN:NE2	2.32	0.43
1:A:364:GLU:HA	1:A:367:PHE:CD2	2.53	0.43
1:B:178:LEU:O	1:B:182:LEU:HB2	2.18	0.43
1:A:92:ILE:H	1:A:92:ILE:HD12	1.83	0.43
1:C:420:THR:HG1	1:C:573:LYS:HB3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:GLU:HG3	1:A:557:LYS:NZ	2.33	0.43
1:D:39:ASN:N	1:D:40:PRO:CD	2.82	0.43
1:D:423:VAL:CG1	1:D:578:THR:HG23	2.48	0.43
1:B:198:PHE:HB2	1:B:580:PHE:HB3	1.99	0.43
1:B:435:ALA:HB2	1:B:518:PHE:HA	2.00	0.43
1:C:230:LEU:N	1:C:230:LEU:HD23	2.33	0.43
1:B:232:HIS:HD2	1:B:233:ILE:HG13	1.84	0.43
1:A:203:GLN:O	1:A:207:HIS:ND1	2.51	0.43
1:A:478:PHE:CE2	1:A:492:LYS:HA	2.53	0.43
1:D:172:PRO:HG3	1:D:495:TYR:CD1	2.54	0.43
1:C:396:ASN:HA	1:C:400:GLN:O	2.19	0.43
1:A:318:GLN:HA	1:A:318:GLN:NE2	2.33	0.43
1:D:92:ILE:HD12	1:D:92:ILE:H	1.82	0.43
1:D:189:PRO:CB	1:D:430:ILE:HD12	2.48	0.43
1:A:281:GLU:C	1:A:283:LEU:H	2.22	0.43
1:C:544:TYR:O	1:C:546:LYS:N	2.51	0.43
1:D:198:PHE:CZ	1:D:352:LEU:HD13	2.53	0.43
1:B:421:GLN:OE1	1:B:424:GLU:HB2	2.19	0.43
1:B:218:PRO:HB2	1:B:458:MET:SD	2.58	0.43
1:A:113:MET:O	1:A:117:LEU:HB2	2.18	0.43
1:C:190:ASP:HA	1:C:191:PRO:HD2	1.84	0.43
1:C:172:PRO:HG3	1:C:495:TYR:CE1	2.54	0.43
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.58	0.43
1:D:380:GLU:HG2	1:D:466:TYR:HE1	1.77	0.43
1:C:525:LEU:N	1:C:525:LEU:HD23	2.33	0.43
1:A:197:MET:HA	1:A:197:MET:HE3	2.01	0.43
1:C:367:PHE:CD1	1:C:542:PRO:HG3	2.53	0.43
1:C:117:LEU:HD12	1:C:117:LEU:HA	1.85	0.43
1:B:459:LYS:HB3	1:B:459:LYS:HE2	1.75	0.43
1:D:148:TYR:CD1	1:D:377:ILE:HG13	2.49	0.43
1:A:544:TYR:O	1:A:546:LYS:N	2.52	0.43
1:C:148:TYR:CE1	1:C:377:ILE:HD11	2.54	0.43
1:B:478:PHE:CD1	1:B:491:LEU:HB3	2.54	0.42
1:A:557:LYS:HA	1:A:557:LYS:HD3	1.81	0.42
1:B:350:GLN:HE22	1:B:359:LEU:H	1.66	0.42
1:C:554:VAL:CG1	1:C:555:GLY:N	2.82	0.42
1:D:525:LEU:O	1:D:528:PRO:HD2	2.19	0.42
1:A:405:LYS:HD2	1:A:405:LYS:H	1.84	0.42
1:B:215:LYS:CD	1:B:215:LYS:N	2.81	0.42
1:C:349:VAL:CG1	4:C:701:FLP:H132	2.49	0.42
1:B:39:ASN:N	1:B:40:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD11	1:B:518:PHE:HZ	1.83	0.42
1:D:396:ASN:HA	1:D:400:GLN:O	2.19	0.42
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.59	0.42
1:C:420:THR:HA	1:C:576:PRO:HG2	2.01	0.42
1:B:183:LEU:HD23	1:B:183:LEU:HA	1.78	0.42
1:D:183:LEU:HD22	1:D:442:ILE:HG12	2.01	0.42
1:D:85:THR:OG1	1:D:88:THR:HG23	2.19	0.42
1:B:396:ASN:HA	1:B:401:GLU:HA	2.02	0.42
1:D:396:ASN:HA	1:D:401:GLU:HA	2.01	0.42
1:C:240:ARG:O	1:C:241:GLN:C	2.58	0.42
1:A:554:VAL:CG1	1:A:555:GLY:N	2.83	0.42
1:C:424:GLU:O	1:C:428:ARG:NE	2.51	0.42
1:D:92:ILE:HD12	1:D:92:ILE:N	2.34	0.42
1:D:303:THR:O	1:D:307:ARG:HD3	2.20	0.42
1:A:263:PRO:HB2	1:A:285:PHE:HB3	2.01	0.42
1:C:316:LEU:HD12	1:C:316:LEU:HA	1.89	0.42
