



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:57 PM GMT

PDB ID : 6COX  
Title : CYCLOOXYGENASE-2 (PROSTAGLANDIN SYNTHASE-2) COM-  
PLEXED WITH A SELECTIVE INHIBITOR, SC-558 IN I222 SPACE  
GROUP  
Authors : Kurumbail, R.; Stallings, W.  
Deposited on : 1996-12-18  
Resolution : 2.80 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

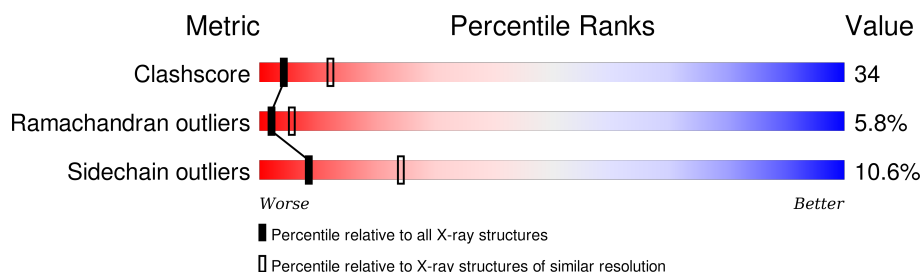
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

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

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9168 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			

There are 4 discrepancies between the modelled and reference sequences:

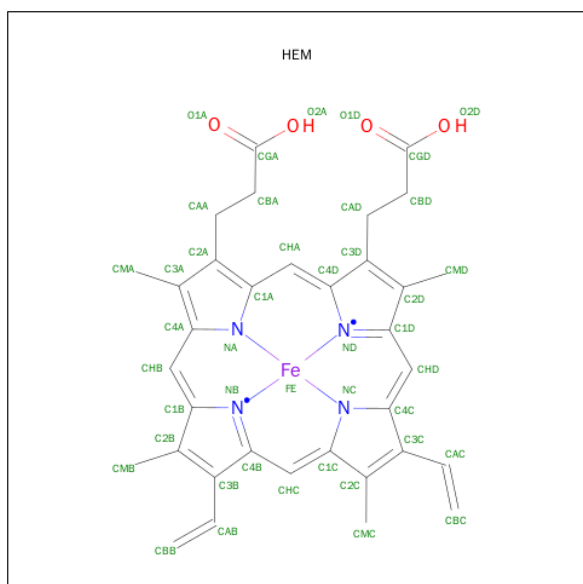
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	CONFLICT	UNP Q05769
A	333	LYS	ARG	CONFLICT	UNP Q05769
B	310	GLN	ASN	CONFLICT	UNP Q05769
B	333	LYS	ARG	CONFLICT	UNP Q05769

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



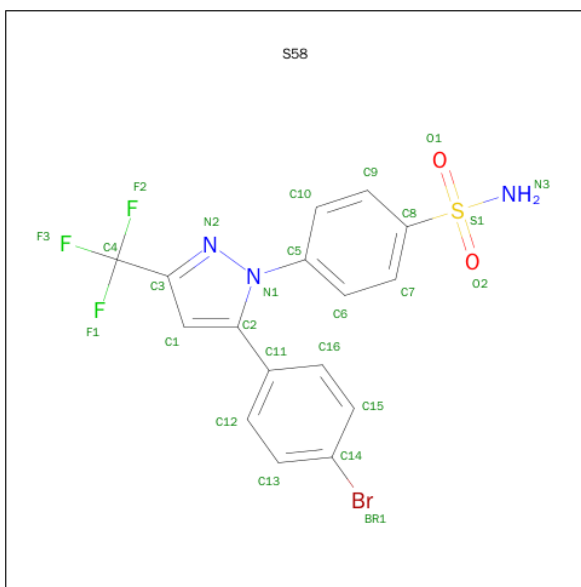
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is 1-PHENYLSULFONAMIDE-3-TRIFLUOROMETHYL-5-PARABROMOPHENYLPYRAZOLE (three-letter code: S58) (formula:  $C_{16}H_{11}BrF_3N_3O_2S$ ).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	F	N	O	S		
4	A	1	26	1	16	3	3	2	1	0	0
4	B	1	26	1	16	3	3	2	1	0	0



ARG SER THR GLU LEU	I539	F470	S403	E322	L246	P172	W100
	S471	S471	F404	W323	F247	D173	M101
	L472	L472	R405	L328	K248	S174	I102
	K473	K473	Q406	F329	K251	E176	N103
	P474	P474	Y409	Q330	L252	V177	N104
	Y475	Y475	R410	T331	K253	L178	N105
	T476	T476	M411	S332	Y254	E179	I105A
	S477	S477	S412	K333	Q255	K180	P106
	F478	F478	I413	L334	P263	V181	F107
	E479	E479	L414	L337	P264	L182	L108
	T482	T482	H417	L341	P265	L183	M109
	G483	G483	G418	T342	V266	R184	S110
	E484	E484	L419	K342			L111
	K485	K485	T420	L343	T269	P189	M112
	A488	A488	Q421	V344	Q270	D190	M113
	A489	A489	F422	L345	V271	P191	K114
	E490	E490	V423			Q192	Y115
	A493	A493	E424	Y348	L274	G193	V116
	G494	G494	S425	Y349	Y275	S194	L117
	L495	L495	F426	Q350	P276	M195	T118
	Y495	Y495	T427	K351	P277	M196	S119
	S496	S496	R428	L352	H278	M197	R120
	D497	D497	Q429		L279	F198	
	I498	I498	I430	Y355	P280		L123
	D499	D499	A431	H356		A202	I124
	N500	N500	F357	F357	L283		D125
	M501	M501	K358	K358	Q284	F205	S126
			V434	L359	F285	T206	P127
			A435	K360	A286	H207	Y130
	Y504	Y504	G436		G287	Q208	M131
PRO	P505	P505	G437	L365	G288	F209	V132
GLU	A506	A506	R438	L366	Q289	F210	H133
PRO	L507	L507	N439	F367	E290	K211	Y134
THR	L508	L508		K368	V291	T212	G135
LYS	V509	V509	I442	Q369	F292		Y136
THR	E510	E510	A443	Q370	G293		K137
ALA	V511	V511	V444	F371	L294		S138
THR	P512	P512	Q445		V295		M139
ILE	R513	R513	A446		P296		
ASN	P514	P514	V447	K376	G297		N144
ALA				L377	H226		
SER	I517	I517		A378	L298	G227	
ALA	P518	P518	S451	S379	M299	V228	Y147
SER	G519	G519	I452	E380	M300	D229	Y148
HIS	E520	E520	D453	F381		L230	T149
SER	T521	T521	Q454	K382	T303	M231	R150
ARG	M522	M522	S455			H232	A151
LEU	V523	V523	R456	Y385	L306	L233	L152
ASP	E524	E524	E457		R307		P153
ASP	L525	L525	M458	H388	E308	E236	
ILE	G526	G526	R459	P389	H309	T237	A156
ASN	A527	A527	Y460		Q310	L238	C159
PRO	P528	P528		K396	R311	D239	P160
THR	F529	F529	L463	L397		R240	
VAL	S530	S530	M464		I315	Q241	G164
LEU				E398	L316	H242	V165
ILE	L534	L534	R467	Q400	H320	L243	
LYS			K468	E401			
ARG	P538	P538	R469	Y402	P321	R245	L171

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.17Å 132.81Å 122.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	88.5 (8.00-2.80)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.220 , 0.309	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9168	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, NAG, S58

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	0.65	0/4600	0.84	1/6237 (0.0%)
1	B	0.65	1/4600 (0.0%)	0.85	2/6237 (0.0%)
All	All	0.65	1/9200 (0.0%)	0.85	3/12474 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	479	GLU	CB-CG	5.55	1.62	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-C	5.54	125.97	111.00
1	B	287	VAL	N-CA-C	5.29	125.28	111.00
1	B	437	GLY	N-CA-C	-5.17	100.17	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4375	324	0
1	B	4473	0	4375	301	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	42	0	39	1	0
2	B	42	0	39	0	0
3	A	43	0	30	2	0
3	B	43	0	30	1	0
4	A	26	0	11	3	0
4	B	26	0	11	2	0
All	All	9168	0	8910	607	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 34.

