



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 09:18 PM BST

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

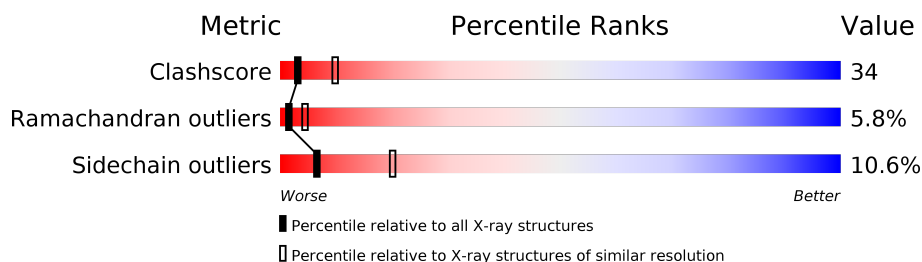
1 Overall quality at a glance

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

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:

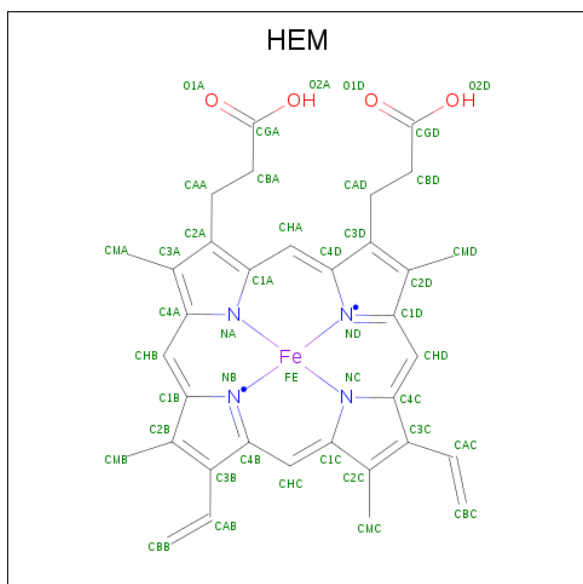
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	GLN	ASN	conflict	UNP Q05769
A	333	LYS	ARG	conflict	UNP Q05769
B	310	GLN	ASN	conflict	UNP Q05769
B	333	LYS	ARG	conflict	UNP Q05769

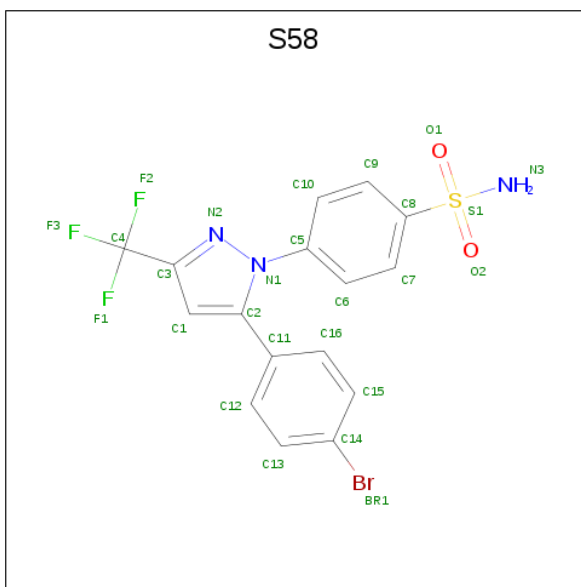
- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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: $C_{34}H_{32}FeN_4O_4$).





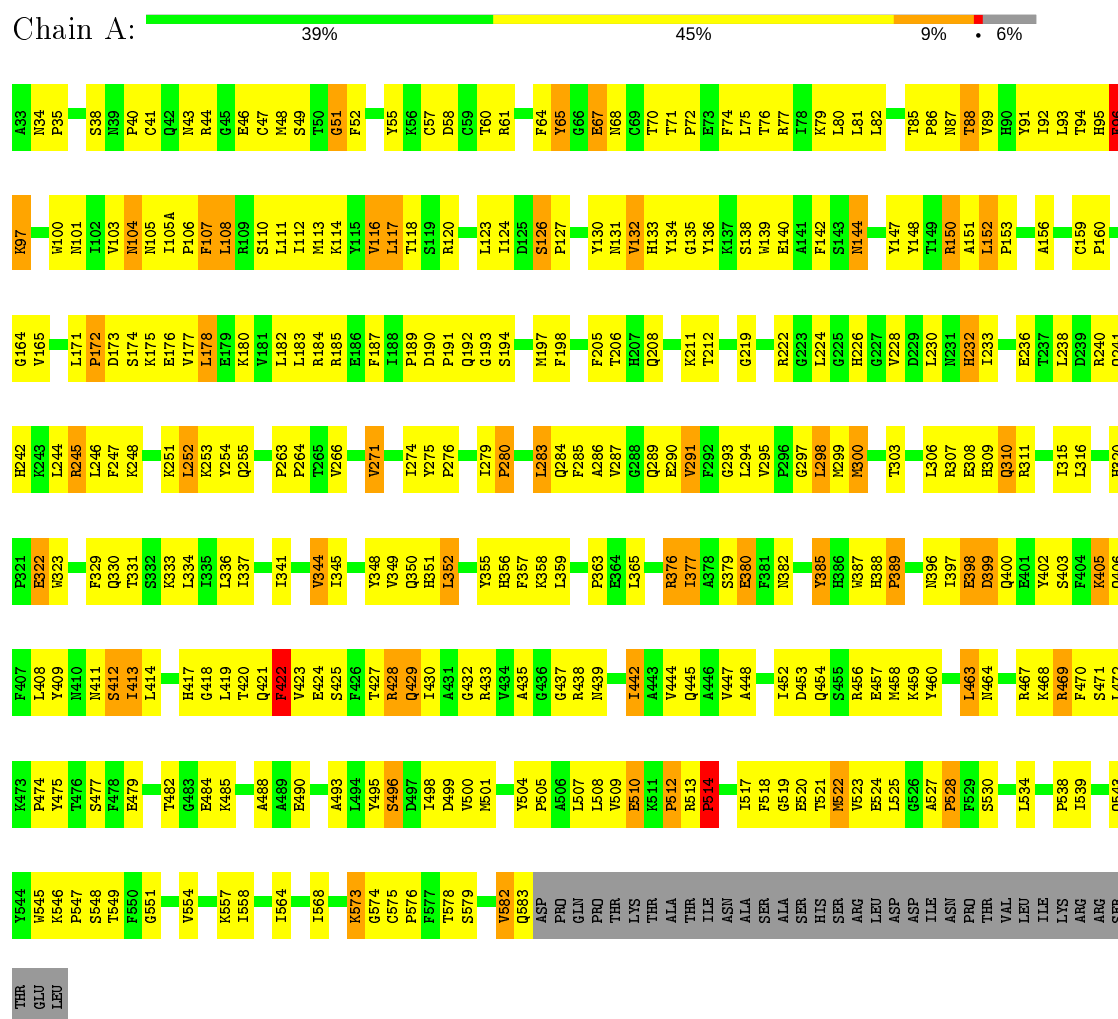
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	F	N	O	S		
4	A	1	26	1	16	3	3	2	1	0	0
4	B	1	26	1	16	3	3	2	1	0	0