1:D:230:LEU:HD13	1:D:233:ILE:HD12	2.01	0.42
1:A:44:ARG:HD2	1:A:469:ARG:HD2	2.01	0.42
1:C:578:THR:HG22	1:C:579:SER:H	1.84	0.42
1:B:45:GLY:HA3	1:B:69:CYS:SG	2.59	0.42
1:B:497:ASP:HB3	1:B:500:VAL:HG23	2.02	0.42
1:C:340:THR:O	1:C:344:VAL:HG23	2.20	0.42
1:D:403:SER:HB2	1:D:405:LYS:CD	2.49	0.42
1:C:388:HIS:HB3	1:C:444:VAL:HG21	2.02	0.42
1:C:435:ALA:HB2	1:C:518:PHE:HA	2.01	0.42
1:A:109:ARG:HG3	1:A:357:PHE:CE1	2.54	0.42
1:D:478:PHE:CE2	1:D:492:LYS:HA	2.54	0.42
1:B:565:GLN:HE21	1:B:565:GLN:HA	1.85	0.42
1:A:216:ARG:HB3	1:A:220:PHE:CD2	2.54	0.42
1:A:83:LYS:O	1:A:83:LYS:HG3	2.20	0.42
1:C:74:PHE:CZ	1:C:78:ILE:HD11	2.55	0.42
1:C:249:ASP:CG	1:C:317:LYS:NZ	2.73	0.42
1:C:94:THR:O	1:C:356:HIS:CE1	2.73	0.42
1:B:194:SER:OG	1:B:351:HIS:HE1	2.03	0.42
1:B:208:GLN:HB3	1:B:232:HIS:ND1	2.35	0.42
1:B:398:GLU:HG3	1:B:421:GLN:CD	2.40	0.42
1:B:387:TRP:HZ2	4:B:701:FLP:C5	2.33	0.42
1:D:525:LEU:N	1:D:525:LEU:HD23	2.35	0.42
1:C:287:VAL:HG23	1:C:288:GLY:N	2.34	0.42
1:A:510:GLU:O	1:A:512:PRO:HD3	2.20	0.42
1:B:245:ARG:HD3	1:B:329:PHE:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:92:ILE:HD12	1:C:92:ILE:N	2.35	0.42
1:C:215:LYS:CD	1:C:215:LYS:N	2.82	0.42
1:C:330:GLN:HB3	1:D:138:SER:HB2	2.02	0.42
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.55	0.41
1:B:210:PHE:CE1	1:B:382:ASN:HA	2.54	0.41
1:B:151:ALA:O	1:B:469:ARG:NH1	2.53	0.41
1:B:388:HIS:C	1:B:390:LEU:H	2.24	0.41
1:A:578:THR:HG22	1:A:579:SER:H	1.85	0.41
1:C:292:PHE:CD1	1:C:292:PHE:N	2.88	0.41
1:B:479:GLU:HG3	1:B:488:ALA:HB1	2.02	0.41
1:A:189:PRO:CB	1:A:430:ILE:HD12	2.50	0.41
1:A:405:LYS:H	1:A:405:LYS:CD	2.33	0.41
1:D:510:GLU:O	1:D:512:PRO:HD3	2.19	0.41
1:D:478:PHE:CD1	1:D:491:LEU:HB3	2.56	0.41
1:D:352:LEU:HD11	1:D:518:PHE:CZ	2.55	0.41
1:D:210:PHE:HB3	3:D:682:HEM:HBD1	2.03	0.41
1:C:44:ARG:HD2	1:C:469:ARG:HD2	2.03	0.41
1:D:108:LEU:O	1:D:111:LEU:HB3	2.20	0.41
1:A:191:PRO:HG3	1:A:433:ARG:NH2	2.35	0.41
1:D:215:LYS:CD	1:D:215:LYS:N	2.83	0.41
1:B:185:ARG:HB2	1:B:186:GLU:H	1.68	0.41
1:D:554:VAL:CG1	1:D:555:GLY:N	2.81	0.41
1:B:482:THR:OG1	1:B:488:ALA:HB2	2.20	0.41
1:D:150:ARG:HD2	1:D:380:GLU:OE2	2.20	0.41
1:C:557:LYS:O	1:C:558:ILE:C	2.57	0.41
1:C:238:LEU:HD22	1:C:242:HIS:CD2	2.54	0.41
1:A:465:GLU:HA	1:A:465:GLU:OE1	2.20	0.41
1:A:396:ASN:HA	1:A:401:GLU:HA	2.03	0.41
1:C:403:SER:HB2	1:C:405:LYS:CD	2.48	0.41
1:A:40:PRO:O	1:A:68:ASN:HB3	2.20	0.41
1:B:340:THR:O	1:B:344:VAL:HG23	2.20	0.41
1:A:92:ILE:N	1:A:92:ILE:HD12	2.36	0.41
1:C:92:ILE:HD12	1:C:92:ILE:H	1.85	0.41
1:B:191:PRO:HB2	1:B:515:ASP:HB3	2.00	0.41
1:C:298:LEU:HD12	1:C:298:LEU:HA	1.80	0.41
1:B:40:PRO:HB3	2:B:661:NAG:H62	2.03	0.41
1:A:388:HIS:HB3	1:A:444:VAL:HG21	2.03	0.41
