



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 10, 2023 – 12:15 pm GMT

PDB ID : 2CA0
Title : Crystal structure of YC-17-bound cytochrome P450 PikC (CYP107L1)
Authors : Yermalitskaya, L.I.; Kim, Y.; Sherman, D.H.; Waterman, M.R.; Podust, L.M.
Deposited on : 2005-12-15
Resolution : 2.85 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

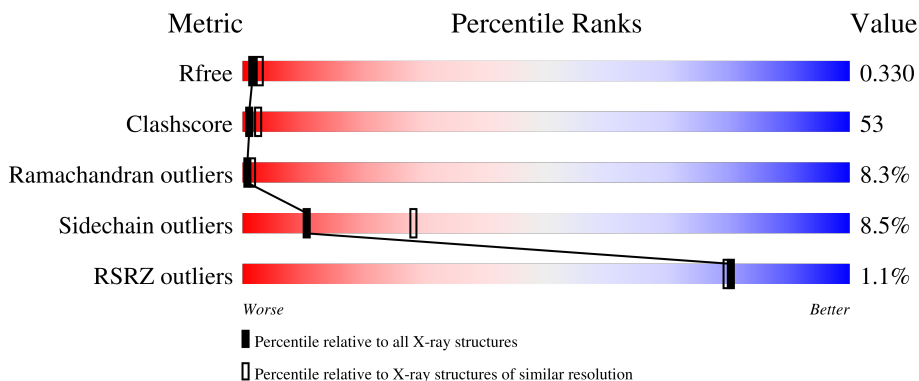
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 Å.

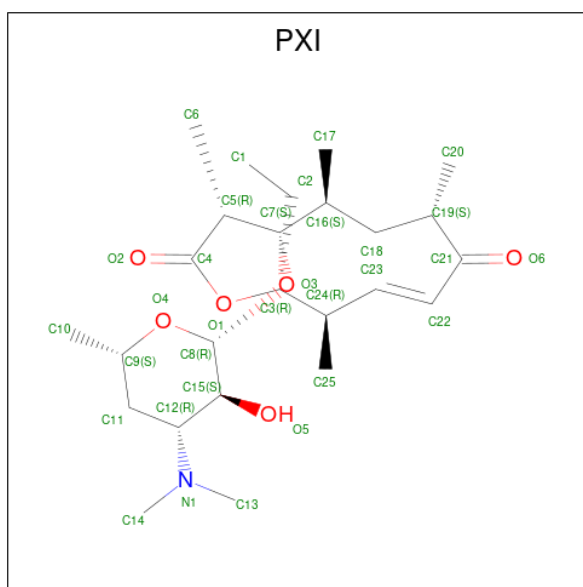
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 of 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	436	 29% 52% 8% 10%
1	B	436	 24% 55% 10% 10%



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	32	25	1	6	0	0
3	B	1	32	25	1	6	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	33	33	33	0	0
4	B	30	30	30	0	0

R374	T247	P310	T112
G375	T248	A311	M113
P376	V249	G312	R114
D377	N250	D313	R115
L378	L251	T314	R116
A379	I252	V315	V117
L380	A253	L316	E117
D381	N254	V317	L118
Y382	G255	V318	L119
S383	M256		R120
P384		D321	P121
G385	L259	A322	R122
E386	L260	H323	V123
E387	S261	R324	Q124
W388	H262	T325	E125
W389	P263	P326	I126
Y390	E327	E327	V127
P391	R328	R328	D128
W392	Q265	F329	G129
P393	L266	P330	G130
M394	A267	D331	L131
I395	A268	P332	D132
R396	L269	H333	A133
G397	R270	R334	M134
L398	A271	F335	L135
K399	D272	D336	A136
A400	M273	I337	A137
L401	T274	R338	P138
P402	L275	R339	D139
I403	L276	D340	G140
R404	L277	T341	R141
W405	G278	A342	A142
R406	E281	G343	D143
ARG	E282	H344	L144
GLY	M283	L345	M145
ARG	L284	A346	E146
GLU	R285	F347	S147
ALA	Y286	G348	L148
GLY	E287	H349	A149
ARG	G288		W150
ARG	P289	C354	P151
THR	V290	I355	L152
GLY	E291	G356	P153
	S292	A357	I154
	A293	P358	T155
	T294	L359	V156
	Y295	A360	I157
	R296	R361	S158
	F297	L362	
	P298	E363	L161
	V299	A364	G162
	E300	R365	V163
		I366	P164
		V368	E165
		A367	P166
		V368	D167
		R369	R168
		A370	A169
		L371	A170
		L372	F171
		E373	R172
			V173
			W174
			T175
			D176
			A177
			F178
			V179
			F180
			P181
			D182
			D183
			P184
			A185
			Q186
			A187
			Q188
			T189
			A190
			M191
			A192
			E193
			Y197
			L198
			L201
			L202
			D203
			S204
			K205
			R206
			L213
			L214
			V218
			R219
			E223
			D224
			G225