3 Residue-property plots

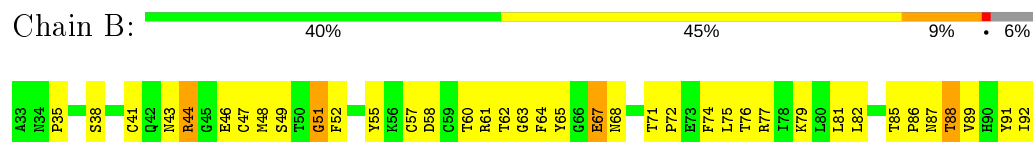
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



ARG SER THR GLU LEU	I539	F470	S403	E322	L246	P172	W100
	Q543	S471	F404	W323	F247	DI73	M101
		L472	K405	L328	K248	S174	I102
			Q406	F329	K251	K175	Y103
				Q330	L252	E176	N104
	K546	P474	Y409	T331	K253	V177	N105
	S548	Y475	M410	T331	Y254	L178	N105A
		T476	M411	S332	Q255	E179	P106
	G551	F477	S412	K333		K180	F107
		F478	L413	L334		V181	L108
	V554	E479	L414		P263	L182	R109
					P264	L183	S110
	K557	T482	H417	L337	T265	R184	L111
	I558	G483	G418	I341	V266	R185	L112
		E484	L419	K342			M113
	I564	K485	T420	V344	T269	P189	M114
			Q421	V345	Q270	D190	Y115
	I568	A488	F422		V271	P191	Y116
		A489	V423	I348		Q192	L117
	K573	E424	E424	V349	I274	G193	L118
	G574	S425	S425	Q350	Y275	S194	N119
	C575	L494	F426	H351	P276	N195	S119
	P576	Y495	T427	L352	P277	M196	R120
	F577	S496	R428		H278	M197	
	T578	D497	Q429		I279	F198	L123
	S579	I498	T430	Y355	P280		I124
	F580	D499	A431	H356		A202	D125
	N581	V500	G432	F357	L283	F205	S126
	V582	M501	R433	K358	Q284	T206	P127
	Q583		V434	L359	F285	G207	
	ASP	Y504	A435	K360	A286	H207	Y130
	PRO	P505	G436		V287	Q208	N131
	GLN	A506	G437	L365	G288	F209	V132
	PRO	L507	R438	L366	Q289	F210	H133
	THR	L508	M439	F367	E290	K211	Y134
	LYS	V509		N368	V291	T212	G135
	THR	E510	I442	Q369	F292		Y136
	ALA	V511	L443	Q370	G293	Q219	R137
	THR	P512	V444	F371	L294		S138
	ILE	R513	Q445		V295	R222	W139
	ASN	P514	A446	R376	P296		
	ALA		V447	I377	G297	H226	N144
	SER	I517		A378	L298	Q227	
	ALA	F518	S451	S379	V299	V228	Y147
	SER	G519	I452	E380	K300	D229	Y148
	HIS	E520	D453	F381		L230	T149
	SER	T521	Q454	N382	T303	N231	R150
	ARG	M522	S455			H232	A151
	LEU	V523	R456	Y385	L306	I233	L152
	ASP	E524	E457		R307		P153
	ASP	L525	M458	H388	E308	E236	
	ILE	G526	K459	P389	R309	T237	A156
	ASN	A527	Y460		Q310	L238	
	PRO	P528		N396	R311	D239	C159
	THR	F529	L463	I397		R240	P160
	VAL	S530	M464			Q241	
	LEU			E398	I315	H242	G164
	ILE	L534	R467	D399	L316	R243	V165
	LYS		K468	Q400	E320	L244	
	ARG	P538	R469	Y402	P321	R245	L171