1:C:232:HIS:HD2	1:C:233:ILE:HG13	1.85	0.41
1:B:355:TYR:CE2	4:B:701:FLP:O1	2.71	0.41
1:C:475:TYR:HD1	1:C:480:GLU:HG2	1.85	0.41
1:A:388:HIS:C	1:A:390:LEU:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:VAL:HG12	1:B:555:GLY:N	2.36	0.41
1:B:465:GLU:OE1	1:B:465:GLU:HA	2.20	0.41
1:C:388:HIS:C	1:C:390:LEU:H	2.24	0.41
1:B:382:ASN:HD21	3:B:682:HEM:CAD	2.29	0.41
1:D:554:VAL:HG12	1:D:555:GLY:N	2.36	0.41
1:B:74:PHE:O	1:B:77:ARG:HB2	2.20	0.41
1:D:398:GLU:HG3	1:D:421:GLN:HE22	1.86	0.41
1:A:210:PHE:HB3	3:A:682:HEM:HBD1	2.03	0.41
1:B:83:LYS:O	1:B:83:LYS:HG3	2.20	0.41
1:C:435:ALA:HB3	1:C:512:PRO:HG3	2.03	0.41
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.35	0.41
1:B:510:GLU:O	1:B:512:PRO:HD3	2.21	0.41
1:C:544:TYR:OH	1:D:142:PHE:HB2	2.20	0.41
1:A:557:LYS:O	1:A:558:ILE:C	2.59	0.41
1:C:320:HIS:HB3	1:C:323:TRP:CG	2.56	0.41
1:A:49:SER:O	1:B:320:HIS:CD2	2.74	0.41
1:B:413:ILE:HG12	2:B:681:NAG:O6	2.21	0.41
1:C:322:GLU:HG3	1:D:51:GLY:O	2.21	0.41
1:A:198:PHE:HB2	1:A:580:PHE:HB3	2.02	0.41
1:C:42:GLN:O	1:C:69:CYS:HB2	2.20	0.41
1:A:292:PHE:N	1:A:292:PHE:CD1	2.89	0.41
1:D:204:HIS:ND1	1:D:292:PHE:CE2	2.88	0.41
1:D:575:CYS:N	1:D:576:PRO:CD	2.84	0.41
1:A:381:PHE:HA	1:A:384:LEU:HG	2.03	0.41
1:D:578:THR:HG22	1:D:579:SER:H	1.85	0.41
1:A:565:GLN:HE21	1:A:565:GLN:HA	1.86	0.41
1:A:146:SER:O	1:A:220:PHE:HA	2.21	0.41
1:C:51:GLY:O	1:D:322:GLU:HG3	2.21	0.41
1:B:420:THR:HG1	1:B:573:LYS:HB3	1.86	0.40
1:B:280:PRO:O	1:B:281:GLU:CB	2.68	0.40
1:A:215:LYS:CD	1:A:215:LYS:N	2.84	0.40
1:A:74:PHE:CZ	1:A:78:ILE:HD11	2.56	0.40
1:A:240:ARG:O	1:A:241:GLN:C	2.60	0.40
1:B:412:SER:O	1:B:416:GLU:HB2	2.21	0.40
1:D:350:GLN:HE22	1:D:359:LEU:H	1.70	0.40
1:C:150:ARG:HD2	1:C:380:GLU:OE2	2.22	0.40
1:D:196:MET:SD	1:D:392:PRO:HD3	2.62	0.40
1:B:108:LEU:O	1:B:111:LEU:HB3	2.21	0.40
1:B:381:PHE:HA	1:B:384:LEU:HG	2.03	0.40
1:C:276:PRO:HD2	1:C:279:ILE:HD11	2.02	0.40
1:C:148:TYR:HE1	1:C:377:ILE:HD11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:HIS:CD2	1:D:49:SER:O	2.74	0.40
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.56	0.40
1:D:191:PRO:HD2	1:D:433:ARG:HG3	2.02	0.40
1:C:327:GLN:HG3	1:D:136:TYR:CE2	2.56	0.40
1:C:550:PHE:CD2	1:C:556:PHE:CD1	3.09	0.40
1:D:192:GLN:OE1	1:D:517:ILE:HG22	2.21	0.40
1:B:181:VAL:CG2	1:B:509:VAL:HG21	2.51	0.40
1:D:114:LYS:HE3	1:D:114:LYS:HB2	1.91	0.40
1:C:495:TYR:CE2	1:C:502:GLU:HG3	2.55	0.40
1:B:85:THR:OG1	1:B:88:THR:HG23	2.21	0.40
1:C:211:LYS:HZ1	1:C:236:GLU:HG3	1.87	0.40
1:D:190:ASP:HA	1:D:191:PRO:HD2	1.87	0.40
1:A:550:PHE:CD2	1:A:556:PHE:CD1	3.09	0.40
1:A:276:PRO:HA	1:A:277:PRO:HD2	1.83	0.40
1:D:203:GLN:HG3	3:D:682:HEM:C2C	2.56	0.40