			S226
			R227
			L228
			E231
			E232
			L233
			M236
			A237
			H238
			I239
			L240
			L241
			V242
			A243
			G244
			H245
			E246

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.09Å 91.97Å 68.90Å 90.00° 89.92° 90.00°	Depositor
Resolution (Å)	32.41 – 2.85 45.74 – 2.85	Depositor EDS
% Data completeness (in resolution range)	92.5 (32.41-2.85) 92.2 (45.74-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 2.86Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.338 0.234 , 0.330	Depositor DCC
R_{free} test set	1675 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtrriage
Anisotropy	0.519	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 16.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	0.427 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6269	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.43	0/3098	0.68	0/4229
1	B	0.41	0/3098	0.71	0/4229
All	All	0.42	0/6196	0.70	0/8458

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3028	0	2986	314	0
1	B	3028	0	2986	342	0
2	A	43	0	30	3	0
2	B	43	0	30	5	0
3	A	32	0	43	1	0
3	B	32	0	43	7	0
4	A	33	0	0	9	0
4	B	30	0	0	9	0
All	All	6269	0	6118	656	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 53.

All (656) 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:B:55:VAL:HG11	1:B:64:VAL:HG21	1.41	1.03
1:B:285:ARG:HH11	1:B:285:ARG:HB3	1.25	1.01
1:A:285:ARG:HH21	1:A:286:TYR:HA	1.26	1.00
1:A:152:LEU:HB3	1:A:153:PRO:HD3	1.48	0.95
1:A:45:ARG:HH21	1:A:49:GLY:H	1.02	0.92
1:B:266:LEU:O	1:B:270:ARG:HB2	1.70	0.92
1:A:91:ASN:HD21	1:A:94:GLU:HG3	1.30	0.92
1:B:121:PRO:O	1:B:125:GLU:HG3	1.70	0.92
1:A:167:ASP:HB2	4:A:2015:HOH:O	1.69	0.91
1:A:97:PRO:HA	1:A:98:PRO:O	1.70	0.91
1:A:141:ARG:HB2	1:A:141:ARG:HH11	1.34	0.90
1:B:265:GLN:HE21	1:B:337:ILE:H	1.20	0.89
1:A:395:ILE:HG22	1:A:396:ARG:H	1.36	0.89
1:B:380:LEU:HD21	1:B:401:LEU:HD11	1.54	0.88
1:B:252:ILE:O	1:B:256:MET:HG2	1.72	0.88
1:A:29:TYR:OH	1:A:287:GLU:HG2	1.72	0.87
1:A:60:ARG:HD2	1:A:304:LEU:HD22	1.56	0.87
1:A:45:ARG:HH21	1:A:49:GLY:N	1.74	0.86
1:A:17:LEU:HB2	1:A:47:PRO:HD3	1.59	0.85
1:A:251:LEU:HD13	1:A:284:LEU:HD23	1.59	0.85
1:B:152:LEU:HB3	1:B:153:PRO:HD3	1.60	0.84
1:A:331:ASP:N	1:A:332:PRO:HD3	1.92	0.83
1:A:395:ILE:HD12	1:A:395:ILE:N	1.94	0.83