All (607) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:HD22	1:A:411:ASN:HB2	1.32	1.11
1:B:280:PRO:HD2	1:B:283:LEU:HD23	1.35	1.09
1:A:279:ILE:HG23	1:A:283:LEU:HG	1.32	1.08
1:B:279:ILE:HG23	1:B:283:LEU:HG	1.37	1.07
1:A:280:PRO:HD2	1:A:283:LEU:HD23	1.41	1.02
1:B:283:LEU:HD22	1:B:411:ASN:HB2	1.39	1.00
1:B:156:ALA:HB3	1:B:159:CYS:SG	2.01	0.99
1:A:156:ALA:HB3	1:A:159:CYS:SG	2.03	0.99
1:B:75:LEU:HD11	1:B:79:LYS:HE2	1.50	0.94
1:A:75:LEU:HD11	1:A:79:LYS:HE2	1.57	0.86
1:B:208:GLN:NE2	1:B:228:VAL:HA	1.90	0.86
1:A:208:GLN:NE2	1:A:228:VAL:HA	1.92	0.84
1:B:283:LEU:HB2	1:B:411:ASN:ND2	1.93	0.83
1:A:124:ILE:HD11	1:A:528:PRO:HB3	1.61	0.82
1:B:341:ILE:HG23	1:B:534:LEU:HD12	1.62	0.82
1:A:191:PRO:HD2	1:A:433:ARG:HG3	1.60	0.82
1:A:104:ASN:ND2	1:A:358:LYS:HB2	1.97	0.80
1:B:104:ASN:ND2	1:B:358:LYS:HB2	1.98	0.79
1:A:341:ILE:HG23	1:A:534:LEU:HD12	1.64	0.79
1:A:283:LEU:HB2	1:A:411:ASN:ND2	1.97	0.79
1:A:294:LEU:HA	1:A:409:TYR:HB3	1.63	0.78
1:B:190:ASP:HB2	1:B:432:GLY:O	1.84	0.77
1:B:530:SER:O	1:B:534:LEU:HD23	1.86	0.76
1:A:190:ASP:HB2	1:A:432:GLY:O	1.86	0.75
1:B:280:PRO:CD	1:B:283:LEU:HD23	2.13	0.74
1:B:124:ILE:HD11	1:B:528:PRO:HB3	1.69	0.74
1:B:41:CYS:SG	1:B:47:CYS:HB2	2.28	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:GLU:HG2	1:B:52:PHE:H	1.51	0.74
1:A:283:LEU:CD2	1:A:411:ASN:HB2	2.15	0.74
1:A:322:GLU:HG2	1:B:52:PHE:N	2.02	0.74
1:B:294:LEU:HA	1:B:409:TYR:HB3	1.69	0.73
1:A:105(A):ILE:HG22	1:A:108:LEU:H	1.52	0.73
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.70	0.72
1:A:52:PHE:H	1:B:322:GLU:HG2	1.54	0.72
1:B:279:ILE:HG13	1:B:283:LEU:HD21	1.71	0.72
1:A:52:PHE:N	1:B:322:GLU:HG2	2.05	0.72
1:A:518:PHE:CD1	1:A:522:MET:HG2	2.25	0.72
1:A:470:PHE:CD1	1:A:525:LEU:HD22	2.24	0.72
1:B:105(A):ILE:HG22	1:B:108:LEU:H	1.53	0.72
1:A:41:CYS:SG	1:A:47:CYS:HB2	2.29	0.72
1:B:244:LEU:HD23	1:B:271:VAL:HG11	1.70	0.72
1:B:518:PHE:CD1	1:B:522:MET:HG2	2.24	0.71
1:A:303:THR:O	1:A:307:ARG:HD3	1.91	0.71
1:A:194:SER:OG	1:A:351:HIS:HE1	1.73	0.71
1:B:295:VAL:HB	1:B:298:LEU:CD2	2.20	0.71
1:A:283:LEU:O	1:A:283:LEU:HD12	1.91	0.70
1:B:388:HIS:CE1	1:B:447:VAL:HG11	2.26	0.70
1:B:283:LEU:HB2	1:B:411:ASN:CG	2.11	0.70
1:B:276:PRO:HD2	1:B:279:ILE:HD13	1.73	0.70
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.73	0.70
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.27	0.70
1:A:530:SER:O	1:A:534:LEU:HD23	1.91	0.69
1:B:303:THR:O	1:B:307:ARG:HD3	1.92	0.69
1:A:244:LEU:HD23	1:A:271:VAL:HG11	1.73	0.69
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.75	0.69
1:A:81:LEU:HD12	1:A:81:LEU:O	1.93	0.69
1:B:578:THR:HG22	1:B:579:SER:N	2.07	0.69
1:B:315:ILE:HG21	1:B:558:ILE:HD11	1.76	0.69
1:A:110:SER:HB2	1:A:365:LEU:HD21	1.75	0.68
1:B:470:PHE:CD1	1:B:525:LEU:HD22	2.29	0.68
1:B:283:LEU:CD2	1:B:411:ASN:HB2	2.21	0.68
1:A:578:THR:HG22	1:A:579:SER:N	2.08	0.68
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.77	0.67
1:A:150:ARG:NH2	1:A:458:MET:O	2.27	0.67
1:A:120:ARG:HG3	1:A:120:ARG:HH11	1.60	0.67
1:A:105(A):ILE:HD12	1:A:108:LEU:HD12	1.75	0.67
1:A:283:LEU:HB2	1:A:411:ASN:CG	2.15	0.67
1:A:279:ILE:HG13	1:A:283:LEU:HD21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.25	0.67
1:B:160:PRO:HG2	1:B:165:VAL:HA	1.77	0.67
1:A:482:THR:HG22	1:A:509:VAL:CG1	2.25	0.66
1:B:385:TYR:CE2	4:B:701:S58:BR1	3.04	0.66
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.61	0.66
1:B:192:GLN:OE1	1:B:517:ILE:HG22	1.96	0.66
1:B:205:PHE:CE1	1:B:344:VAL:HG21	2.31	0.66
1:A:427:THR:HB	1:A:428:ARG:NH1	2.10	0.66
1:A:123:LEU:O	1:A:469:ARG:NH2	2.29	0.66
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	1.76	0.66
1:A:485:LYS:HA	1:A:488:ALA:HB3	1.77	0.66
1:A:192:GLN:OE1	1:A:517:ILE:HG22	1.95	0.66
1:A:152:LEU:HD23	1:A:153:PRO:HD2	1.78	0.66
1:B:574:GLY:O	1:B:576:PRO:HD3	1.94	0.66
1:A:124:ILE:HD11	1:A:528:PRO:CB	2.26	0.66
1:B:274:ILE:HD12	1:B:291:VAL:HG23	1.78	0.66
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.60	0.65
1:B:400:GLN:OE1	1:B:400:GLN:HA	1.96	0.65
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.31	0.65
1:A:173:ASP:HB3	1:A:176:GLU:HB2	1.78	0.65
1:B:175:LYS:HE3	1:B:175:LYS:HA	1.78	0.65
1:A:388:HIS:CE1	1:A:447:VAL:HG11	2.31	0.65
1:A:568:ILE:CG2	1:A:576:PRO:HD2	2.26	0.65
1:B:81:LEU:O	1:B:81:LEU:HD12	1.96	0.65
1:A:85:THR:O	1:A:89:VAL:HG23	1.96	0.65
1:A:279:ILE:HG23	1:A:283:LEU:CG	2.19	0.65
1:B:472:LEU:HD21	1:B:524:GLU:HG3	1.78	0.64
1:B:182:LEU:O	1:B:438:ARG:HA	1.97	0.64
1:B:568:ILE:CG2	1:B:576:PRO:HD2	2.27	0.64
1:B:283:LEU:HD12	1:B:283:LEU:O	1.97	0.64
1:B:295:VAL:HB	1:B:298:LEU:HD23	1.79	0.64
1:A:264:PRO:HG2	1:A:286:ALA:HB3	1.80	0.64
1:A:454:GLN:HA	1:A:457:GLU:HG3	1.80	0.64
1:A:191:PRO:CD	1:A:433:ARG:HG3	2.27	0.64
1:B:48:MET:HE3	1:B:49:SER:H	1.62	0.64
1:A:160:PRO:HG2	1:A:165:VAL:HA	1.78	0.64
1:A:280:PRO:CD	1:A:283:LEU:HD23	2.23	0.64
1:A:574:GLY:O	1:A:576:PRO:HD3	1.97	0.64
1:A:463:LEU:O	1:A:467:ARG:HG3	1.98	0.64
1:B:244:LEU:CD2	1:B:271:VAL:HG11	2.27	0.64
1:A:105(A):ILE:HB	1:A:108:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:ASP:HB3	1:B:176:GLU:HB2	1.80	0.63
1:A:548:SER:OG	1:B:58:ASP:HB2	1.99	0.63
1:B:477:SER:HB2	1:B:479:GLU:OE1	1.98	0.63
1:B:500:VAL:HG12	1:B:500:VAL:O	1.99	0.63
1:A:107:PHE:N	1:A:107:PHE:CD1	2.67	0.63
1:B:482:THR:HG22	1:B:509:VAL:CG1	2.29	0.63
1:A:458:MET:CE	1:A:460:TYR:HE1	2.12	0.62
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.34	0.62
1:B:479:GLU:HG3	1:B:488:ALA:HB1	1.80	0.62
1:A:52:PHE:CD1	1:B:322:GLU:HB3	2.35	0.62
1:A:359:LEU:HD11	4:A:701:S58:F1	1.90	0.62
1:A:306:LEU:HD23	1:A:306:LEU:O	2.00	0.62
1:A:205:PHE:CE1	1:A:344:VAL:HG21	2.34	0.62
1:B:420:THR:OG1	1:B:573:LYS:HB3	1.99	0.61
1:A:573:LYS:HG3	1:A:574:GLY:N	2.14	0.61
1:A:295:VAL:HB	1:A:298:LEU:CD2	2.30	0.61
1:B:107:PHE:N	1:B:107:PHE:CD1	2.66	0.61
1:A:315:ILE:HG21	1:A:558:ILE:HD11	1.80	0.61
1:A:96:PHE:CD1	1:A:96:PHE:N	2.67	0.61
1:B:124:ILE:HD11	1:B:528:PRO:CB	2.31	0.61
1:B:110:SER:HB2	1:B:365:LEU:HD21	1.82	0.61
1:A:105:ASN:O	1:A:106:PRO:HD3	1.99	0.61
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.36	0.61
1:B:105(A):ILE:CG2	1:B:108:LEU:HB2	2.30	0.61
1:B:397:ILE:HA	1:B:425:SER:HB3	1.83	0.61
1:A:279:ILE:CG2	1:A:284:GLN:HG2	2.31	0.61
1:B:51:GLY:O	1:B:52:PHE:HB2	2.01	0.61
1:B:485:LYS:HA	1:B:488:ALA:HB3	1.83	0.61
1:A:58:ASP:HB2	1:B:548:SER:OG	2.00	0.61
1:A:208:GLN:HE21	1:A:228:VAL:HA	1.66	0.61
1:B:150:ARG:NH2	1:B:458:MET:O	2.33	0.61
1:B:96:PHE:N	1:B:96:PHE:CD1	2.69	0.61
1:A:60:THR:HG22	1:A:61:ARG:HG3	1.83	0.60
1:B:171:LEU:HD23	1:B:456:ARG:HE	1.65	0.60
1:A:420:THR:OG1	1:A:573:LYS:HB3	2.02	0.60
1:A:48:MET:HE3	1:A:49:SER:H	1.66	0.60
1:B:573:LYS:HG3	1:B:574:GLY:N	2.17	0.60
1:A:64:PHE:CE2	1:A:72:PRO:HB3	2.36	0.60
1:B:458:MET:CE	1:B:460:TYR:HE1	2.15	0.60
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.83	0.60
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:SER:OG	1:B:351:HIS:HE1	1.84	0.60