1:B:117:LEU:HA	1:B:117:LEU:HD12	1.85	0.40
1:D:281:GLU:C	1:D:283:LEU:H	2.24	0.40
1:C:569:CYS:HA	1:C:575:CYS:HA	2.03	0.40
1:A:388:HIS:N	1:A:389:PRO:CD	2.85	0.40
1:A:320:HIS:CD2	1:B:49:SER:O	2.74	0.40
1:A:231:ASN:C	1:A:231:ASN:OD1	2.58	0.40
1:A:424:GLU:CA	1:A:428:ARG:HH21	2.16	0.40
1:B:479:GLU:CD	1:B:479:GLU:N	2.75	0.40
1:D:294:LEU:HD22	1:D:409:TYR:CD1	2.56	0.40
1:A:122:TYR:CE1	1:A:123:LEU:CD2	3.05	0.40
1:B:109:ARG:HG3	1:B:357:PHE:CE1	2.57	0.40
1:C:281:GLU:C	1:C:283:LEU:H	2.24	0.40
1:A:553:GLU:HG3	1:A:557:LYS:HE3	2.02	0.40
1:C:391:LEU:HB2	1:C:441:PRO:HG2	2.03	0.40
1:C:583:GLN:CD	1:C:583:GLN:H	2.25	0.40
1:C:48:MET:O	1:C:56:LYS:N	2.55	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%)	473 (86%)	62 (11%)	15 (3%)	6	9
1	B	550/587 (94%)	484 (88%)	49 (9%)	17 (3%)	5	7
1	C	550/587 (94%)	479 (87%)	54 (10%)	17 (3%)	5	7
1	D	550/587 (94%)	477 (87%)	57 (10%)	16 (3%)	6	8
All	All	2200/2348 (94%)	1913 (87%)	222 (10%)	65 (3%)	5	7

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PHE
1	A	82	LEU
1	A	130	TYR
1	A	138	SER
1	A	282	ASN
1	A	398	GLU
1	A	419	LEU
1	A	514	PRO
1	B	52	PHE
1	B	82	LEU
1	B	130	TYR
1	B	138	SER
1	B	282	ASN
1	B	398	GLU
1	B	419	LEU
1	B	514	PRO
1	C	52	PHE
1	C	82	LEU
1	C	138	SER
1	C	282	ASN
1	C	398	GLU
1	C	419	LEU
1	C	514	PRO
1	D	52	PHE
1	D	82	LEU
1	D	130	TYR
1	D	138	SER
1	D	282	ASN
1	D	398	GLU
1	D	419	LEU

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Mol	Chain	Res	Type
1	D	514	PRO
1	A	422	PHE
1	B	422	PHE
1	B	499	ASP
1	C	130	TYR
1	C	422	PHE
1	C	545	TRP
1	D	422	PHE
1	A	277	PRO
1	A	499	ASP
1	B	277	PRO
1	B	399	ASP
1	C	277	PRO
1	C	499	ASP
1	D	277	PRO
1	D	399	ASP
1	D	499	ASP
1	A	280	PRO
1	A	399	ASP
1	B	162	PRO
1	C	399	ASP
1	A	162	PRO
1	B	280	PRO
1	B	545	TRP
1	B	573	LYS
1	C	162	PRO
1	C	280	PRO
1	C	573	LYS
1	D	162	PRO
1	D	280	PRO
1	D	573	LYS
1	A	226	HIS
1	C	226	HIS
1	B	51	GLY
1	D	51	GLY

### 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%)	436 (88%)	57 (12%)	7	13
1	B	493/525 (94%)	437 (89%)	56 (11%)	7	13
1	C	493/525 (94%)	437 (89%)	56 (11%)	7	13
1	D	493/525 (94%)	437 (89%)	56 (11%)	7	13
All	All	1972/2100 (94%)	1747 (89%)	225 (11%)	7	13

All (225) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	52	PHE
1	A	71	THR
1	A	83	LYS
1	A	106	PRO
1	A	107	PHE
1	A	111	LEU
1	A	116	VAL
1	A	117	LEU
1	A	120	ARG
1	A	122	TYR
1	A	137	LYS
1	A	138	SER
1	A	165	VAL
1	A	178	LEU
1	A	186	GLU
1	A	197	MET
1	A	216	ARG
1	A	232	HIS
1	A	238	LEU
1	A	245	ARG
1	A	248	LYS
1	A	252	LEU
1	A	270	GLN
1	A	271	VAL
1	A	272	GLU
1	A	282	ASN
1	A	289	GLN
1	A	291	VAL
1	A	298	LEU
1	A	300	MET

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Mol	Chain	Res	Type
1	A	310	GLN
1	A	316	LEU
1	A	322	GLU