1:A:45:ARG:HE	1:A:49:GLY:CA	1.92	0.83
1:B:122:ARG:HA	1:B:125:GLU:OE2	1.78	0.83
1:B:127:VAL:HG22	1:B:152:LEU:HD11	1.60	0.83
1:B:162:GLY:HA3	1:B:205:LYS:HZ1	1.42	0.83
1:B:296:ARG:HG3	1:B:296:ARG:HH11	1.41	0.83
1:B:58:TYR:CD2	1:B:328:ARG:HG3	2.14	0.83
1:B:254:ASN:HD22	1:B:287:GLU:HB3	1.44	0.83
1:A:242:VAL:O	1:A:244:GLY:N	2.13	0.82
1:A:350:GLY:O	1:A:352:HIS:N	2.12	0.81
1:A:261:SER:O	1:A:263:PRO:HD3	1.80	0.81
1:A:91:ASN:ND2	1:A:94:GLU:HG3	1.95	0.80
1:B:388:VAL:HG11	1:B:399:LYS:HD2	1.61	0.79
1:B:62:ARG:HH12	1:B:349:HIS:CE1	2.00	0.79
1:A:98:PRO:O	1:A:100:HIS:N	2.16	0.79
1:A:174:TRP:HE1	1:A:193:GLU:CD	1.86	0.78
1:B:82:THR:HG23	1:B:85:GLU:OE1	1.82	0.78
1:A:398:LEU:HD12	1:A:401:LEU:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:H	1:A:332:PRO:HD3	1.47	0.78
1:B:369:ARG:HG3	1:B:369:ARG:HH11	1.48	0.78
1:A:45:ARG:NH2	1:A:49:GLY:H	1.81	0.77
1:A:137:ALA:HA	4:A:2014:HOH:O	1.84	0.77
1:A:15:LEU:HD11	1:A:20:LEU:HD11	1.66	0.77
1:A:285:ARG:HD3	1:A:339:ARG:HD3	1.67	0.77
1:B:179:VAL:HG22	1:B:395:ILE:CD1	2.15	0.77
1:B:243:ALA:HA	3:B:1408:PXI:O2	1.84	0.76
1:B:276:LEU:HD13	1:B:276:LEU:O	1.84	0.76
1:B:361:ARG:HB3	1:B:365:ARG:HH12	1.51	0.76
1:A:282:GLU:OE2	1:A:339:ARG:HD2	1.86	0.76
1:B:206:ARG:HB2	1:B:218:VAL:HG11	1.66	0.75
1:B:265:GLN:NE2	1:B:337:ILE:H	1.85	0.75
1:B:162:GLY:HA3	1:B:205:LYS:NZ	2.01	0.75
1:B:361:ARG:HB3	1:B:365:ARG:NH1	2.01	0.75
1:B:62:ARG:NH1	1:B:349:HIS:CE1	2.55	0.75
1:A:250:ASN:HB2	1:A:289:PRO:HB3	1.69	0.75
1:B:214:LEU:O	1:B:218:VAL:HG23	1.86	0.75
1:B:114:ARG:H	1:B:114:ARG:HD3	1.52	0.75
1:B:270:ARG:HH12	1:B:372:LEU:HD22	1.51	0.74
1:B:63:ALA:O	1:B:67:ASP:HB2	1.87	0.74
1:A:141:ARG:HB2	1:A:141:ARG:NH1	2.02	0.73
1:B:249:VAL:HG12	1:B:249:VAL:O	1.88	0.73
1:B:67:ASP:OD1	1:B:69:ARG:HG3	1.88	0.73
1:B:65:LEU:HA	1:B:296:ARG:HE	1.54	0.73
1:A:156:VAL:O	1:A:160:LEU:HD12	1.89	0.73
1:A:150:TRP:HB3	1:A:151:PRO:HD3	1.68	0.73
1:A:285:ARG:C	1:A:285:ARG:HE	1.92	0.73
1:A:154:ILE:HB	1:A:245:HIS:NE2	2.04	0.72
1:A:45:ARG:HH11	1:A:45:ARG:HG2	1.54	0.72
1:B:227:ARG:O	1:B:228:LEU:HB2	1.88	0.72
1:A:74:TRP:CD2	1:A:81:LEU:HD21	2.25	0.72
1:A:382:VAL:HG22	1:A:383:SER:N	2.04	0.72
1:B:171:PHE:CE2	1:B:241:LEU:HD22	2.24	0.72
1:A:285:ARG:NH2	1:A:286:TYR:HA	2.04	0.71
1:A:148:LEU:O	1:A:151:PRO:HD2	1.89	0.71