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.67	0.59
1:A:477:SER:HB2	1:A:479:GLU:OE1	2.01	0.59
1:A:388:HIS:HB3	1:A:444:VAL:HG11	1.84	0.59
1:B:458:MET:HE3	1:B:460:TYR:HE1	1.67	0.59
1:A:414:LEU:HA	1:A:422:PHE:CE2	2.38	0.59
1:A:333:LYS:O	1:A:337:ILE:HG13	2.03	0.59
1:B:333:LYS:O	1:B:337:ILE:HG13	2.03	0.59
1:B:482:THR:HG22	1:B:509:VAL:HG13	1.85	0.59
1:A:182:LEU:O	1:A:438:ARG:HA	2.02	0.58
1:A:104:ASN:HD21	1:A:358:LYS:HB2	1.67	0.58
1:B:388:HIS:HB3	1:B:444:VAL:HG11	1.85	0.58
1:A:197:MET:CE	1:A:423:VAL:HG13	2.32	0.58
1:A:419:LEU:O	1:A:423:VAL:HG23	2.02	0.58
1:B:427:THR:HB	1:B:428:ARG:NH1	2.18	0.58
1:A:51:GLY:O	1:A:52:PHE:HB2	2.01	0.58
1:B:91:TYR:O	1:B:95:HIS:HD2	1.87	0.58
1:B:60:THR:HG22	1:B:61:ARG:HG3	1.86	0.58
1:B:64:PHE:CE2	1:B:72:PRO:HB3	2.38	0.58
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.38	0.58
1:A:175:LYS:HE3	1:A:175:LYS:HA	1.86	0.58
1:A:418:GLY:O	1:A:422:PHE:HB2	2.03	0.58
1:B:280:PRO:HD2	1:B:283:LEU:CD2	2.24	0.57
1:A:352:LEU:HD11	1:A:518:PHE:CE2	2.39	0.57
1:B:123:LEU:O	1:B:469:ARG:NH2	2.36	0.57
1:B:85:THR:O	1:B:89:VAL:HG23	2.04	0.57
1:A:458:MET:HE3	1:A:460:TYR:HE1	1.68	0.57
1:A:424:GLU:O	1:A:428:ARG:HD2	2.05	0.57
1:A:500:VAL:HG12	1:A:500:VAL:O	2.04	0.57
1:A:525:LEU:O	1:A:528:PRO:HD2	2.04	0.57
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.39	0.57
1:B:264:PRO:HG2	1:B:286:ALA:HB3	1.86	0.57
1:A:398:GLU:O	1:A:399:ASP:HB3	2.04	0.57
1:B:525:LEU:O	1:B:528:PRO:HD2	2.04	0.57
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.39	0.57
1:B:389:PRO:HG2	1:B:508:LEU:HD22	1.87	0.57
1:A:509:VAL:HG12	1:A:510:GLU:N	2.20	0.57
1:A:320:HIS:HB3	1:A:323:TRP:CG	2.40	0.57
1:B:463:LEU:O	1:B:467:ARG:HG3	2.05	0.57
1:B:513:ARG:HH21	1:B:520:GLU:HG3	1.69	0.57
1:A:105(A):ILE:CG2	1:A:108:LEU:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:SER:HB2	1:A:405:LYS:HZ2	1.69	0.57
1:A:397:ILE:HA	1:A:425:SER:HB3	1.86	0.57
1:A:197:MET:HG3	1:A:578:THR:CG2	2.35	0.56
1:A:87:ASN:C	1:A:89:VAL:H	2.08	0.56
1:A:171:LEU:HD23	1:A:456:ARG:HE	1.70	0.56
1:B:124:ILE:N	1:B:124:ILE:HD12	2.20	0.56
1:B:105(A):ILE:HB	1:B:108:LEU:HB2	1.87	0.56
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.21	0.56
1:B:43:ASN:O	1:B:44:ARG:HB2	2.04	0.56
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.87	0.56
1:B:279:ILE:CG2	1:B:284:GLN:HG2	2.34	0.56
1:A:194:SER:OG	1:A:351:HIS:CE1	2.58	0.56
1:A:127:PRO:HD2	1:B:543:GLN:HE22	1.71	0.56
1:A:97:LYS:HG3	1:A:356:HIS:CD2	2.40	0.56
1:B:104:ASN:HD21	1:B:358:LYS:HB2	1.71	0.56
1:A:295:VAL:HB	1:A:298:LEU:HD23	1.88	0.56
1:B:208:GLN:HE21	1:B:228:VAL:HA	1.67	0.56
1:A:198:PHE:HZ	1:A:352:LEU:HD13	1.71	0.56
1:B:578:THR:CG2	1:B:579:SER:N	2.69	0.56
1:A:295:VAL:HG12	1:A:297:GLY:H	1.71	0.56
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.88	0.55
1:B:185:ARG:HH21	1:B:438:ARG:HD3	1.70	0.55
1:B:306:LEU:O	1:B:306:LEU:HD23	2.07	0.55
1:A:46:GLU:OE2	1:B:546:LYS:HD2	2.06	0.55
1:B:103:VAL:HG11	1:B:112:ILE:HG13	1.89	0.55
1:A:568:ILE:HG22	1:A:576:PRO:HD2	1.88	0.55
1:B:74:PHE:O	1:B:77:ARG:HB2	2.06	0.55
1:B:352:LEU:HD11	1:B:518:PHE:CE2	2.42	0.55
1:A:124:ILE:N	1:A:124:ILE:HD12	2.21	0.55
1:A:112:ILE:HB	1:A:357:PHE:CZ	2.42	0.55
1:B:105:ASN:O	1:B:106:PRO:HD3	2.06	0.55
1:A:578:THR:CG2	1:A:579:SER:N	2.69	0.54
1:A:482:THR:HG22	1:A:509:VAL:HG13	1.87	0.54
1:B:458:MET:HE3	1:B:460:TYR:CE1	2.42	0.54
1:A:344:VAL:O	1:A:349:VAL:HG23	2.07	0.54
1:A:148:TYR:HD1	1:A:377:ILE:HG13	1.72	0.54
1:A:58:ASP:OD2	1:B:546:LYS:HD3	2.08	0.54
1:A:94:THR:O	1:A:356:HIS:ND1	2.40	0.54
1:B:509:VAL:HG12	1:B:510:GLU:N	2.23	0.54
1:A:120:ARG:HG3	1:A:120:ARG:NH1	2.23	0.54
1:B:295:VAL:HB	1:B:298:LEU:HD22	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HD22	1:B:183:LEU:HG	1.88	0.54
1:B:419:LEU:O	1:B:423:VAL:HG23	2.07	0.54
1:B:87:ASN:C	1:B:89:VAL:H	2.11	0.54
1:A:178:LEU:HD22	1:A:183:LEU:HG	1.90	0.54
1:B:252:LEU:O	1:B:310:GLN:NE2	2.41	0.54
1:A:578:THR:HG22	1:A:579:SER:H	1.72	0.54
1:B:176:GLU:OE1	1:B:180:LYS:HE3	2.08	0.54
1:A:279:ILE:CG2	1:A:283:LEU:HG	2.23	0.54
1:A:134:TYR:HB3	1:A:136:TYR:O	2.08	0.54
1:A:385:TYR:CE2	4:A:701:S58:BR1	3.16	0.54
1:B:197:MET:HG3	1:B:578:THR:CG2	2.38	0.54
1:A:108:LEU:O	1:A:112:ILE:HG12	2.08	0.53
1:B:197:MET:CE	1:B:423:VAL:HG13	2.38	0.53
1:B:320:HIS:HB3	1:B:323:TRP:CG	2.43	0.53
1:B:230:LEU:HG	1:B:337:ILE:HG12	1.91	0.53
1:B:417:HIS:HB3	1:B:421:GLN:O	2.09	0.53
1:A:400:GLN:OE1	1:A:400:GLN:HA	2.08	0.53
1:A:582:VAL:O	1:A:582:VAL:HG13	2.09	0.53
1:A:424:GLU:HA	1:A:428:ARG:NH1	2.24	0.53
1:A:463:LEU:HD21	1:A:475:TYR:HD2	1.73	0.53
1:B:418:GLY:O	1:B:422:PHE:HB2	2.08	0.53
1:B:424:GLU:HA	1:B:428:ARG:NH1	2.23	0.53
1:B:95:HIS:HB2	1:B:96:PHE:CE1	2.44	0.53
1:A:103:VAL:HG11	1:A:112:ILE:HG13	1.90	0.53
1:B:148:TYR:HD1	1:B:377:ILE:HG13	1.74	0.53
1:B:133:HIS:ND1	1:B:147:TYR:HE2	2.07	0.53
1:B:295:VAL:HG12	1:B:297:GLY:H	1.73	0.53
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.43	0.52
1:B:279:ILE:HG23	1:B:283:LEU:CG	2.25	0.52
1:B:173:ASP:OD1	1:B:175:LYS:HB3	2.10	0.52
1:A:46:GLU:O	1:A:57:CYS:HA	2.10	0.52
1:B:276:PRO:O	1:B:279:ILE:HB	2.09	0.52
1:A:513:ARG:HH21	1:A:520:GLU:HG3	1.73	0.52
1:A:274:ILE:HD12	1:A:291:VAL:HG23	1.92	0.52
1:A:197:MET:HE2	1:A:423:VAL:HG13	1.91	0.52
1:A:574:GLY:O	1:A:576:PRO:CD	2.58	0.52
1:B:479:GLU:HG2	1:B:485:LYS:HD3	1.92	0.52
1:B:194:SER:OG	1:B:351:HIS:CE1	2.63	0.52
1:B:114:LYS:O	1:B:118:THR:HG23	2.09	0.52
1:A:185:ARG:HH21	1:A:438:ARG:HD3	1.74	0.52
1:A:294:LEU:HD22	1:A:409:TYR:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:O	1:A:117:LEU:HB2	2.10	0.52
1:B:105(A):ILE:CD1	1:B:108:LEU:HD12	2.40	0.52
1:A:276:PRO:O	1:A:279:ILE:HB	2.10	0.51
1:B:85:THR:HB	1:B:86:PRO:HD2	1.90	0.51
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.92	0.51
1:A:142:PHE:O	1:A:376:ARG:NH2	2.37	0.51
1:A:151:ALA:HB3	1:A:380:GLU:HG3	1.92	0.51
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.92	0.51
1:A:150:ARG:HD2	1:A:380:GLU:OE1	2.10	0.51
1:A:246:LEU:O	1:A:247:PHE:HB2	2.11	0.51
1:A:283:LEU:HD13	1:A:411:ASN:CA	2.41	0.51
1:A:266:VAL:O	1:A:266:VAL:HG12	2.09	0.51
1:B:276:PRO:HD2	1:B:279:ILE:CD1	2.40	0.51
1:A:458:MET:CE	1:A:460:TYR:CE1	2.93	0.51
1:A:458:MET:HE3	1:A:460:TYR:CE1	2.45	0.51
1:B:458:MET:CE	1:B:460:TYR:CE1	2.93	0.51
1:A:403:SER:HB2	1:A:405:LYS:NZ	2.25	0.51
1:B:279:ILE:HG22	1:B:284:GLN:HG2	1.92	0.51
4:B:701:S58:H10	4:B:701:S58:C11	2.41	0.51
1:B:152:LEU:HD23	1:B:153:PRO:HD2	1.92	0.51
1:B:280:PRO:O	1:B:283:LEU:HB3	2.11	0.51
1:B:252:LEU:HD22	1:B:309:HIS:CG	2.46	0.51
1:A:43:ASN:O	1:A:44:ARG:HB2	2.09	0.51
1:B:479:GLU:HB3	1:B:485:LYS:HE2	1.92	0.51
1:A:148:TYR:CD1	1:A:377:ILE:HG13	2.45	0.51
1:B:46:GLU:O	1:B:57:CYS:HA	2.11	0.50
1:A:435:ALA:O	1:A:512:PRO:HG3	2.10	0.50
1:A:173:ASP:O	1:A:177:VAL:HG23	2.11	0.50
1:A:105(A):ILE:CD1	1:A:108:LEU:HD12	2.41	0.50
1:B:424:GLU:O	1:B:428:ARG:HD2	2.11	0.50