1	A	382	ASN
1	A	385	TYR
1	A	399	ASP
1	A	405	LYS
1	A	409	TYR
1	A	416	GLU
1	A	422	PHE
1	A	430	ILE
1	A	433	ARG
1	A	459	LYS
1	A	463	LEU
1	A	484	GLU
1	A	485	LYS
1	A	514	PRO
1	A	518	PHE
1	A	543	GLN
1	A	554	VAL
1	A	556	PHE
1	A	565	GLN
1	A	569	CYS
1	A	575	CYS
1	A	578	THR
1	A	583	GLN
1	B	44	ARG
1	B	52	PHE
1	B	54	GLN
1	B	71	THR
1	B	83	LYS
1	B	106	PRO
1	B	107	PHE
1	B	111	LEU
1	B	117	LEU
1	B	120	ARG
1	B	122	TYR
1	B	137	LYS
1	B	138	SER
1	B	165	VAL
1	B	171	LEU
1	B	178	LEU

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Mol	Chain	Res	Type
1	B	186	GLU
1	B	197	MET
1	B	216	ARG
1	B	232	HIS
1	B	238	LEU
1	B	245	ARG
1	B	248	LYS
1	B	252	LEU
1	B	270	GLN
1	B	271	VAL
1	B	272	GLU
1	B	282	ASN
1	B	289	GLN
1	B	291	VAL
1	B	298	LEU
1	B	300	MET
1	B	310	GLN
1	B	316	LEU
1	B	322	GLU
1	B	376	ARG
1	B	382	ASN
1	B	385	TYR
1	B	399	ASP
1	B	405	LYS
1	B	409	TYR
1	B	422	PHE
1	B	430	ILE
1	B	459	LYS
1	B	484	GLU
1	B	485	LYS
1	B	514	PRO
1	B	518	PHE
1	B	534	LEU
1	B	543	GLN
1	B	554	VAL
1	B	565	GLN
1	B	569	CYS
1	B	575	CYS
1	B	578	THR
1	B	583	GLN
1	C	44	ARG
1	C	52	PHE

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Mol	Chain	Res	Type
1	C	71	THR
1	C	83	LYS
1	C	107	PHE
1	C	111	LEU
1	C	116	VAL
1	C	117	LEU
1	C	120	ARG
1	C	122	TYR
1	C	137	LYS
1	C	138	SER
1	C	165	VAL
1	C	178	LEU
1	C	197	MET
1	C	215	LYS
1	C	216	ARG
1	C	232	HIS
1	C	238	LEU
1	C	245	ARG
1	C	248	LYS
1	C	252	LEU
1	C	270	GLN
1	C	272	GLU
1	C	282	ASN
1	C	289	GLN
1	C	291	VAL
1	C	298	LEU
1	C	300	MET
1	C	310	GLN
1	C	316	LEU
1	C	322	GLU
1	C	376	ARG
1	C	382	ASN
1	C	385	TYR
1	C	399	ASP
1	C	405	LYS
1	C	409	TYR
1	C	421	GLN
1	C	422	PHE
1	C	430	ILE
1	C	459	LYS
1	C	484	GLU
1	C	485	LYS

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Mol	Chain	Res	Type
1	C	505	PRO
1	C	514	PRO
1	C	518	PHE
1	C	534	LEU
1	C	543	GLN
1	C	554	VAL
1	C	556	PHE
1	C	565	GLN
1	C	569	CYS
1	C	575	CYS
1	C	578	THR
1	C	583	GLN
1	D	44	ARG
1	D	52	PHE
1	D	71	THR
1	D	83	LYS
1	D	106	PRO
1	D	107	PHE
1	D	111	LEU
1	D	117	LEU
1	D	120	ARG
1	D	122	TYR
1	D	137	LYS
1	D	138	SER
1	D	165	VAL
1	D	171	LEU
1	D	178	LEU
1	D	197	MET
1	D	216	ARG
1	D	232	HIS
1	D	238	LEU
1	D	248	LYS
1	D	252	LEU
1	D	270	GLN
1	D	271	VAL
1	D	272	GLU
1	D	282	ASN
1	D	289	GLN
1	D	291	VAL
1	D	298	LEU
1	D	300	MET
1	D	310	GLN

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	322	GLU
1	D	376	ARG
1	D	382	ASN
1	D	385	TYR
1	D	399	ASP
1	D	405	LYS
1	D	409	TYR
1	D	422	PHE
1	D	430	ILE
1	D	459	LYS
1	D	484	GLU
1	D	485	LYS
1	D	505	PRO
1	D	514	PRO
1	D	518	PHE
1	D	528	PRO
1	D	534	LEU
1	D	543	GLN
1	D	554	VAL
1	D	565	GLN
1	D	569	CYS
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 (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	95	HIS