1:A:66:ALA:HB2	1:A:350:GLY:HA3	1.73	0.71
1:A:144:LEU:CD2	1:A:256:MET:HG3	2.20	0.71
1:B:115:ARG:HG3	1:B:118:LEU:HD12	1.73	0.70
1:A:127:VAL:HG22	1:A:152:LEU:CD1	2.21	0.70
1:A:336:ASP:OD1	1:A:338:ARG:HB2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ALA:HB1	1:B:389:TRP:O	1.91	0.70
1:B:150:TRP:O	1:B:153:PRO:HD2	1.92	0.70
1:A:382:VAL:HG22	1:A:383:SER:H	1.55	0.70
1:B:406:ARG:HH11	1:B:406:ARG:HB2	1.56	0.69
1:A:53:TRP:O	1:A:54:LEU:HD23	1.92	0.69
1:A:259:LEU:HD11	1:A:266:LEU:HA	1.73	0.69
1:B:289:PRO:HA	1:B:396:ARG:HB3	1.75	0.69
1:B:395:ILE:HD11	3:B:1408:PXI:O6	1.93	0.69
1:B:309:ILE:HG13	4:B:2027:HOH:O	1.92	0.69
1:B:66:ALA:HB2	1:B:349:HIS:CD2	2.29	0.68
1:A:165:GLU:HB3	1:A:166:PRO:HD3	1.74	0.68
1:B:56:VAL:HB	1:B:321:ASP:OD1	1.93	0.68
1:B:95:SER:HB3	1:B:99:ARG:HH11	1.58	0.68
1:A:272:ASP:OD2	1:A:275:LEU:HG	1.92	0.68
1:B:306:GLY:O	1:B:308:VAL:HG23	1.93	0.68
1:A:170:ALA:O	1:A:173:VAL:HB	1.94	0.68
1:A:183:ASP:OD1	1:A:185:ALA:HB3	1.94	0.68
1:A:336:ASP:C	1:A:338:ARG:H	1.97	0.68
1:B:150:TRP:HB3	1:B:151:PRO:HD3	1.76	0.68
1:B:238:HIS:NE2	3:B:1408:PXI:H102	2.08	0.68
1:A:45:ARG:NE	1:A:49:GLY:HA2	2.09	0.68
1:B:147:SER:O	1:B:151:PRO:HG2	1.94	0.67
1:B:236:MET:O	1:B:239:ILE:HG22	1.95	0.67
1:A:395:ILE:HD12	1:A:395:ILE:H	1.60	0.66
1:A:251:LEU:HD13	1:A:284:LEU:CD2	2.24	0.66
1:A:175:THR:O	1:A:179:VAL:HG23	1.94	0.66
1:B:144:LEU:HD21	1:B:256:MET:HG3	1.76	0.66
1:B:269:LEU:O	1:B:271:ALA:N	2.29	0.66
1:A:331:ASP:N	1:A:332:PRO:CD	2.58	0.66
1:A:276:LEU:HD11	1:A:365:ARG:HB3	1.78	0.65
1:A:327:GLU:N	1:A:327:GLU:OE1	2.29	0.65
1:B:74:TRP:CD2	1:B:81:LEU:HD21	2.30	0.65
1:A:149:ALA:O	1:A:249:VAL:HG22	1.97	0.65
1:B:287:GLU:HB2	4:B:2023:HOH:O	1.95	0.65
1:B:14:VAL:HG12	1:B:15:LEU:H	1.62	0.65
1:A:371:LEU:O	1:A:375:CYS:HB2	1.97	0.65
1:B:238:HIS:O	1:B:242:VAL:HG23	1.97	0.65
1:B:329:PHE:O	1:B:332:PRO:HG3	1.96	0.65
1:A:131:VAL:O	1:A:135:LEU:HG	1.96	0.65
1:B:201:LEU:HD12	1:B:204:SER:OG	1.96	0.65
1:B:405:TRP:O	1:B:406:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:TYR:HB2	4:B:2025:HOH:O	1.95	0.65
1:B:114:ARG:HD3	1:B:114:ARG:N	2.12	0.65
1:A:174:TRP:CZ2	1:A:193:GLU:HB3	2.32	0.64
1:A:259:LEU:O	1:A:266:LEU:HB2	1.97	0.64
1:B:389:TRP:HA	1:B:397:GLY:O	1.98	0.64
1:A:323:HIS:NE2	1:A:345:LEU:N	2.42	0.64