4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	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 ²)	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:A:191:PRO:HD2	1:A:433:ARG:HG3	1.60	0.82
1:B:341:ILE:HG23	1:B:534:LEU:HD12	1.62	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:A:52:PHE:H	1:B:322:GLU:HG2	1.54	0.72
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.70	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:A:81:LEU:HD12	1:A:81:LEU:O	1.93	0.69
1:B:191:PRO:HD2	1:B:433:ARG:HG3	1.75	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:A:578:THR:HG22	1:A:579:SER:N	2.08	0.68
1:B:283:LEU:CD2	1:B:411:ASN:HB2	2.21	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:105(A):ILE:HD12	1:A:108:LEU:HD12	1.75	0.67
1:A:120:ARG:HH11	1:A:120:ARG:HG3	1.60	0.67
1:A:283:LEU:HB2	1:A:411:ASN:CG	2.15	0.67
1:A:244:LEU:CD2	1:A:271:VAL:HG11	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:ILE:HG13	1:A:283:LEU:HD21	1.76	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:427:THR:HB	1:A:428:ARG:NH1	2.10	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:123:LEU:O	1:A:469:ARG:NH2	2.29	0.66
1:A:485:LYS:HA	1:A:488:ALA:HB3	1.77	0.66
1:B:105(A):ILE:HD12	1:B:108:LEU:HD12	1.76	0.66
1:A:152:LEU:HD23	1:A:153:PRO:HD2	1.78	0.66
1:A:192:GLN:OE1	1:A:517:ILE:HG22	1.95	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:400:GLN:OE1	1:B:400:GLN:HA	1.96	0.65
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.60	0.65
1:A:173:ASP:HB3	1:A:176:GLU:HB2	1.78	0.65
1:A:322:GLU:HB3	1:B:52:PHE:CD1	2.31	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:175:LYS:HE3	1:B:175:LYS:HA	1.78	0.65
1:A:85:THR:O	1:A:89:VAL:HG23	1.96	0.65
1:B:81:LEU:O	1:B:81:LEU:HD12	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:A:264:PRO:HG2	1:A:286:ALA:HB3	1.80	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: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:A:160:PRO:HG2	1:A:165:VAL:HA	1.78	0.64
1:B:48:MET:HE3	1:B:49:SER:H	1.62	0.64
1:A:280:PRO:CD	1:A:283:LEU:HD23	2.23	0.64
1:A:463:LEU:O	1:A:467:ARG:HG3	1.98	0.64
1:A:574:GLY:O	1:A:576:PRO:HD3	1.97	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:306:LEU:HD23	1:A:306:LEU:O	2.00	0.62
1:A:359:LEU:HD11	4:A:701:S58:F1	1.90	0.62
1:A:205:PHE:CE1	1:A:344:VAL:HG21	2.34	0.62
1:A:295:VAL:HB	1:A:298:LEU:CD2	2.30	0.61
1:A:573:LYS:HG3	1:A:574:GLY:N	2.14	0.61
1:B:107:PHE:N	1:B:107:PHE:CD1	2.66	0.61
1:B:420:THR:OG1	1:B:573:LYS:HB3	1.99	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: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:110:SER:HB2	1:B:365:LEU:HD21	1.82	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:A:64:PHE:CE2	1:A:72:PRO:HB3	2.36	0.60
1:B:573:LYS:HG3	1:B:574:GLY:N	2.17	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:194:SER:OG	1:B:351:HIS:HE1	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.83	0.60
1:B:120:ARG:HG3	1:B:120:ARG:HH11	1.67	0.59
1:A:388:HIS:HB3	1:A:444:VAL:HG11	1.84	0.59
1:A:477:SER:HB2	1:A:479:GLU:OE1	2.01	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:104:ASN:HD21	1:A:358:LYS:HB2	1.67	0.58
1:A:182:LEU:O	1:A:438:ARG:HA	2.02	0.58
1:A:197:MET:CE	1:A:423:VAL:HG13	2.32	0.58
1:B:388:HIS:HB3	1:B:444:VAL:HG11	1.85	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: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:91:TYR:O	1:B:95:HIS:HD2	1.87	0.58
1:A:175:LYS:HE3	1:A:175:LYS:HA	1.86	0.58
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.38	0.58
1:A:418:GLY:O	1:A:422:PHE:HB2	2.03	0.58
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:280:PRO:HD2	1:B:283:LEU:CD2	2.24	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:398:GLU:O	1:A:399:ASP:HB3	2.04	0.57
1:A:525:LEU:O	1:A:528:PRO:HD2	2.04	0.57
1:B:264:PRO:HG2	1:B:286:ALA:HB3	1.86	0.57
1:B:198:PHE:CZ	1:B:352:LEU:HD13	2.39	0.57
1:A:320:HIS:HB3	1:A:323:TRP:CG	2.40	0.57
1:A:509:VAL:HG12	1:A:510:GLU:N	2.20	0.57
1:B:112:ILE:HB	1:B:357:PHE:CZ	2.39	0.57
1:B:463:LEU:O	1:B:467:ARG:HG3	2.05	0.57
1:B:389:PRO:HG2	1:B:508:LEU:HD22	1.87	0.57
1:B:513:ARG:HH21	1:B:520:GLU:HG3	1.69	0.57
1:B:525:LEU:O	1:B:528:PRO:HD2	2.04	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:171:LEU:HD23	1:A:456:ARG:HE	1.70	0.56
1:A:87:ASN:C	1:A:89:VAL:H	2.08	0.56
1:B:124:ILE:N	1:B:124:ILE:HD12	2.20	0.56
1:B:226:HIS:ND1	1:B:376:ARG:HD2	2.21	0.56
1:B:403:SER:HB2	1:B:405:LYS:HD2	1.87	0.56
1:B:43:ASN:O	1:B:44:ARG:HB2	2.04	0.56
1:B:105(A):ILE:HB	1:B:108:LEU:HB2	1.87	0.56
1:B:279:ILE:CG2	1:B:284:GLN:HG2	2.34	0.56
1:A:127:PRO:HD2	1:B:543:GLN:HE22	1.71	0.56
1:A:194:SER:OG	1:A:351:HIS:CE1	2.58	0.56
1:A:97:LYS:HG3	1:A:356:HIS:CD2	2.40	0.56
1:A:295:VAL:HB	1:A:298:LEU:HD23	1.88	0.56
1:B:104:ASN:HD21	1:B:358:LYS:HB2	1.71	0.56
1:A:198:PHE:HZ	1:A:352:LEU:HD13	1.71	0.56
1:A:295:VAL:HG12	1:A:297:GLY:H	1.71	0.56
1:B:208:GLN:HE21	1:B:228:VAL:HA	1.67	0.56
1:B:578:THR:CG2	1:B:579:SER:N	2.69	0.56
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.88	0.55
1:B:306:LEU:O	1:B:306:LEU:HD23	2.07	0.55
1:B:185:ARG:HH21	1:B:438:ARG:HD3	1.70	0.55
1:A:46:GLU:OE2	1:B:546:LYS:HD2	2.06	0.55
1:A:568:ILE:HG22	1:A:576:PRO:HD2	1.88	0.55
1:B:103:VAL:HG11	1:B:112:ILE:HG13	1.89	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:482:THR:HG22	1:A:509:VAL:HG13	1.87	0.54
1:A:578:THR:CG2	1:A:579:SER:N	2.69	0.54
1:B:458:MET:HE3	1:B:460:TYR:CE1	2.42	0.54
1:A:148:TYR:HD1	1:A:377:ILE:HG13	1.72	0.54
1:A:344:VAL:O	1:A:349:VAL:HG23	2.07	0.54
1:A:94:THR:O	1:A:356:HIS:ND1	2.40	0.54
1:A:58:ASP:OD2	1:B:546:LYS:HD3	2.08	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:178:LEU:HD22	1:B:183:LEU:HG	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:VAL:HB	1:B:298:LEU:HD22	1.87	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:134:TYR:HB3	1:A:136:TYR:O	2.08	0.54
1:A:279:ILE:CG2	1:A:283:LEU:HG	2.23	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:320:HIS:HB3	1:B:323:TRP:CG	2.43	0.53
1:B:197:MET:CE	1:B:423:VAL:HG13	2.38	0.53
1:A:400:GLN:OE1	1:A:400:GLN:HA	2.08	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: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:133:HIS:ND1	1:B:147:TYR:HE2	2.07	0.53
1:B:148:TYR:HD1	1:B:377:ILE:HG13	1.74	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:A:46:GLU:O	1:A:57:CYS:HA	2.10	0.52
1:B:173:ASP:OD1	1:B:175:LYS:HB3	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:197:MET:HE2	1:A:423:VAL:HG13	1.91	0.52
1:A:274:ILE:HD12	1:A:291:VAL:HG23	1.92	0.52
1:A:574:GLY:O	1:A:576:PRO:CD	2.58	0.52
1:B:114:LYS:O	1:B:118:THR:HG23	2.09	0.52
1:B:194:SER:OG	1:B:351:HIS:CE1	2.63	0.52
1:B:479:GLU:HG2	1:B:485:LYS:HD3	1.92	0.52
1:A:185:ARG:HH21	1:A:438:ARG:HD3	1.74	0.52
1:A:113:MET:O	1:A:117:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:LEU:HD22	1:A:409:TYR:CD2	2.45	0.52
1:B:105(A):ILE:CD1	1:B:108:LEU:HD12	2.40	0.52
1:A:142:PHE:O	1:A:376:ARG:NH2	2.37	0.51
1:A:276:PRO:O	1:A:279:ILE:HB	2.10	0.51
1:A:403:SER:HB2	1:A:405:LYS:HD2	1.92	0.51
1:B:85:THR:HB	1:B:86:PRO:HD2	1.90	0.51
1:A:151:ALA:HB3	1:A:380:GLU:HG3	1.92	0.51
1:A:150:ARG:HD2	1:A:380:GLU:OE1	2.10	0.51
1:A:230:LEU:HD13	1:A:233:ILE:HD12	1.92	0.51
1:A:246:LEU:O	1:A:247:PHE:HB2	2.11	0.51
1:A:266:VAL:O	1:A:266:VAL:HG12	2.09	0.51
1:A:283:LEU:HD13	1:A:411:ASN:CA	2.41	0.51
1:A:403:SER:HB2	1:A:405:LYS:NZ	2.25	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:276:PRO:HD2	1:B:279:ILE:CD1	2.40	0.51
1:B:458:MET:CE	1:B:460:TYR:CE1	2.93	0.51
1:B:152:LEU:HD23	1:B:153:PRO:HD2	1.92	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:A:43:ASN:O	1:A:44:ARG:HB2	2.09	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:148:TYR:CD1	1:A:377:ILE:HG13	2.45	0.51
1:B:479:GLU:HB3	1:B:485:LYS:HE2	1.92	0.51
1:A:435:ALA:O	1:A:512:PRO:HG3	2.10	0.50
1:B:46:GLU:O	1:B:57:CYS:HA	2.11	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:176:GLU:O	1:B:180:LYS:HG3	2.11	0.50
1:B:178:LEU:HD23	1:B:182:LEU:HB2	1.94	0.50
1:A:232:HIS:ND1	1:A:233:ILE:HG13	2.27	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:A:546:LYS:HD3	1:B:58:ASP:OD2	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:134:TYR:HB3	1:B:136:TYR:O	2.11	0.50
1:B:574:GLY:O	1:B:576:PRO:CD	2.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:HA	1:B:96:PHE:HE1	1.76	0.50
1:A:211:LYS:NZ	1:A:236:GLU:HG3	2.27	0.50
1:A:252:LEU:O	1:A:310:GLN:NE2	2.44	0.50
1:A:184:ARG:HB2	1:A:439:ASN:C	2.32	0.50
1:B:242:HIS:ND1	1:B:247:PHE:HZ	2.10	0.50
1:B:379:SER:O	1:B:382:ASN:N	2.45	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:226:HIS:CE1	1:B:376:ARG:HD2	2.47	0.49
1:B:72:PRO:HB2	1:B:76:THR:HB	1.94	0.49
1:A:252:LEU:HD22	1:A:309:HIS:CG	2.47	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:B:246:LEU:O	1:B:247:PHE:HB2	2.12	0.49
1:B:345:ILE:HD11	1:B:534:LEU:HG	1.94	0.49
1:B:134:TYR:HD1	1:B:136:TYR:CE1	2.30	0.49
1:B:148:TYR:CD1	1:B:377:ILE:HG13	2.47	0.49
1:B:414:LEU:HA	1:B:422:PHE:CE2	2.48	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:A:176:GLU:O	1:A:180:LYS:HG3	2.12	0.49