1	A	101	ASN
1	A	133	HIS
1	A	203	GLN
1	A	232	HIS
1	A	318	GLN
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	356	HIS
1	A	369	GLN

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Mol	Chain	Res	Type
1	A	382	ASN
1	A	396	ASN
1	A	411	ASN
1	A	417	HIS
1	A	454	GLN
1	A	464	ASN
1	A	543	GLN
1	B	42	GLN
1	B	101	ASN
1	B	105	ASN
1	B	133	HIS
1	B	203	GLN
1	B	232	HIS
1	B	318	GLN
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	356	HIS
1	B	369	GLN
1	B	382	ASN
1	B	396	ASN
1	B	411	ASN
1	B	417	HIS
1	B	454	GLN
1	B	464	ASN
1	C	90	HIS
1	C	95	HIS
1	C	101	ASN
1	C	133	HIS
1	C	203	GLN
1	C	232	HIS
1	C	278	HIS
1	C	318	GLN
1	C	320	HIS
1	C	350	GLN
1	C	351	HIS
1	C	356	HIS
1	C	369	GLN
1	C	382	ASN
1	C	396	ASN
1	C	411	ASN
1	C	417	HIS

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Mol	Chain	Res	Type
1	C	454	GLN
1	C	464	ASN
1	C	543	GLN
1	D	95	HIS
1	D	101	ASN
1	D	105	ASN
1	D	133	HIS
1	D	203	GLN
1	D	232	HIS
1	D	318	GLN
1	D	320	HIS
1	D	350	GLN
1	D	351	HIS
1	D	356	HIS
1	D	369	GLN
1	D	382	ASN
1	D	396	ASN
1	D	411	ASN
1	D	417	HIS
1	D	454	GLN
1	D	464	ASN
1	D	581	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

20 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	NAG	A	661	1	14,14,15	0.58	0	15,19,21	0.91	1 (6%)
2	NAG	A	671	1	14,14,15	0.70	0	15,19,21	1.41	3 (20%)
2	NAG	A	681	1	14,14,15	0.77	0	15,19,21	0.67	0
3	HEM	A	682	1	30,50,50	3.38	10 (33%)	24,82,82	2.05	6 (25%)
4	FLP	A	701	-	16,19,19	1.49	3 (18%)	21,26,26	1.41	4 (19%)
2	NAG	B	661	1	14,14,15	0.51	0	15,19,21	1.13	1 (6%)
2	NAG	B	671	1	14,14,15	0.74	0	15,19,21	1.42	3 (20%)
2	NAG	B	681	1	14,14,15	0.72	0	15,19,21	0.84	1 (6%)
3	HEM	B	682	1	30,50,50	3.21	10 (33%)	24,82,82	2.09	7 (29%)
4	FLP	B	701	-	16,19,19	1.75	4 (25%)	21,26,26	1.46	4 (19%)
2	NAG	C	661	1	14,14,15	0.25	0	15,19,21	0.94	1 (6%)
2	NAG	C	671	1	14,14,15	0.81	1 (7%)	15,19,21	1.48	3 (20%)
2	NAG	C	681	1	14,14,15	0.60	0	15,19,21	0.72	0
3	HEM	C	682	1	30,50,50	3.28	10 (33%)	24,82,82	2.12	6 (25%)
4	FLP	C	701	-	16,19,19	1.09	1 (6%)	21,26,26	1.46	3 (14%)
2	NAG	D	661	1	14,14,15	0.64	0	15,19,21	1.06	1 (6%)
2	NAG	D	671	1	14,14,15	0.61	0	15,19,21	1.27	2 (13%)
2	NAG	D	681	1	14,14,15	0.78	0	15,19,21	0.86	0
3	HEM	D	682	1	30,50,50	3.34	10 (33%)	24,82,82	2.06	7 (29%)
4	FLP	D	701	-	16,19,19	1.55	2 (12%)	21,26,26	1.33	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	NAG	A	661	1	-	0/6/23/26	0/1/1/1
2	NAG	A	671	1	-	0/6/23/26	0/1/1/1
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	HEM	A	682	1	-	0/10/54/54	0/0/8/8
4	FLP	A	701	-	-	0/8/12/12	0/2/2/2
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	671	1	-	0/6/23/26	0/1/1/1