1:B:178:LEU:HD23	1:B:182:LEU:HB2	1.94	0.50
1:B:176:GLU:O	1:B:180:LYS:HG3	2.11	0.50
1:A:232:HIS:ND1	1:A:233:ILE:HG13	2.27	0.50
1:A:546:LYS:HD3	1:B:58:ASP:OD2	2.11	0.50
1:A:92:ILE:HA	1:A:96:PHE:HE1	1.76	0.50
1:B:379:SER:HB3	1:B:460:TYR:OH	2.12	0.50
1:B:582:VAL:O	1:B:582:VAL:HG13	2.11	0.50
1:B:463:LEU:HD21	1:B:475:TYR:HD2	1.77	0.50
1:A:578:THR:CG2	1:A:579:SER:H	2.24	0.50
1:B:574:GLY:O	1:B:576:PRO:CD	2.58	0.50
1:B:92:ILE:HA	1:B:96:PHE:HE1	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:TYR:HB3	1:B:136:TYR:O	2.11	0.50
1:A:184:ARG:HB2	1:A:439:ASN:C	2.32	0.50
1:B:379:SER:O	1:B:382:ASN:N	2.45	0.50
1:A:252:LEU:O	1:A:310:GLN:NE2	2.44	0.50
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.27	0.50
1:B:242:HIS:ND1	1:B:247:PHE:HZ	2.10	0.50
1:A:279:ILE:HG22	1:A:284:GLN:HG2	1.94	0.50
1:A:97:LYS:HG3	1:A:356:HIS:NE2	2.26	0.50
1:A:379:SER:HB3	1:A:460:TYR:OH	2.12	0.49
1:A:320:HIS:HE1	1:A:551:GLY:O	1.95	0.49
1:A:230:LEU:HD23	1:A:230:LEU:N	2.26	0.49
1:A:190:ASP:OD1	1:A:517:ILE:HB	2.12	0.49
1:A:91:TYR:O	1:A:95:HIS:HD2	1.95	0.49
1:B:72:PRO:HB2	1:B:76:THR:HB	1.94	0.49
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.47	0.49
1:B:345:ILE:HD11	1:B:534:LEU:HG	1.94	0.49
1:B:103:VAL:HG22	1:B:108:LEU:HD13	1.95	0.49
1:B:193:GLY:O	1:B:582:VAL:N	2.41	0.49
1:A:252:LEU:HD22	1:A:309:HIS:CG	2.47	0.49
1:B:246:LEU:O	1:B:247:PHE:HB2	2.12	0.49
1:B:414:LEU:HA	1:B:422:PHE:CE2	2.48	0.49
1:B:148:TYR:CD1	1:B:377:ILE:HG13	2.47	0.49
1:B:134:TYR:HD1	1:B:136:TYR:CE1	2.30	0.49
1:A:134:TYR:HD1	1:A:136:TYR:CE1	2.31	0.49
1:A:543:GLN:HE22	1:B:127:PRO:HD2	1.78	0.49
1:B:344:VAL:O	1:B:349:VAL:HG23	2.13	0.49
1:B:413:ILE:O	1:B:422:PHE:HE2	1.96	0.49
1:A:389:PRO:HG2	1:A:508:LEU:HD22	1.94	0.49
1:A:280:PRO:O	1:A:283:LEU:HB3	2.13	0.49
1:B:113:MET:O	1:B:117:LEU:HB2	2.12	0.49
1:B:294:LEU:HD22	1:B:409:TYR:CD2	2.47	0.49
1:A:176:GLU:O	1:A:180:LYS:HG3	2.12	0.49
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.42	0.49
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	0.49
1:B:197:MET:HE2	1:B:423:VAL:HG13	1.94	0.49
1:B:132:VAL:HG21	1:B:219:GLY:HA3	1.95	0.49
1:B:94:THR:O	1:B:356:HIS:ND1	2.46	0.49
1:A:417:HIS:HB3	1:A:421:GLN:O	2.13	0.48
1:A:421:GLN:OE1	1:A:424:GLU:HB2	2.13	0.48
1:B:308:GLU:OE1	1:B:311:ARG:HD3	2.13	0.48
1:B:92:ILE:HA	1:B:96:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:NH1	1:B:120:ARG:HG3	2.28	0.48
1:A:171:LEU:HB3	1:A:456:ARG:HH21	1.78	0.48
1:A:131:ASN:ND2	1:A:147:TYR:CD2	2.81	0.48
1:A:92:ILE:HA	1:A:96:PHE:CE1	2.48	0.48
1:B:454:GLN:O	1:B:457:GLU:N	2.46	0.48
1:B:108:LEU:O	1:B:112:ILE:HG12	2.12	0.48
1:B:490:GLU:O	1:B:493:ALA:HB3	2.14	0.48
1:A:85:THR:HB	1:A:86:PRO:HD2	1.95	0.48
1:B:230:LEU:N	1:B:230:LEU:HD23	2.27	0.48
1:A:142:PHE:CD1	1:A:142:PHE:C	2.87	0.48
1:B:398:GLU:O	1:B:399:ASP:HB3	2.13	0.48
1:A:447:VAL:HG13	3:A:682:HEM:HBA2	1.94	0.48
1:A:251:LYS:HD3	1:A:310:GLN:HG3	1.96	0.48
1:A:197:MET:HG3	1:A:578:THR:HG23	1.94	0.48
1:B:173:ASP:O	1:B:177:VAL:HG23	2.13	0.48
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.29	0.48
1:B:184:ARG:HB2	1:B:439:ASN:C	2.34	0.48
1:A:95:HIS:HB2	1:A:96:PHE:CE1	2.49	0.48
1:B:331:THR:O	1:B:334:LEU:HB2	2.13	0.48
1:B:113:MET:HG2	1:B:360:LYS:HB3	1.95	0.48
1:A:133:HIS:ND1	1:A:147:TYR:HE2	2.12	0.48
1:A:103:VAL:HG22	1:A:108:LEU:HD13	1.96	0.47
1:A:546:LYS:HD2	1:B:46:GLU:OE2	2.14	0.47
1:B:255:GLN:HG2	1:B:263:PRO:O	2.14	0.47
1:B:546:LYS:HB2	1:B:547:PRO:HD2	1.95	0.47
4:A:701:S58:H10	4:A:701:S58:C11	2.44	0.47
1:A:479:GLU:HG3	1:A:488:ALA:HB1	1.95	0.47
1:A:85:THR:OG1	1:A:88:THR:HG23	2.15	0.47
1:A:582:VAL:O	1:A:583:GLN:HB2	2.14	0.47
1:B:190:ASP:OD1	1:B:517:ILE:HB	2.14	0.47
1:A:519:GLY:O	1:A:523:VAL:HG23	2.14	0.47
1:B:264:PRO:HB2	1:B:269:THR:HG23	1.96	0.47
1:A:254:TYR:HD2	1:A:310:GLN:HE21	1.61	0.47
1:A:495:TYR:O	1:A:496:SER:HB2	2.14	0.47
1:A:254:TYR:C	1:A:254:TYR:CD1	2.88	0.47
1:A:178:LEU:HD23	1:A:182:LEU:HB2	1.96	0.47
1:A:105(A):ILE:CB	1:A:108:LEU:HB2	2.44	0.47
1:A:264:PRO:HG2	1:A:286:ALA:CB	2.45	0.47
1:B:91:TYR:O	1:B:95:HIS:CD2	2.67	0.47
1:A:72:PRO:HB2	1:A:76:THR:HB	1.95	0.47
1:A:35:PRO:HB2	1:A:55:TYR:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:NH2	1:B:236:GLU:HG2	2.29	0.47
1:A:232:HIS:CE1	1:A:233:ILE:HG13	2.49	0.47
1:A:413:ILE:O	1:A:422:PHE:HE2	1.97	0.47
1:A:454:GLN:O	1:A:457:GLU:N	2.48	0.47
1:A:114:LYS:O	1:A:118:THR:HG23	2.15	0.47
1:B:130:TYR:CE1	1:B:135:GLY:O	2.68	0.47
1:B:403:SER:HB2	1:B:405:LYS:NZ	2.29	0.47
1:B:197:MET:HG3	1:B:578:THR:HG23	1.97	0.47
1:B:133:HIS:ND1	1:B:147:TYR:CE2	2.82	0.47
1:A:495:TYR:CE2	1:A:501:MET:SD	3.07	0.47
1:A:132:VAL:HG21	1:A:219:GLY:HA3	1.97	0.47
1:B:100:TRP:O	1:B:104:ASN:HB2	2.15	0.46
1:A:222:ARG:NH2	1:A:236:GLU:HG2	2.29	0.46
1:B:454:GLN:HA	1:B:457:GLU:HG3	1.96	0.46
1:A:113:MET:HA	1:A:116:VAL:HG13	1.97	0.46
1:A:442:ILE:O	1:A:445:GLN:HG2	2.16	0.46
1:B:254:TYR:CD1	1:B:254:TYR:C	2.88	0.46
1:B:495:TYR:O	1:B:496:SER:HB2	2.16	0.46
1:B:291:VAL:HG22	1:B:294:LEU:HD12	1.98	0.46
1:B:297:GLY:O	1:B:300:MET:HB3	2.14	0.46
1:A:130:TYR:CE1	1:A:135:GLY:O	2.68	0.46
1:A:140:GLU:OE2	1:A:144:ASN:HB2	2.16	0.46
1:A:185:ARG:NE	1:A:438:ARG:HD3	2.27	0.46
1:B:232:HIS:ND1	1:B:233:ILE:HG13	2.30	0.46
1:A:490:GLU:O	1:A:493:ALA:HB3	2.15	0.46
1:A:230:LEU:HG	1:A:337:ILE:HG12	1.97	0.46
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.98	0.46
1:B:402:TYR:OH	1:B:417:HIS:HE1	1.98	0.46
1:A:159:CYS:HB3	1:A:164:GLY:O	2.16	0.46
1:A:548:SER:OG	1:B:58:ASP:CB	2.64	0.46
1:B:513:ARG:O	1:B:514:PRO:O	2.32	0.46
1:A:113:MET:HE3	1:A:117:LEU:HD13	1.96	0.46
1:A:139:TRP:CZ3	1:B:538:PRO:HG2	2.51	0.46
1:B:521:THR:O	1:B:523:VAL:N	2.49	0.46
1:B:151:ALA:HB3	1:B:380:GLU:HG3	1.96	0.46
1:B:232:HIS:CE1	1:B:233:ILE:HG13	2.51	0.46
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.51	0.46
1:B:578:THR:HG22	1:B:579:SER:H	1.78	0.46
1:B:568:ILE:HG22	1:B:576:PRO:HD2	1.98	0.46
1:A:388:HIS:N	1:A:389:PRO:CD	2.79	0.46
1:A:546:LYS:HB2	1:A:547:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:PRO:HB2	1:B:55:TYR:HB3	1.98	0.46
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.98	0.46
1:B:433:ARG:H	1:B:439:ASN:ND2	2.14	0.46
1:B:251:LYS:HD3	1:B:310:GLN:HG3	1.98	0.46
1:A:242:HIS:ND1	1:A:247:PHE:HZ	2.14	0.46
1:B:479:GLU:HG3	1:B:488:ALA:CB	2.45	0.45
1:B:91:TYR:CD1	1:B:95:HIS:CD2	3.03	0.45
1:A:337:ILE:O	1:A:341:ILE:HG13	2.16	0.45
1:B:184:ARG:HA	1:B:438:ARG:O	2.17	0.45
1:A:193:GLY:O	1:A:582:VAL:N	2.46	0.45
1:A:189:PRO:HB2	1:A:430:ILE:HD13	1.98	0.45
1:A:295:VAL:HB	1:A:298:LEU:HD22	1.97	0.45
1:A:240:ARG:CZ	1:A:271:VAL:HG23	2.46	0.45
1:B:578:THR:CG2	1:B:579:SER:H	2.29	0.45
1:A:379:SER:O	1:A:382:ASN:N	2.49	0.45
1:B:240:ARG:CZ	1:B:271:VAL:HG23	2.46	0.45
1:B:507:LEU:HD21	1:B:521:THR:HG22	1.99	0.45
1:A:295:VAL:HG22	1:A:408:LEU:HD22	1.99	0.45
1:A:498:ILE:C	1:A:500:VAL:H	2.20	0.45
1:A:285:PHE:HD2	1:A:299:MET:SD	2.40	0.45
1:B:498:ILE:C	1:B:500:VAL:H	2.19	0.45