1:B:294:LEU:HD22	1:B:409:TYR:CD2	2.47	0.49
1:B:479:GLU:HG2	1:B:485:LYS:CE	2.42	0.49
1:B:132:VAL:HG21	1:B:219:GLY:HA3	1.95	0.49
1:B:197:MET:HE2	1:B:423:VAL:HG13	1.94	0.49
1:B:94:THR:O	1:B:356:HIS:ND1	2.46	0.49
1:B:183:LEU:O	1:B:438:ARG:HB3	2.13	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:A:131:ASN:ND2	1:A:147:TYR:CD2	2.81	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:LEU:HB3	1:A:456:ARG:HH21	1.78	0.48
1:B:120:ARG:NH1	1:B:120:ARG:HG3	2.28	0.48
1:B:92:ILE:HA	1:B:96:PHE:CE1	2.48	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:142:PHE:CD1	1:A:142:PHE:C	2.87	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:B:398:GLU:O	1:B:399:ASP:HB3	2.13	0.48
1:A:251:LYS:HD3	1:A:310:GLN:HG3	1.96	0.48
1:A:447:VAL:HG13	3:A:682:HEM:HBA2	1.94	0.48
1:A:226:HIS:ND1	1:A:376:ARG:HD2	2.29	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: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:184:ARG:HB2	1:B:439:ASN:C	2.34	0.48
1:A:133:HIS:ND1	1:A:147:TYR:HE2	2.12	0.48
1:B:113:MET:HG2	1:B:360:LYS:HB3	1.95	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
1:A:479:GLU:HG3	1:A:488:ALA:HB1	1.95	0.47
1:A:582:VAL:O	1:A:583:GLN:HB2	2.14	0.47
4:A:701:S58:C11	4:A:701:S58:H10	2.44	0.47
1:A:85:THR:OG1	1:A:88:THR:HG23	2.15	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: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:B:190:ASP:OD1	1:B:517:ILE:HB	2.14	0.47
1:A:254:TYR:C	1:A:254:TYR:CD1	2.88	0.47
1:A:105(A):ILE:CB	1:A:108:LEU:HB2	2.44	0.47
1:A:178:LEU:HD23	1:A:182:LEU:HB2	1.96	0.47
1:A:35:PRO:HB2	1:A:55:TYR:HB3	1.97	0.47
1:B:222:ARG:NH2	1:B:236:GLU:HG2	2.29	0.47
1:B:91:TYR:O	1:B:95:HIS:CD2	2.67	0.47
1:A:264:PRO:HG2	1:A:286:ALA:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HB2	1:A:76:THR:HB	1.95	0.47
1:A:114:LYS:O	1:A:118:THR:HG23	2.15	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: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:A:132:VAL:HG21	1:A:219:GLY:HA3	1.97	0.47
1:A:495:TYR:CE2	1:A:501:MET:SD	3.07	0.47
1:B:133:HIS:ND1	1:B:147:TYR:CE2	2.82	0.47
1:B:197:MET:HG3	1:B:578:THR:HG23	1.97	0.47
1:A:222:ARG:NH2	1:A:236:GLU:HG2	2.29	0.46
1:B:100:TRP:O	1:B:104:ASN:HB2	2.15	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: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: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:185:ARG:NE	1:A:438:ARG:HD3	2.27	0.46
1:A:490:GLU:O	1:A:493:ALA:HB3	2.15	0.46
1:B:232:HIS:ND1	1:B:233:ILE:HG13	2.30	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:113:MET:HE3	1:A:117:LEU:HD13	1.96	0.46
1:A:159:CYS:HB3	1:A:164:GLY:O	2.16	0.46
1:B:513:ARG:O	1:B:514:PRO:O	2.32	0.46
1:A:139:TRP:CZ3	1:B:538:PRO:HG2	2.51	0.46
1:A:548:SER:OG	1:B:58:ASP:CB	2.64	0.46
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.51	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:B:521:THR:O	1:B:523:VAL:N	2.49	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
1:B:35:PRO:HB2	1:B:55:TYR:HB3	1.98	0.46
1:B:568:ILE:HG22	1:B:576:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:THR:HG22	1:B:579:SER:H	1.78	0.46
1:A:242:HIS:ND1	1:A:247:PHE:HZ	2.14	0.46
1:A:184:ARG:HB2	1:A:439:ASN:HA	1.98	0.46
1:B:251:LYS:HD3	1:B:310:GLN:HG3	1.98	0.46
1:B:433:ARG:H	1:B:439:ASN:ND2	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:189:PRO:HB2	1:A:430:ILE:HD13	1.98	0.45
1:A:193:GLY:O	1:A:582:VAL:N	2.46	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: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:A:379:SER:O	1:A:382:ASN:N	2.49	0.45
1:B:578:THR:CG2	1:B:579:SER:H	2.29	0.45
1:A:295:VAL:HG22	1:A:408:LEU:HD22	1.99	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:285:PHE:HD2	1:A:299:MET:SD	2.40	0.45
1:A:498:ILE:C	1:A:500:VAL:H	2.20	0.45
1:B:149:THR:O	1:B:378:ALA:HA	2.17	0.45
1:B:266:VAL:HG12	1:B:266:VAL:O	2.16	0.45
1:B:498:ILE:C	1:B:500:VAL:H	2.19	0.45
1:B:211:LYS:NZ	1:B:236:GLU:HG3	2.32	0.45
1:B:198:PHE:HZ	1:B:352:LEU:HD13	1.79	0.45
1:B:468:LYS:HG2	1:B:474:PRO:HG3	1.99	0.45
1:B:470:PHE:O	1:B:471:SER:HB2	2.17	0.45
1:B:306:LEU:HD23	1:B:306:LEU:C	2.37	0.44
1:B:283:LEU:HD13	1:B:411:ASN:CA	2.46	0.44
1:A:403:SER:O	1:A:406:GLN:HG2	2.17	0.44
1:B:417:HIS:HB2	1:B:422:PHE:CD2	2.53	0.44
1:A:283:LEU:HD13	1:A:411:ASN:HA	1.99	0.44
1:A:454:GLN:O	1:A:457:GLU:HB2	2.18	0.44
1:A:513:ARG:O	1:A:514:PRO:O	2.35	0.44
1:B:479:GLU:HG2	1:B:485:LYS:CD	2.47	0.44
1:A:105(A):ILE:O	1:A:108:LEU:N	2.50	0.44
1:A:345:ILE:HD11	1:A:534:LEU:HG	1.99	0.44
1:A:414:LEU:HD11	1:A:419:LEU:HD22	2.00	0.44
1:B:434:VAL:HG23	1:B:517:ILE:HD11	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:B:171:LEU:HB3	1:B:456:ARG:HH21	1.83	0.44
1:A:58:ASP:CB	1:B:548:SER:OG	2.66	0.44
1:A:230:LEU:HD23	1:A:230:LEU:H	1.83	0.44
1:A:472:LEU:HD11	1:A:524:GLU:HB2	2.00	0.44
1:B:105(A):ILE:CB	1:B:108:LEU:HB2	2.47	0.44
1:B:254:TYR:HD2	1:B:310:GLN:HE21	1.65	0.44
1:A:211:LYS:HZ3	1:A:236:GLU:HG3	1.81	0.44
1:A:297:GLY:O	1:A:300:MET:HB3	2.18	0.44
1:B:328:LEU:HD23	1:B:328:LEU:HA	1.86	0.44
1:B:184:ARG:HB2	1:B:439:ASN:HA	1.99	0.43
1:A:322:GLU:HB3	1:B:52:PHE:CE1	2.53	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:B:185:ARG:NE	1:B:438:ARG:HD3	2.28	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:131:ASN:ND2	1:A:147:TYR:CG	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:222:ARG:HH22	1:A:236:GLU:HG2	1.84	0.43
1:A:448:ALA:O	1:A:452:ILE:HG13	2.18	0.43
1:B:435:ALA:O	1:B:512:PRO:HG3	2.18	0.43
1:A:306:LEU:HD23	1:A:306:LEU:C	2.39	0.43
1:A:197:MET:HE1	1:A:423:VAL:HG13	2.01	0.43
1:A:100:TRP:O	1:A:104:ASN:HB2	2.17	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: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: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:A:308:GLU:O	1:A:309:HIS:C	2.54	0.42
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.42
1:B:185:ARG:NH2	1:B:438:ARG:HD3	2.34	0.42
1:B:513:ARG:O	1:B:514:PRO:C	2.58	0.42
1:B:447:VAL:HG13	3:B:682:HEM:HBA2	2.00	0.42
1:A:463:LEU:HD21	1:A:475:TYR:CD2	2.54	0.42
1:A:538:PRO:HG2	1:B:139:TRP:CZ3	2.54	0.42
1:B:322:GLU:HG3	1:B:322:GLU:H	1.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:ILE:O	1:B:568:ILE:HD13	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:159:CYS:HB3	1:B:164:GLY:O	2.19	0.42
1:B:230:LEU:H	1:B:230:LEU:HD23	1.83	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: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:458:MET:HE2	1:A:460:TYR:HE1	1.82	0.42
1:B:451:SER:HB2	1:B:504:TYR:CE2	2.54	0.42
1:A:74:PHE:O	1:A:77:ARG:HB2	2.20	0.42
1:B:495:TYR:CE2	1:B:501:MET:SD	3.12	0.42
1:B:472:LEU:HD11	1:B:524:GLU:HB2	2.02	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:A:458:MET:HE2	1:A:460:TYR:CE1	2.55	0.42
1:B:62:THR:OG1	1:B:63:GLY:N	2.51	0.42
1:A:126:SER:HA	1:A:127:PRO:HA	1.85	0.42
1:A:470:PHE:O	1:A:471:SER:HB2	2.20	0.42
1:A:521:THR:O	1:A:523:VAL:N	2.52	0.42
1:B:278:HIS:O	1:B:278:HIS:CD2	2.73	0.42
1:B:343:ILE:O	1:B:345:ILE:N	2.53	0.42
1:A:105(A):ILE:HG23	1:A:107:PHE:CD2	2.54	0.42
1:B:202:ALA:HB2	1:B:348:TYR:HE1	1.84	0.42
1:B:67:GLU:HG2	1:B:68:ASN:OD1	2.20	0.42
1:A:293:GLY:HA2	1:A:299:MET:HE3	2.01	0.42
1:A:472:LEU:HD22	1:A:520:GLU:CD	2.40	0.42
1:B:275:TYR:CE2	1:B:284:GLN:HA	2.55	0.42
1:B:582:VAL:O	1:B:583:GLN:HB2	2.20	0.42
1:A:224:LEU:HD23	1:A:224:LEU:HA	1.79	0.41
1:A:65:TYR:N	1:A:65:TYR:CD1	2.88	0.41
1:B:453:ASP:O	1:B:457:GLU:HG3	2.19	0.41
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:A:521:THR:O	1:A:522:MET:C	2.58	0.41
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.02	0.41
1:B:150:ARG:HD2	1:B:380:GLU:OE1	2.19	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: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:388:HIS:N	1:B:389:PRO:CD	2.84	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: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:A:97:LYS:HB2	1:A:356:HIS:CE1	2.56	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:428:ARG:O	1:A:429:GLN:HB2	2.20	0.41
1:A:437:GLY:O	1:A:438:ARG:C	2.58	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:479:GLU:HG2	1:A:485:LYS:CE	2.51	0.41
1:A:507:LEU:HD21	1:A:521:THR:HG22	2.02	0.41
1:A:64:PHE:HD2	1:A:70:THR:O	2.04	0.41
1:B:195:ASN:HB2	1:B:196:MET:H	1.78	0.41
1:A:173:ASP:OD1	1:A:175:LYS:HB3	2.21	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:500:VAL:CG1	1:A:500:VAL:O	2.68	0.41
1:B:230:LEU:HB3	1:B:233:ILE:HD12	2.02	0.41
1:A:130:TYR:HB3	1:A:134:TYR:O	2.21	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: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:210:PHE:HB3	1:B:382:ASN:ND2	2.35	0.40
1:B:437:GLY:O	1:B:438:ARG:C	2.58	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: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:A:387:TRP:HB2	3:A:682:HEM:HAC	2.03	0.40
1:A:67:GLU:HG2	1:A:68:ASN:OD1	2.21	0.40
1:B:334:LEU:HD23	1:B:334:LEU:HA	1.80	0.40
1:B:442:ILE:O	1:B:445:GLN:HB3	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	5
1	B	550/587 (94%)	431 (78%)	86 (16%)	33 (6%)	1	4
All	All	1100/1174 (94%)	866 (79%)	170 (16%)	64 (6%)	1	4