1:B:41:ALA:HB3	1:B:307:THR:HG21	1.79	0.64
1:B:359:LEU:O	1:B:363:GLU:HG3	1.98	0.64
1:A:61:ALA:HB1	1:A:317:VAL:HG13	1.80	0.64
1:B:291:GLU:N	1:B:394:MET:O	2.31	0.64
1:A:130:LEU:HD21	1:A:151:PRO:HB3	1.80	0.63
1:A:137:ALA:HB3	1:A:405:TRP:HZ2	1.63	0.63
1:B:250:ASN:O	1:B:254:ASN:HB2	1.99	0.63
1:A:122:ARG:C	1:A:124:GLN:H	2.02	0.63
1:A:282:GLU:OE1	1:A:285:ARG:HB3	1.99	0.63
1:B:344:HIS:O	1:B:345:LEU:HD23	1.98	0.63
1:B:69:ARG:O	1:B:299:VAL:HG23	1.99	0.63
1:B:36:ARG:HH12	1:B:326:PRO:HD2	1.64	0.62
1:B:124:GLN:OE1	1:B:366:ILE:HG23	1.99	0.62
1:A:120:ARG:HB3	1:A:121:PRO:HD3	1.81	0.62
1:B:164:PRO:O	1:B:168:ARG:HG3	2.00	0.62
1:A:67:ASP:HB3	1:A:70:PHE:CD1	2.35	0.62
1:B:102:ARG:O	1:B:106:LEU:HD13	1.99	0.62
1:B:202:ILE:HG22	1:B:206:ARG:NH1	2.13	0.62
1:B:152:LEU:HB3	1:B:153:PRO:CD	2.29	0.62
1:A:183:ASP:O	1:A:185:ALA:N	2.32	0.61
1:A:22:GLN:NE2	1:A:388:VAL:HA	2.15	0.61
1:A:122:ARG:NH2	4:A:2010:HOH:O	2.33	0.61
1:B:295:TYR:CE1	1:B:316:LEU:HD21	2.36	0.61
1:A:118:LEU:O	1:A:121:PRO:HD2	2.00	0.61
1:B:43:ARG:HH12	1:B:51:GLU:C	2.03	0.61
1:B:344:HIS:HD2	1:B:346:ALA:HB3	1.65	0.61
1:A:238:HIS:NE2	3:A:1408:PXI:H102	2.16	0.61
1:B:270:ARG:NH1	1:B:372:LEU:HB3	2.15	0.61
1:B:145:MET:HA	1:B:149:ALA:HB3	1.81	0.61
1:B:35:LEU:HB3	1:B:42:HIS:CD2	2.35	0.61
1:B:57:GLY:N	1:B:321:ASP:OD1	2.33	0.61
1:B:259:LEU:HD23	1:B:266:LEU:HD13	1.81	0.61
1:B:84:ALA:HB3	1:B:188:GLN:NE2	2.15	0.60
1:A:267:ALA:O	1:A:270:ARG:HB2	2.01	0.60
1:B:36:ARG:HH22	1:B:325:THR:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:TRP:NE1	1:A:172:ARG:HB2	2.15	0.60
1:B:285:ARG:HD2	1:B:329:PHE:CE2	2.36	0.60
1:A:24:PHE:HE1	1:A:31:THR:HB	1.67	0.60
1:A:61:ALA:HB1	1:A:317:VAL:CG1	2.31	0.60
1:A:204:SER:O	1:A:208:GLN:HG2	2.01	0.60
1:B:178:PHE:HD2	1:B:178:PHE:N	2.00	0.60
1:B:296:ARG:HG3	1:B:296:ARG:NH1	2.16	0.60
1:A:395:ILE:HG22	1:A:396:ARG:N	2.13	0.60
1:A:127:VAL:HG22	1:A:152:LEU:HD11	1.83	0.60
1:A:144:LEU:HD21	1:A:371:LEU:HD11	1.82	0.60
1:B:178:PHE:N	1:B:178:PHE:CD2	2.67	0.60
1:A:141:ARG:NH1	1:A:141:ARG:CB	2.65	0.60
1:A:122:ARG:NE	1:A:126:ILE:HD11	2.16	0.59
1:A:137:ALA:HB3	1:A:405:TRP:CZ2	2.36	0.59
1:B:285:ARG:HB3	1:B:285:ARG:NH1	2.07	0.59
1:B:390:TYR:CD1	1:B:397:GLY:HA3	2.37	0.59
1:B:245:HIS:O	1:B:249:VAL:HG23	2.02	0.59
1:B:369:ARG:HG3	1:B:369:ARG:NH1	2.16	0.59