1:B:266:VAL:O	1:B:266:VAL:HG12	2.16	0.45
1:B:149:THR:O	1:B:378:ALA:HA	2.17	0.45
1:B:470:PHE:O	1:B:471:SER:HB2	2.17	0.45
1:B:198:PHE:HZ	1:B:352:LEU:HD13	1.79	0.45
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.32	0.45
1:B:468:LYS:HG2	1:B:474:PRO:HG3	1.99	0.45
1:B:283:LEU:HD13	1:B:411:ASN:CA	2.46	0.44
1:B:306:LEU:HD23	1:B:306:LEU:C	2.37	0.44
1:B:417:HIS:HB2	1:B:422:PHE:CD2	2.53	0.44
1:A:403:SER:O	1:A:406:GLN:HG2	2.17	0.44
1:A:283:LEU:HD13	1:A:411:ASN:HA	1.99	0.44
1:A:513:ARG:O	1:A:514:PRO:O	2.35	0.44
1:A:454:GLN:O	1:A:457:GLU:HB2	2.18	0.44
1:B:479:GLU:HG2	1:B:485:LYS:CD	2.47	0.44
1:A:345:ILE:HD11	1:A:534:LEU:HG	1.99	0.44
1:B:434:VAL:HG23	1:B:517:ILE:HD11	2.00	0.44
1:A:105(A):ILE:O	1:A:108:LEU:N	2.50	0.44
1:A:414:LEU:HD11	1:A:419:LEU:HD22	2.00	0.44
1:A:275:TYR:CE2	1:A:284:GLN:HA	2.53	0.44
1:B:182:LEU:CD1	1:B:452:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ASP:CB	1:B:548:SER:OG	2.66	0.44
1:B:171:LEU:HB3	1:B:456:ARG:HH21	1.83	0.44
1:A:230:LEU:HD23	1:A:230:LEU:H	1.83	0.44
1:B:105(A):ILE:CB	1:B:108:LEU:HB2	2.47	0.44
1:A:472:LEU:HD11	1:A:524:GLU:HB2	2.00	0.44
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.65	0.44
1:A:297:GLY:O	1:A:300:MET:HB3	2.18	0.44
1:A:211:LYS:HZ3	1:A:236:GLU:HG3	1.81	0.44
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.86	0.44
1:A:322:GLU:HB3	1:B:52:PHE:CE1	2.53	0.43
1:B:184:ARG:HB2	1:B:439:ASN:HA	1.99	0.43
1:B:185:ARG:NE	1:B:438:ARG:HD3	2.28	0.43
1:A:564:ILE:O	1:A:568:ILE:HD13	2.19	0.43
1:B:222:ARG:HH22	1:B:236:GLU:HG2	1.83	0.43
1:A:184:ARG:NE	1:A:439:ASN:OD1	2.49	0.43
1:B:105(A):ILE:O	1:B:108:LEU:N	2.51	0.43
1:B:131:ASN:ND2	1:B:147:TYR:CD2	2.86	0.43
1:A:184:ARG:HA	1:A:438:ARG:O	2.18	0.43
1:B:403:SER:O	1:B:406:GLN:HG2	2.17	0.43
1:A:131:ASN:ND2	1:A:147:TYR:CG	2.86	0.43
1:A:448:ALA:O	1:A:452:ILE:HG13	2.18	0.43
1:A:222:ARG:HH22	1:A:236:GLU:HG2	1.84	0.43
1:B:435:ALA:O	1:B:512:PRO:HG3	2.18	0.43
1:A:197:MET:HE1	1:A:423:VAL:HG13	2.01	0.43
1:A:306:LEU:HD23	1:A:306:LEU:C	2.39	0.43
1:A:100:TRP:O	1:A:104:ASN:HB2	2.17	0.43
1:B:521:THR:O	1:B:522:MET:C	2.56	0.43
1:B:85:THR:OG1	1:B:88:THR:HG23	2.19	0.43
1:A:242:HIS:HE1	1:A:245:ARG:NH2	2.17	0.43
1:A:40:PRO:HB3	2:A:661:NAG:H62	1.99	0.43
1:B:367:PHE:C	1:B:369:GLN:H	2.22	0.43
1:A:350:GLN:HE22	1:A:358:LYS:HA	1.84	0.43
1:A:87:ASN:O	1:A:89:VAL:N	2.52	0.43
1:B:447:VAL:HG13	3:B:682:HEM:HBA2	2.00	0.42
1:B:185:ARG:NH2	1:B:438:ARG:HD3	2.34	0.42
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.42
1:B:513:ARG:O	1:B:514:PRO:C	2.58	0.42
1:A:308:GLU:O	1:A:309:HIS:C	2.54	0.42
1:B:322:GLU:HG3	1:B:322:GLU:H	1.45	0.42
1:B:564:ILE:O	1:B:568:ILE:HD13	2.19	0.42
1:A:463:LEU:HD21	1:A:475:TYR:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:PRO:HG2	1:B:139:TRP:CZ3	2.54	0.42
1:B:159:CYS:HB3	1:B:164:GLY:O	2.19	0.42
1:A:402:TYR:OH	1:A:417:HIS:HE1	2.02	0.42
1:A:479:GLU:HG3	1:A:485:LYS:HG3	2.00	0.42
1:B:230:LEU:H	1:B:230:LEU:HD23	1.83	0.42
1:A:433:ARG:H	1:A:439:ASN:ND2	2.16	0.42
1:A:453:ASP:O	1:A:457:GLU:HG3	2.19	0.42
1:B:211:LYS:HZ3	1:B:236:GLU:HG3	1.84	0.42
1:A:255:GLN:HG2	1:A:263:PRO:O	2.18	0.42
1:A:93:LEU:HB3	1:A:355:TYR:CD1	2.55	0.42
1:B:451:SER:HB2	1:B:504:TYR:CE2	2.54	0.42
1:A:458:MET:HE2	1:A:460:TYR:HE1	1.82	0.42
1:B:472:LEU:HD11	1:B:524:GLU:HB2	2.02	0.42
1:B:495:TYR:CE2	1:B:501:MET:SD	3.12	0.42
1:A:74:PHE:O	1:A:77:ARG:HB2	2.20	0.42
1:A:458:MET:HE2	1:A:460:TYR:CE1	2.55	0.42
1:A:242:HIS:CE1	1:A:245:ARG:NH2	2.88	0.42
1:A:308:GLU:OE1	1:A:311:ARG:HD3	2.19	0.42
1:A:331:THR:O	1:A:334:LEU:HB2	2.19	0.42
1:B:62:THR:OG1	1:B:63:GLY:N	2.51	0.42
1:A:470:PHE:O	1:A:471:SER:HB2	2.20	0.42
1:B:343:ILE:O	1:B:345:ILE:N	2.53	0.42
1:A:521:THR:O	1:A:523:VAL:N	2.52	0.42
1:A:126:SER:HA	1:A:127:PRO:HA	1.85	0.42
1:B:278:HIS:O	1:B:278:HIS:CD2	2.73	0.42
1:A:105(A):ILE:HG23	1:A:107:PHE:CD2	2.54	0.42
1:B:67:GLU:HG2	1:B:68:ASN:OD1	2.20	0.42
1:B:202:ALA:HB2	1:B:348:TYR:HE1	1.84	0.42
1:B:275:TYR:CE2	1:B:284:GLN:HA	2.55	0.42
1:A:472:LEU:HD22	1:A:520:GLU:CD	2.40	0.42
1:B:582:VAL:O	1:B:583:GLN:HB2	2.20	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE3	2.01	0.42
1:B:500:VAL:CG1	1:B:500:VAL:O	2.67	0.41
1:B:581:ASN:C	1:B:583:GLN:H	2.23	0.41
1:B:453:ASP:O	1:B:457:GLU:HG3	2.19	0.41
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.79	0.41
1:A:65:TYR:CD1	1:A:65:TYR:N	2.88	0.41
1:A:521:THR:O	1:A:522:MET:C	2.58	0.41
1:B:150:ARG:HD2	1:B:380:GLU:OE1	2.19	0.41
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.02	0.41
1:B:189:PRO:HB2	1:B:430:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:HIS:N	1:B:389:PRO:CD	2.84	0.41
1:A:244:LEU:HD21	1:A:271:VAL:HG11	2.01	0.41
1:B:316:LEU:HA	1:B:316:LEU:HD12	1.92	0.41
1:B:557:LYS:HE3	1:B:557:LYS:HA	2.01	0.41
1:A:120:ARG:HB3	1:A:528:PRO:HG3	2.02	0.41
1:B:113:MET:HA	1:B:116:VAL:HG13	2.02	0.41
1:B:370:GLN:O	1:B:371:PHE:HB2	2.20	0.41
1:A:283:LEU:HD13	1:A:411:ASN:CB	2.51	0.41
1:A:97:LYS:HB2	1:A:356:HIS:CE1	2.56	0.41
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.70	0.41
1:A:468:LYS:HG2	1:A:474:PRO:HG3	2.03	0.41
1:B:93:LEU:HB3	1:B:355:TYR:CD1	2.55	0.41
1:A:276:PRO:HD2	1:A:279:ILE:HD13	2.03	0.41
1:A:437:GLY:O	1:A:438:ARG:C	2.58	0.41
1:A:428:ARG:O	1:A:429:GLN:HB2	2.20	0.41
1:A:513:ARG:O	1:A:514:PRO:C	2.59	0.41
1:B:421:GLN:OE1	1:B:424:GLU:HB2	2.20	0.41
1:A:184:ARG:CZ	1:A:187:PHE:HD1	2.34	0.41
1:A:291:VAL:HG22	1:A:294:LEU:HD12	2.02	0.41
1:A:507:LEU:HD21	1:A:521:THR:HG22	2.02	0.41
1:A:479:GLU:HG2	1:A:485:LYS:CE	2.51	0.41
1:A:173:ASP:OD1	1:A:175:LYS:HB3	2.21	0.41
1:A:64:PHE:HD2	1:A:70:THR:O	2.04	0.41
1:B:230:LEU:HB3	1:B:233:ILE:HD12	2.02	0.41
1:A:500:VAL:CG1	1:A:500:VAL:O	2.68	0.41
1:B:195:ASN:HB2	1:B:196:MET:H	1.78	0.41
1:A:518:PHE:CG	1:A:522:MET:HG2	2.56	0.41
1:A:320:HIS:CE1	1:A:551:GLY:O	2.74	0.41
1:A:130:TYR:HB3	1:A:134:TYR:O	2.21	0.41
1:B:97:LYS:HB2	1:B:356:HIS:CE1	2.56	0.41
1:A:110:SER:HB2	1:A:365:LEU:CD2	2.48	0.40
1:A:174:SER:HB3	1:A:456:ARG:NH1	2.36	0.40
1:A:334:LEU:HD13	1:A:549:THR:HG22	2.03	0.40
1:A:182:LEU:CD1	1:A:452:ILE:HD11	2.51	0.40
1:B:112:ILE:HB	1:B:357:PHE:CE1	2.55	0.40
1:B:437:GLY:O	1:B:438:ARG:C	2.58	0.40
1:B:210:PHE:HB3	1:B:382:ASN:ND2	2.35	0.40
1:A:230:LEU:CD1	1:A:336:LEU:HB3	2.51	0.40
1:A:80:LEU:HA	1:A:80:LEU:HD23	1.94	0.40
1:A:91:TYR:O	1:A:95:HIS:CD2	2.73	0.40
1:B:320:HIS:HE1	1:B:551:GLY:O	2.05	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:TRP:HB2	3:A:682:HEM:HAC	2.03	0.40
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.80	0.40
1:A:299:MET:HB2	1:A:299:MET:HE3	1.89	0.40
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.57	0.40
1:B:442:ILE:O	1:B:445:GLN:HB3	2.21	0.40
1:A:67:GLU:HG2	1:A:68:ASN:OD1	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	550/587 (94%)	435 (79%)	84 (15%)	31 (6%)	2	6
1	B	550/587 (94%)	431 (78%)	86 (16%)	33 (6%)	2	5
All	All	1100/1174 (94%)	866 (79%)	170 (16%)	64 (6%)	2	5