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%)	6	19
1	B	493/525 (94%)	442 (90%)	51 (10%)	7	21
All	All	986/1050 (94%)	881 (89%)	105 (11%)	6	20

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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$
4	S58	A	701	-	27,28,28	2.58	7 (25%)	37,43,43	1.99	9 (24%)
2	NAG	A	681	1	14,14,15	0.32	0	17,19,21	0.97	1 (5%)
3	HEM	B	682	1	27,50,50	1.92	6 (22%)	17,82,82	0.63	0
2	NAG	A	671	1	14,14,15	0.42	0	17,19,21	0.81	1 (5%)
2	NAG	A	661	1	14,14,15	0.64	0	17,19,21	0.52	0
4	S58	B	701	-	27,28,28	2.50	7 (25%)	37,43,43	1.75	8 (21%)
2	NAG	B	661	1	14,14,15	0.57	0	17,19,21	0.59	0
2	NAG	B	681	1	14,14,15	0.68	0	17,19,21	0.84	0
2	NAG	B	671	1	14,14,15	0.55	0	17,19,21	0.91	1 (5%)
3	HEM	A	682	1	27,50,50	1.87	6 (22%)	17,82,82	0.74	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	S58	A	701	-	-	2/20/20/20	0/3/3/3
2	NAG	A	681	1	-	0/6/23/26	0/1/1/1
3	HEM	B	682	1	-	1/6/54/54	-
2	NAG	A	671	1	-	2/6/23/26	0/1/1/1
2	NAG	A	661	1	-	2/6/23/26	0/1/1/1
4	S58	B	701	-	-	2/20/20/20	0/3/3/3
2	NAG	B	661	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	681	1	-	0/6/23/26	0/1/1/1
2	NAG	B	671	1	-	2/6/23/26	0/1/1/1
3	HEM	A	682	1	-	1/6/54/54	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	701	S58	S1-N3	8.09	1.76	1.60
4	B	701	S58	S1-N3	7.31	1.74	1.60
4	B	701	S58	C1-C3	6.12	1.47	1.39
4	A	701	S58	C1-C3	5.83	1.47	1.39
3	B	682	HEM	C3B-CAB	-4.88	1.38	1.47
3	A	682	HEM	C3B-CAB	-4.68	1.38	1.47
3	A	682	HEM	C3C-CAC	-4.57	1.38	1.47
3	B	682	HEM	C3C-CAC	-4.35	1.38	1.47
4	B	701	S58	C8-S1	4.21	1.83	1.77
4	A	701	S58	C3-N2	-4.03	1.28	1.33
3	B	682	HEM	C3B-C2B	-4.01	1.34	1.40
4	A	701	S58	C1-C2	-3.90	1.32	1.39
4	B	701	S58	BR1-C14	-3.74	1.82	1.90
3	A	682	HEM	C3B-C2B	-3.68	1.35	1.40
4	B	701	S58	N2-N1	3.62	1.46	1.39
4	A	701	S58	BR1-C14	-3.61	1.83	1.90
3	B	682	HEM	C3C-C2C	-3.59	1.35	1.40
3	A	682	HEM	C3C-C2C	-3.57	1.35	1.40
4	B	701	S58	C3-N2	-2.97	1.30	1.33
4	B	701	S58	C1-C2	-2.83	1.34	1.39
4	A	701	S58	N2-N1	2.71	1.44	1.39
4	A	701	S58	C8-S1	2.67	1.81	1.77
3	A	682	HEM	CBC-CAC	2.52	1.45	1.29
3	B	682	HEM	CBB-CAB	2.34	1.44	1.29
3	A	682	HEM	CBB-CAB	2.33	1.44	1.29
3	B	682	HEM	CBC-CAC	2.19	1.43	1.29