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	0/10/54/54	0/0/8/8
4	FLP	B	701	-	-	0/8/12/12	0/2/2/2
2	NAG	C	661	1	-	0/6/23/26	0/1/1/1
2	NAG	C	671	1	-	0/6/23/26	0/1/1/1
2	NAG	C	681	1	-	0/6/23/26	0/1/1/1
3	HEM	C	682	1	-	0/10/54/54	0/0/8/8
4	FLP	C	701	-	-	0/8/12/12	0/2/2/2
2	NAG	D	661	1	-	0/6/23/26	0/1/1/1
2	NAG	D	671	1	-	0/6/23/26	0/1/1/1
2	NAG	D	681	1	-	0/6/23/26	0/1/1/1
3	HEM	D	682	1	-	0/10/54/54	0/0/8/8
4	FLP	D	701	-	-	0/8/12/12	0/2/2/2

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3B-C4B	-10.57	1.42	1.51
3	C	682	HEM	C3B-C4B	-10.53	1.42	1.51
3	D	682	HEM	C3B-C4B	-9.98	1.42	1.51
3	B	682	HEM	C3B-C4B	-9.40	1.43	1.51
3	D	682	HEM	C3C-CAC	-7.52	1.37	1.51
3	B	682	HEM	C3B-CAB	-7.24	1.37	1.51
3	A	682	HEM	C3C-CAC	-7.10	1.38	1.51
3	C	682	HEM	C3C-CAC	-7.01	1.38	1.51
3	D	682	HEM	C3B-CAB	-6.84	1.38	1.51
3	B	682	HEM	C3C-CAC	-6.77	1.38	1.51
3	A	682	HEM	C3B-CAB	-6.73	1.38	1.51
3	D	682	HEM	C2D-C3D	-6.71	1.34	1.54
3	B	682	HEM	C2D-C3D	-6.70	1.34	1.54
3	C	682	HEM	C2D-C3D	-6.41	1.35	1.54
3	A	682	HEM	C2D-C3D	-6.39	1.35	1.54
3	C	682	HEM	C3B-CAB	-6.37	1.39	1.51
3	A	682	HEM	C3D-C4D	-6.13	1.43	1.51
3	D	682	HEM	C3D-C4D	-5.63	1.44	1.51
3	C	682	HEM	C2C-C1C	-5.19	1.42	1.52
3	B	682	HEM	C2C-C1C	-4.93	1.43	1.52
3	C	682	HEM	C3D-C4D	-4.77	1.45	1.51
3	B	682	HEM	C3D-C4D	-4.65	1.45	1.51
3	D	682	HEM	C2C-C1C	-4.62	1.43	1.52
3	A	682	HEM	C2C-C1C	-4.39	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C2D-C1D	-2.86	1.42	1.51
3	A	682	HEM	C2B-C1B	-2.67	1.43	1.51
3	C	682	HEM	C2D-C1D	-2.45	1.43	1.51
3	C	682	HEM	C2B-C1B	-2.27	1.44	1.51
3	D	682	HEM	C2D-C1D	-2.21	1.44	1.51
3	B	682	HEM	C2D-C1D	-2.19	1.44	1.51
4	B	701	FLP	C10-C11	2.02	1.41	1.37
2	C	671	NAG	C1-C2	2.18	1.55	1.52
4	D	701	FLP	C6-C2	2.22	1.53	1.49
3	B	682	HEM	CBB-CAB	2.29	1.42	1.29
3	B	682	HEM	CBC-CAC	2.38	1.43	1.29
3	A	682	HEM	CBB-CAB	2.45	1.43	1.29
3	D	682	HEM	CBC-CAC	2.48	1.43	1.29
3	C	682	HEM	CBB-CAB	2.52	1.43	1.29
4	A	701	FLP	C8-C7	2.52	1.43	1.38
3	C	682	HEM	CBC-CAC	2.53	1.43	1.29
3	D	682	HEM	CBB-CAB	2.54	1.44	1.29
3	A	682	HEM	CBC-CAC	2.56	1.44	1.29
3	B	682	HEM	C1C-NC	2.60	1.39	1.36
4	B	701	FLP	C6-C11	2.61	1.42	1.38
4	C	701	FLP	C8-C7	2.74	1.43	1.38
3	D	682	HEM	C1C-NC	2.83	1.39	1.36
4	B	701	FLP	C8-C9	3.01	1.44	1.39
4	A	701	FLP	C6-C11	3.02	1.42	1.38
4	A	701	FLP	C8-C9	3.15	1.44	1.39
4	B	701	FLP	C7-C6	3.23	1.45	1.39
4	D	701	FLP	C6-C11	3.83	1.43	1.38

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	FLP	C2-C6-C11	-3.39	118.70	123.05
2	A	671	NAG	C4-C3-C2	-3.26	106.17	111.23
2	B	671	NAG	C4-C3-C2	-3.24	106.19	111.23
2	D	671	NAG	C4-C3-C2	-3.01	106.55	111.23
4	B	701	FLP	C2-C6-C11	-2.98	119.23	123.05
4	B	701	FLP	C10-C11-C6	-2.94	120.54	124.24