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	348	TYR
1	A	398	GLU
1	A	510	GLU
1	A	514	PRO
1	A	573	LYS
1	B	138	SER
1	B	348	TYR
1	B	398	GLU
1	B	459	LYS
1	B	510	GLU
1	B	514	PRO

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Mol	Chain	Res	Type
1	B	573	LYS
1	A	51	GLY
1	A	82	LEU
1	A	96	PHE
1	A	212	THR
1	A	422	PHE
1	A	429	GLN
1	A	459	LYS
1	A	582	VAL
1	B	51	GLY
1	B	82	LEU
1	B	96	PHE
1	B	212	THR
1	B	429	GLN
1	B	554	VAL
1	B	582	VAL
1	A	67	GLU
1	A	329	PHE
1	A	399	ASP
1	A	554	VAL
1	B	67	GLU
1	B	144	ASN
1	B	399	ASP
1	B	422	PHE
1	B	522	MET
1	A	88	THR
1	A	132	VAL
1	A	352	LEU
1	A	496	SER
1	A	499	ASP
1	B	132	VAL
1	B	309	HIS
1	B	329	PHE
1	B	352	LEU
1	B	412	SER
1	A	144	ASN
1	A	522	MET
1	B	44	ARG
1	B	172	PRO
1	B	344	VAL
1	B	380	GLU
1	B	496	SER