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	701	S58	C4-C3-N2	5.59	126.29	119.72
4	A	701	S58	C4-C3-N2	5.39	126.05	119.72
4	A	701	S58	O2-S1-O1	-5.26	110.11	118.76
4	B	701	S58	O2-S1-O1	-4.51	111.34	118.76
4	A	701	S58	O1-S1-N3	4.35	113.81	107.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	701	S58	O2-S1-C8	3.49	111.25	107.35
4	A	701	S58	C1-C2-C11	-2.96	123.39	128.10
4	B	701	S58	F2-C4-C3	-2.91	107.49	112.47
2	B	671	NAG	C2-N2-C7	-2.78	118.94	122.90
4	A	701	S58	F2-C4-C3	-2.67	107.91	112.47
4	A	701	S58	C1-C3-N2	-2.59	107.66	111.41
4	B	701	S58	C1-C2-C11	-2.57	124.01	128.10
2	A	671	NAG	C2-N2-C7	-2.55	119.28	122.90
4	B	701	S58	C1-C3-N2	-2.54	107.73	111.41
4	B	701	S58	O1-S1-N3	2.25	110.70	107.36
4	B	701	S58	O2-S1-C8	2.18	109.78	107.35
4	A	701	S58	C3-N2-N1	2.17	108.17	105.66
2	A	681	NAG	C1-C2-N2	-2.13	106.85	110.49
4	A	701	S58	F3-C4-C3	-2.09	108.90	112.47
4	B	701	S58	C3-N2-N1	2.07	108.06	105.66

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	S58	C6-C5-N1-C2
4	A	701	S58	C10-C5-N1-C2
3	B	682	HEM	C2A-CAA-CBA-CGA
4	B	701	S58	C6-C5-N1-C2
4	B	701	S58	C10-C5-N1-C2
3	A	682	HEM	C2A-CAA-CBA-CGA
2	A	671	NAG	O5-C5-C6-O6
2	B	671	NAG	O5-C5-C6-O6
2	A	671	NAG	C4-C5-C6-O6
2	A	661	NAG	O5-C5-C6-O6
2	B	671	NAG	C4-C5-C6-O6
2	B	661	NAG	O5-C5-C6-O6
2	A	661	NAG	C4-C5-C6-O6
2	B	661	NAG	C4-C5-C6-O6

There are no ring outliers.

5 monomers are involved in 9 short contacts:

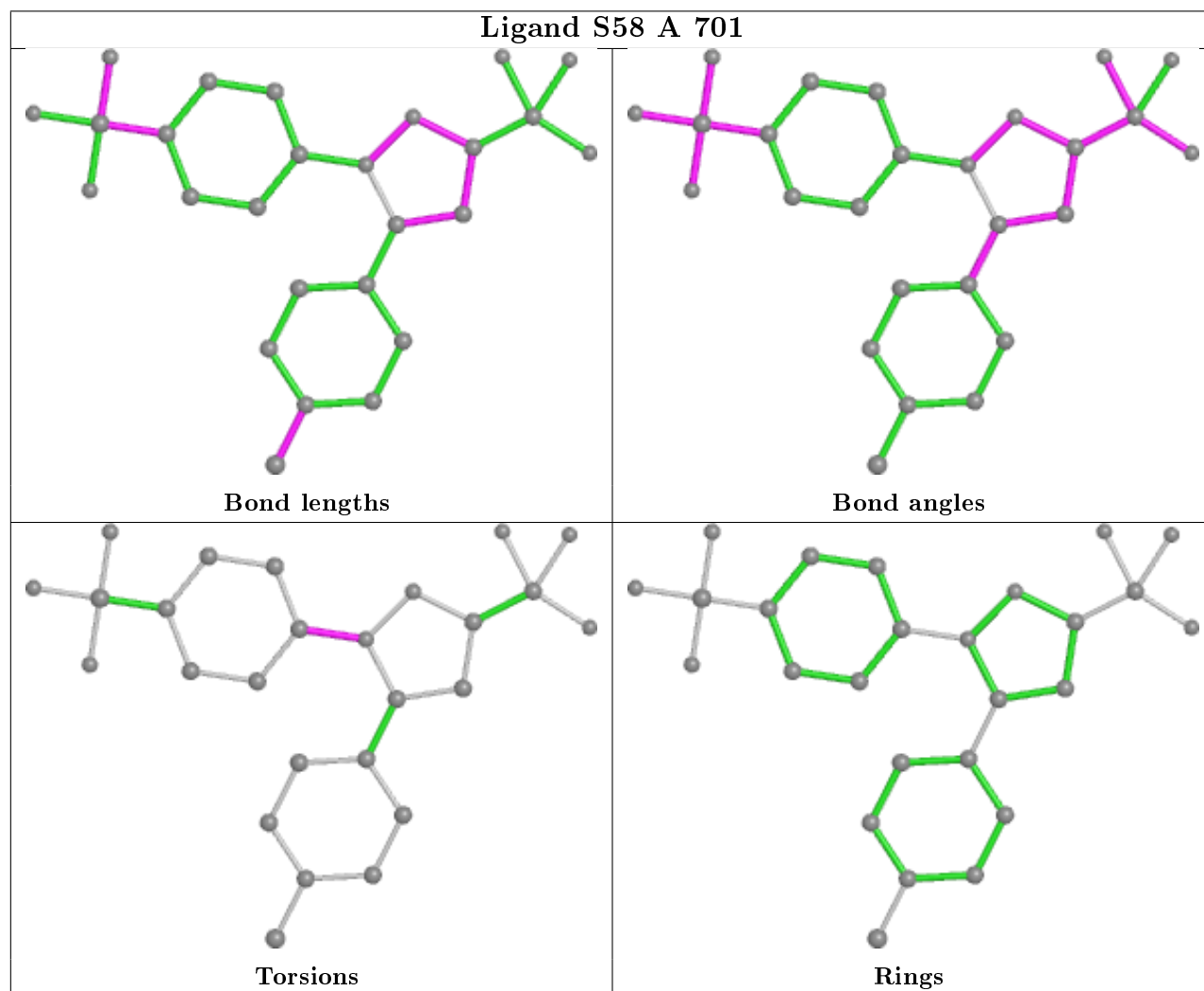
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	701	S58	3	0
3	B	682	HEM	1	0