2	C	671	NAG	C2-N2-C7	-2.87	119.35	123.04
4	A	701	FLP	C2-C6-C11	-2.87	119.36	123.05
2	B	661	NAG	C3-C4-C5	-2.74	105.41	110.20
4	A	701	FLP	C10-C11-C6	-2.70	120.84	124.24
4	D	701	FLP	C2-C6-C11	-2.63	119.68	123.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	701	FLP	C10-C11-C6	-2.62	120.94	124.24
2	D	661	NAG	C3-C4-C5	-2.51	105.81	110.20
2	B	671	NAG	C6-C5-C4	-2.50	106.85	113.02
2	A	661	NAG	C3-C4-C5	-2.46	105.90	110.20
4	B	701	FLP	C14-C12-C9	-2.46	107.48	112.32
4	D	701	FLP	C10-C11-C6	-2.46	121.14	124.24
2	C	671	NAG	C4-C3-C2	-2.32	107.63	111.23
2	B	681	NAG	C2-N2-C7	-2.29	120.10	123.04
4	A	701	FLP	C14-C12-C9	-2.21	107.97	112.32
3	B	682	HEM	CMA-C3A-C4A	-2.11	124.86	128.36
4	D	701	FLP	C14-C12-C9	-2.11	108.17	112.32
2	C	661	NAG	C3-C4-C5	-2.11	106.52	110.20
3	D	682	HEM	C3C-CAC-CBC	-2.04	121.32	124.46
2	A	671	NAG	C6-C5-C4	-2.02	108.03	113.02
2	D	671	NAG	C1-O5-C5	2.13	114.95	112.25
2	A	671	NAG	C1-O5-C5	2.14	114.97	112.25
2	B	671	NAG	C1-O5-C5	2.26	115.12	112.25
3	B	682	HEM	CMD-C2D-C3D	2.62	125.92	114.35
3	D	682	HEM	CMD-C2D-C3D	2.70	126.29	114.35
3	A	682	HEM	CMD-C2D-C3D	2.98	127.54	114.35
3	C	682	HEM	CMD-C2D-C3D	3.06	127.90	114.35
4	B	701	FLP	C7-C6-C11	3.09	118.97	115.90
3	C	682	HEM	C2D-C3D-C4D	3.15	106.85	101.50
2	C	671	NAG	C1-O5-C5	3.23	116.35	112.25
3	A	682	HEM	C2D-C3D-C4D	3.25	107.01	101.50
4	D	701	FLP	C7-C6-C11	3.25	119.13	115.90
3	D	682	HEM	C2D-C3D-C4D	3.27	107.04	101.50
3	B	682	HEM	C2D-C3D-C4D	3.30	107.09	101.50
4	A	701	FLP	C7-C6-C11	3.37	119.25	115.90
4	C	701	FLP	C7-C6-C11	3.54	119.42	115.90
3	C	682	HEM	CAD-C3D-C4D	3.67	125.42	112.47
3	A	682	HEM	CAD-C3D-C4D	3.76	125.74	112.47
3	D	682	HEM	CAD-C3D-C4D	3.86	126.07	112.47
3	B	682	HEM	CAD-C3D-C2D	4.06	124.89	113.22
3	B	682	HEM	CMB-C2B-C3B	4.14	126.87	116.53
3	B	682	HEM	CAD-C3D-C4D	4.18	127.21	112.47
3	A	682	HEM	CMB-C2B-C3B	4.24	127.12	116.53
3	A	682	HEM	CMC-C2C-C3C	4.26	127.16	116.53
3	C	682	HEM	CMC-C2C-C3C	4.29	127.24	116.53
3	D	682	HEM	CMC-C2C-C3C	4.34	127.37	116.53
3	D	682	HEM	CMB-C2B-C3B	4.42	127.55	116.53
3	C	682	HEM	CMB-C2B-C3B	4.54	127.86	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	682	HEM	CAD-C3D-C2D	4.54	126.27	113.22
3	B	682	HEM	CMC-C2C-C3C	4.65	128.13	116.53
3	A	682	HEM	CAD-C3D-C2D	4.67	126.64	113.22
3	C	682	HEM	CAD-C3D-C2D	4.76	126.90	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 50 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	671	NAG	4	0
3	A	682	HEM	6	0
4	A	701	FLP	1	0
2	B	661	NAG	1	0
2	B	671	NAG	1	0
2	B	681	NAG	1	0
3	B	682	HEM	9	0
4	B	701	FLP	6	0
3	C	682	HEM	6	0
4	C	701	FLP	3	0
3	D	682	HEM	9	0
4	D	701	FLP	3	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.