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Mol	Chain	Res	Type
1	B	575	CYS
1	A	104	ASN
1	A	172	PRO
1	A	412	SER
1	B	88	THR
1	A	575	CYS
1	B	413	ILE
1	B	287	VAL
1	A	413	ILE
1	A	344	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	493/525 (94%)	439 (89%)	54 (11%)	8	23
1	B	493/525 (94%)	442 (90%)	51 (10%)	9	26
All	All	986/1050 (94%)	881 (89%)	105 (11%)	8	24

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	65	TYR
1	A	71	THR
1	A	96	PHE
1	A	97	LYS
1	A	101	ASN
1	A	107	PHE
1	A	108	LEU
1	A	111	LEU
1	A	116	VAL
1	A	117	LEU
1	A	126	SER
1	A	150	ARG

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Mol	Chain	Res	Type
1	A	152	LEU
1	A	172	PRO
1	A	178	LEU
1	A	232	HIS
1	A	238	LEU
1	A	241	GLN
1	A	245	ARG
1	A	248	LYS
1	A	252	LEU
1	A	253	LYS
1	A	271	VAL
1	A	280	PRO
1	A	283	LEU
1	A	289	GLN
1	A	290	GLU
1	A	291	VAL
1	A	298	LEU
1	A	300	MET
1	A	310	GLN
1	A	316	LEU
1	A	322	GLU
1	A	376	ARG
1	A	377	ILE
1	A	380	GLU
1	A	385	TYR
1	A	389	PRO
1	A	396	ASN
1	A	405	LYS
1	A	412	SER
1	A	422	PHE
1	A	428	ARG
1	A	442	ILE
1	A	463	LEU
1	A	464	ASN
1	A	469	ARG
1	A	484	GLU
1	A	512	PRO
1	A	514	PRO
1	A	528	PRO
1	A	539	ILE
1	A	557	LYS
1	B	38	SER