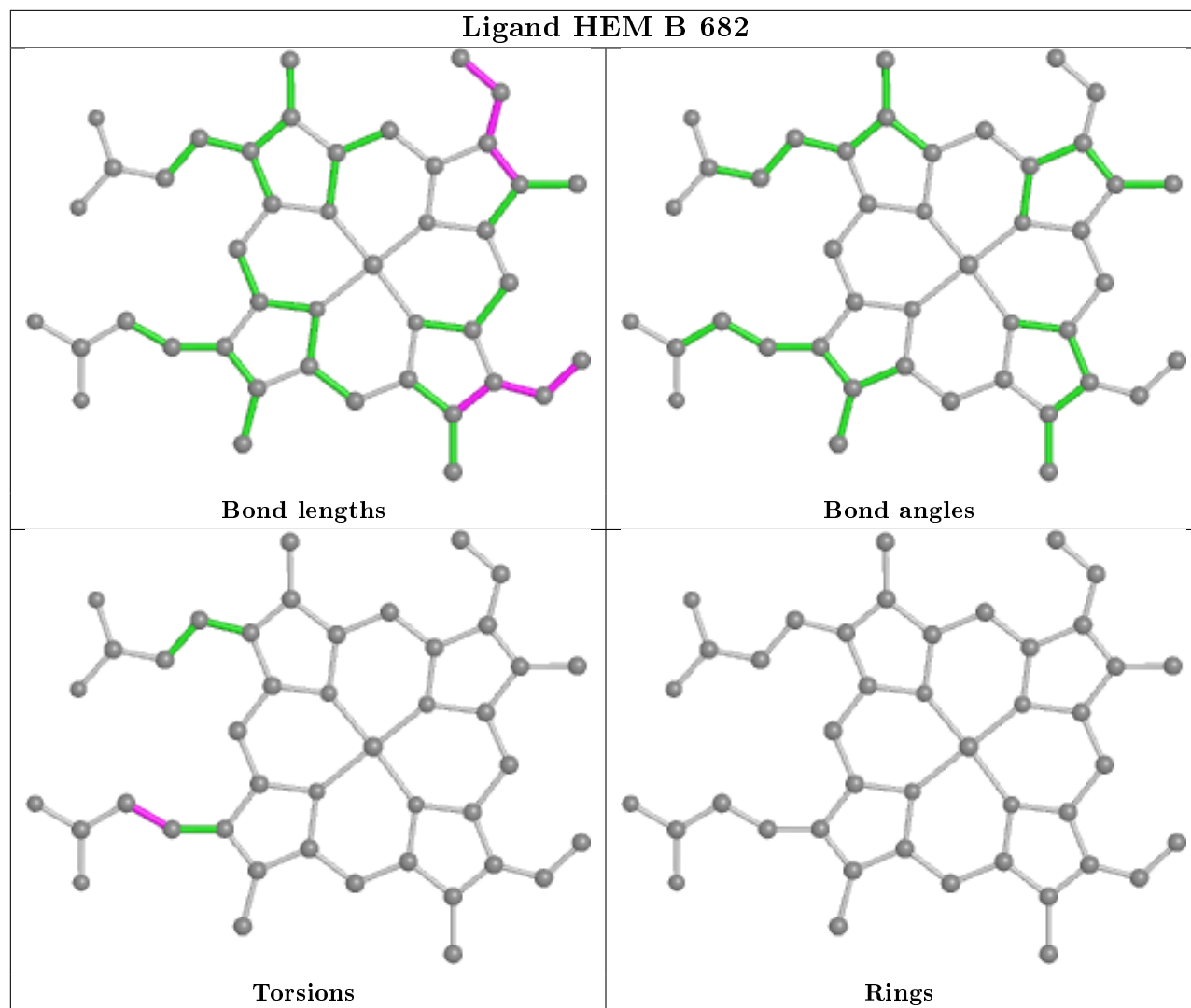
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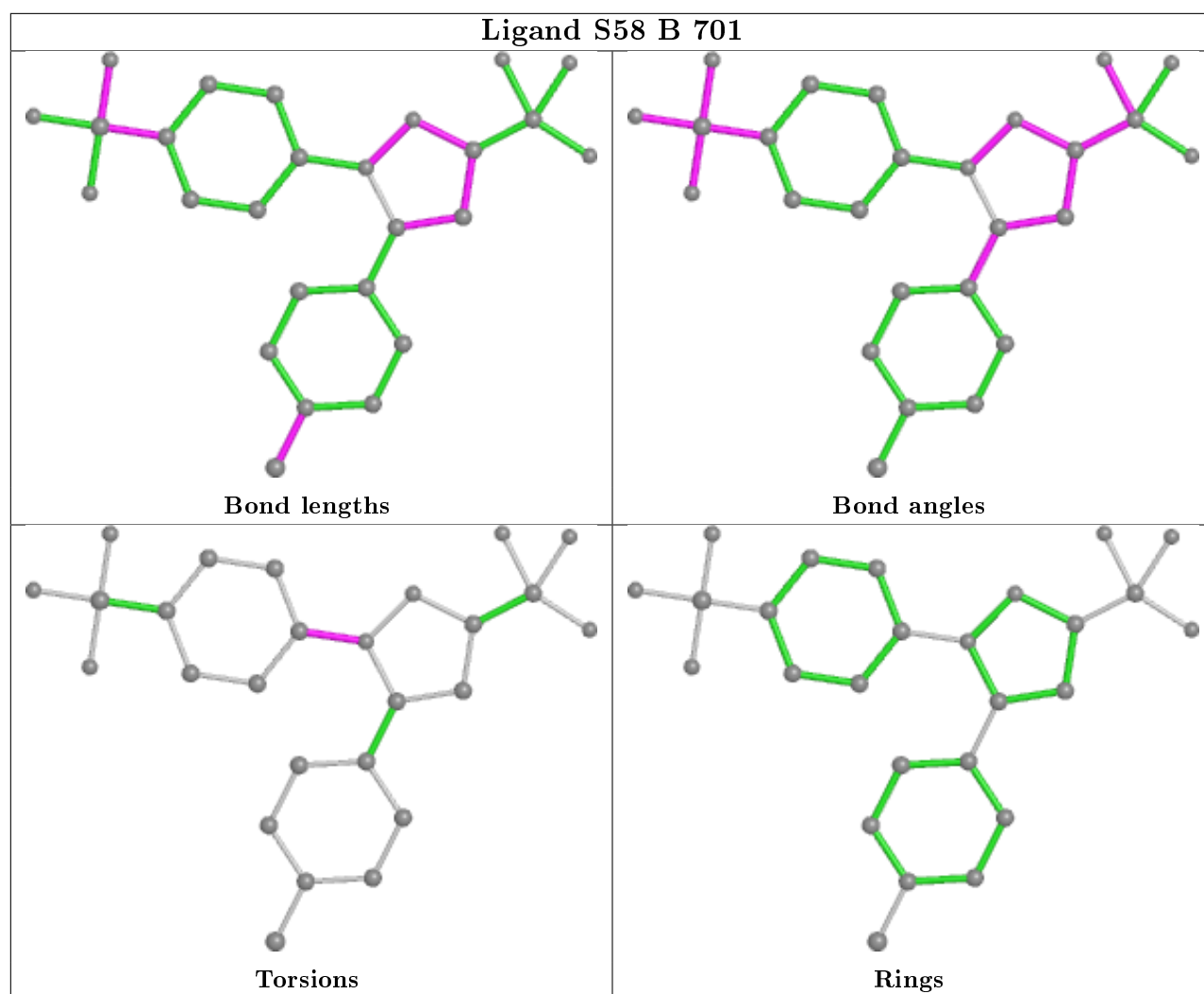
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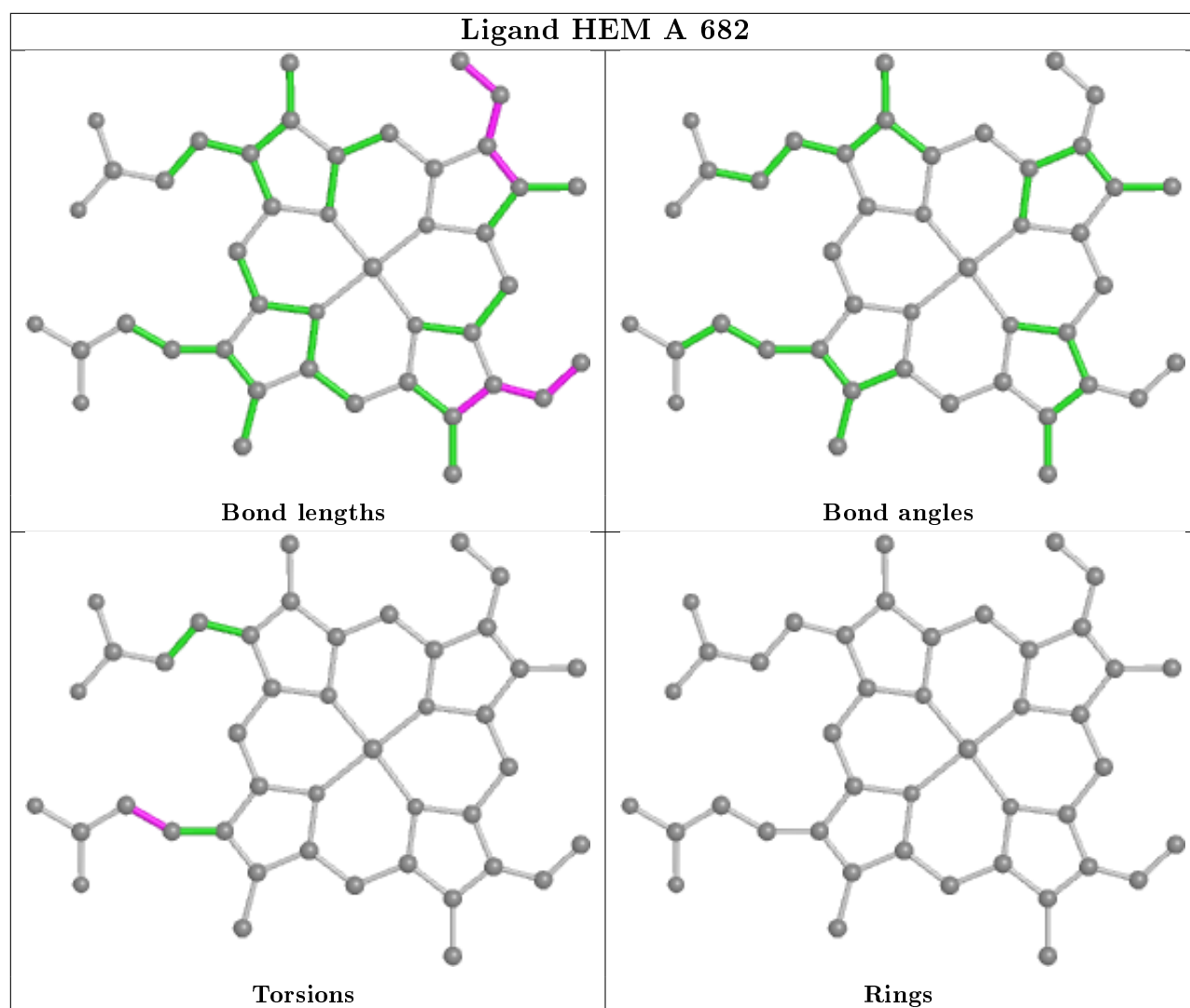
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	661	NAG	1	0
4	B	701	S58	2	0
3	A	682	HEM	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.