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Mol	Chain	Res	Type
1	B	65	TYR
1	B	71	THR
1	B	96	PHE
1	B	101	ASN
1	B	107	PHE
1	B	108	LEU
1	B	111	LEU
1	B	116	VAL
1	B	117	LEU
1	B	126	SER
1	B	150	ARG
1	B	152	LEU
1	B	172	PRO
1	B	176	GLU
1	B	178	LEU
1	B	232	HIS
1	B	238	LEU
1	B	241	GLN
1	B	248	LYS
1	B	252	LEU
1	B	253	LYS
1	B	271	VAL
1	B	280	PRO
1	B	283	LEU
1	B	289	GLN
1	B	290	GLU
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	377	ILE
1	B	380	GLU
1	B	385	TYR
1	B	389	PRO
1	B	396	ASN
1	B	405	LYS
1	B	412	SER
1	B	422	PHE
1	B	428	ARG

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Mol	Chain	Res	Type
1	B	442	ILE
1	B	463	LEU
1	B	464	ASN
1	B	469	ARG
1	B	484	GLU
1	B	514	PRO
1	B	539	ILE
1	B	557	LYS

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

Mol	Chain	Res	Type
1	A	43	ASN
1	A	95	HIS
1	A	203	GLN
1	A	278	HIS
1	A	320	HIS
1	A	350	GLN
1	A	351	HIS
1	A	417	HIS
1	A	565	GLN
1	B	43	ASN
1	B	95	HIS
1	B	203	GLN
1	B	278	HIS
1	B	320	HIS
1	B	350	GLN
1	B	351	HIS
1	B	417	HIS
1	B	454	GLN
1	B	543	GLN
1	B	565	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	NAG	A	661	1	14,14,15	0.64	0	15,19,21	0.55	0
2	NAG	A	671	1	14,14,15	0.43	0	15,19,21	0.91	1 (6%)
2	NAG	A	681	1	14,14,15	0.31	0	15,19,21	0.87	1 (6%)
3	HEM	A	682	1	30,50,50	3.11	11 (36%)	24,82,82	2.02	7 (29%)
4	S58	A	701	-	27,28,28	2.48	7 (25%)	40,43,43	2.06	10 (25%)
2	NAG	B	661	1	14,14,15	0.57	0	15,19,21	0.67	0
2	NAG	B	671	1	14,14,15	0.57	0	15,19,21	1.02	1 (6%)
2	NAG	B	681	1	14,14,15	0.68	0	15,19,21	0.80	1 (6%)
3	HEM	B	682	1	30,50,50	2.95	11 (36%)	24,82,82	1.94	7 (29%)
4	S58	B	701	-	27,28,28	2.43	7 (25%)	40,43,43	1.82	9 (22%)

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	S58	A	701	-	-	0/20/20/20	0/3/3/3
2	NAG	B	661	1	-	0/6/23/26	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	B	682	1	-	0/10/54/54	0/0/8/8
4	S58	B	701	-	-	0/20/20/20	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	682	HEM	C3B-C4B	-7.46	1.45	1.51
3	B	682	HEM	C3B-CAB	-7.11	1.38	1.51
3	A	682	HEM	C3B-CAB	-6.89	1.38	1.51
3	A	682	HEM	C3C-CAC	-6.87	1.38	1.51
3	B	682	HEM	C3B-C4B	-6.82	1.45	1.51
3	A	682	HEM	C2D-C3D	-6.78	1.34	1.54
3	B	682	HEM	C2D-C3D	-6.75	1.34	1.54
3	B	682	HEM	C3C-CAC	-6.63	1.38	1.51
3	A	682	HEM	C3D-C4D	-6.05	1.43	1.51
3	B	682	HEM	C3D-C4D	-4.75	1.45	1.51
3	A	682	HEM	C2C-C1C	-4.15	1.44	1.52
4	A	701	S58	C3-N2	-4.11	1.28	1.33
3	B	682	HEM	C2C-C1C	-3.71	1.45	1.52
4	A	701	S58	C1-C2	-3.66	1.32	1.39
4	B	701	S58	BR1-C14	-3.43	1.82	1.90
4	A	701	S58	BR1-C14	-3.31	1.83	1.90
4	B	701	S58	C3-N2	-3.00	1.30	1.33
4	B	701	S58	C1-C2	-2.65	1.34	1.39
3	A	682	HEM	C2B-C1B	-2.15	1.44	1.51
3	B	682	HEM	C2B-C1B	-2.02	1.45	1.51
3	A	682	HEM	C4C-NC	2.06	1.38	1.36
3	B	682	HEM	C1C-NC	2.38	1.38	1.36
3	B	682	HEM	C4C-NC	2.46	1.39	1.36
3	A	682	HEM	C1C-NC	2.49	1.39	1.36
3	B	682	HEM	CBC-CAC	2.50	1.43	1.29
3	A	682	HEM	CBB-CAB	2.66	1.44	1.29
3	B	682	HEM	CBB-CAB	2.68	1.44	1.29
4	A	701	S58	N2-N1	2.80	1.44	1.39
4	A	701	S58	C8-S1	2.81	1.81	1.77
3	A	682	HEM	CBC-CAC	2.88	1.45	1.29
4	B	701	S58	N2-N1	3.78	1.46	1.39
4	B	701	S58	C8-S1	4.41	1.83	1.77
4	A	701	S58	C1-C3	5.83	1.47	1.39
4	B	701	S58	C1-C3	6.12	1.47	1.39
4	B	701	S58	S1-N3	6.52	1.74	1.60
4	A	701	S58	S1-N3	7.22	1.76	1.60



All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	S58	O2-S1-O1	-6.18	110.11	118.80
4	B	701	S58	O2-S1-O1	-5.31	111.34	118.80
2	B	671	NAG	C2-N2-C7	-3.19	118.94	123.04
2	A	671	NAG	C2-N2-C7	-2.93	119.28	123.04
4	B	701	S58	F2-C4-C3	-2.85	107.49	112.55
4	A	701	S58	C1-C2-C11	-2.84	123.39	128.12
4	A	701	S58	F2-C4-C3	-2.62	107.91	112.55
3	B	682	HEM	C3B-CAB-CBB	-2.52	120.60	124.46
4	B	701	S58	C1-C2-C11	-2.47	124.01	128.12
4	A	701	S58	C1-C3-N2	-2.47	107.66	111.53
4	B	701	S58	C1-C3-N2	-2.42	107.73	111.53
3	A	682	HEM	C3B-CAB-CBB	-2.34	120.87	124.46
4	B	701	S58	C5-N1-C2	-2.18	128.00	130.11
2	B	681	NAG	C2-N2-C7	-2.11	120.33	123.04
4	A	701	S58	F3-C4-C3	-2.06	108.90	112.55
2	A	681	NAG	C2-N2-C7	-2.05	120.40	123.04
4	B	701	S58	C11-C2-N1	2.27	127.16	123.23
4	A	701	S58	C2-C1-C3	2.30	107.79	104.81
3	B	682	HEM	CMD-C2D-C3D	2.31	124.55	114.35
4	B	701	S58	C2-C1-C3	2.40	107.92	104.81
3	A	682	HEM	CMD-C2D-C3D	2.55	125.62	114.35
4	A	701	S58	C11-C2-N1	2.61	127.74	123.23
4	B	701	S58	O1-S1-N3	2.64	110.70	107.28
3	A	682	HEM	C2D-C3D-C4D	2.98	106.56	101.50
3	B	682	HEM	C2D-C3D-C4D	2.99	106.58	101.50
4	A	701	S58	O2-S1-C8	3.13	111.25	107.39
3	B	682	HEM	CMC-C2C-C3C	3.52	125.31	116.53
3	A	682	HEM	CMC-C2C-C3C	3.69	125.75	116.53
3	B	682	HEM	CMB-C2B-C3B	3.74	125.86	116.53
3	A	682	HEM	CAD-C3D-C4D	3.75	125.70	112.47
3	B	682	HEM	CAD-C3D-C4D	3.92	126.30	112.47
3	A	682	HEM	CMB-C2B-C3B	3.97	126.45	116.53
3	B	682	HEM	CAD-C3D-C2D	4.67	126.64	113.22
3	A	682	HEM	CAD-C3D-C2D	4.80	127.00	113.22
4	A	701	S58	O1-S1-N3	5.04	113.81	107.28
4	A	701	S58	C4-C3-N2	5.09	126.05	119.65
4	B	701	S58	C4-C3-N2	5.28	126.29	119.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
3	A	682	HEM	2	0
4	A	701	S58	3	0
3	B	682	HEM	1	0
4	B	701	S58	2	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 [i](#)

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

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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