1:B:93:LEU:HD21	1:B:294:THR:HG21	1.83	0.59
1:B:265:GLN:HG3	1:B:335:PHE:O	2.02	0.59
1:B:285:ARG:O	1:B:323:HIS:HB3	2.03	0.59
1:B:78:THR:HG23	1:B:312:GLY:HA3	1.85	0.59
1:A:183:ASP:OD2	1:B:138:PRO:HG2	2.03	0.59
1:A:357:ALA:HB3	1:A:358:PRO:HD3	1.85	0.59
1:B:115:ARG:HG3	1:B:118:LEU:CD1	2.31	0.59
1:A:55:VAL:HG11	1:A:64:VAL:HG21	1.85	0.59
1:A:114:ARG:HG3	1:A:114:ARG:HH11	1.68	0.59
1:A:282:GLU:OE1	1:A:282:GLU:HA	2.03	0.59
1:A:17:LEU:HG	1:A:45:ARG:O	2.03	0.59
1:A:45:ARG:HE	1:A:49:GLY:HA2	1.61	0.59
1:A:22:GLN:HE22	1:A:388:VAL:HA	1.68	0.58
1:A:170:ALA:HB1	1:A:174:TRP:CH2	2.37	0.58
1:A:251:LEU:HD22	1:A:284:LEU:HD21	1.83	0.58
1:B:119:LEU:O	1:B:123:VAL:HG23	2.03	0.58
1:B:114:ARG:O	1:B:117:GLU:HB3	2.03	0.58
1:A:15:LEU:C	1:A:15:LEU:HD12	2.24	0.58
1:B:251:LEU:HD13	1:B:284:LEU:CD2	2.33	0.58
1:A:71:SER:OG	1:A:76:ASN:ND2	2.35	0.58
1:A:45:ARG:NE	1:A:49:GLY:CA	2.65	0.58
1:A:395:ILE:N	1:A:395:ILE:CD1	2.65	0.58
1:B:395:ILE:HG22	1:B:396:ARG:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:TRP:CE2	1:B:81:LEU:HD21	2.38	0.58
1:A:355:ILE:HG12	1:A:355:ILE:O	2.03	0.58
1:A:193:GLU:O	1:A:196:GLY:N	2.36	0.57
1:A:336:ASP:O	1:A:338:ARG:N	2.37	0.57
1:A:123:VAL:HG21	1:A:362:LEU:HD23	1.85	0.57
1:A:336:ASP:O	1:A:339:ARG:N	2.37	0.57
1:B:147:SER:O	1:B:151:PRO:HD2	2.04	0.57
1:A:35:LEU:HD22	1:A:42:HIS:CD2	2.39	0.57
1:B:148:LEU:HD23	1:B:371:LEU:HD11	1.85	0.57
1:B:251:LEU:O	1:B:255:GLY:N	2.36	0.57
1:B:406:ARG:HH11	1:B:406:ARG:CB	2.17	0.57
1:A:387:LEU:HB2	4:A:2026:HOH:O	2.03	0.57
1:B:175:THR:O	1:B:179:VAL:HG23	2.04	0.57
1:B:148:LEU:CD2	1:B:371:LEU:HD11	2.34	0.57
1:A:174:TRP:HD1	1:A:190:ALA:HB1	1.70	0.57
1:B:169:ALA:O	1:B:173:VAL:HG23	2.05	0.57
1:B:331:ASP:OD1	1:B:334:ARG:HB2	2.05	0.56
1:A:67:ASP:HB3	1:A:70:PHE:HD1	1.70	0.56
1:A:123:VAL:HG12	1:A:123:VAL:O	2.05	0.56
1:A:279:ALA:HA	1:A:337:ILE:HG22	1.86	0.56
1:B:147:SER:O	1:B:151:PRO:CG	2.53	0.56
1:B:228:LEU:HA	1:B:232:GLU:OE2	2.04	0.56
1:B:270:ARG:HH11	1:B:270:ARG:HG2	1.69	0.56
1:A:133:ALA:O	1:A:136:ALA:HB3	2.05	0.56
1:A:377:ASP:HB2	1:A:406:ARG:CA	2.36	0.56
1:B:104:ARG:HG3	1:B:104:ARG:HH11	1.70	0.56
1:B:127:VAL:HG12	1:B:128:ASP:N	2.19	0.56
1:B:187:ALA:O	1:B:191:MET:HG3	2.05	0.56
1:B:293:ALA:HB1	2:B:1407:HEM:O2A	2.05	0.56
1:B:304:LEU:O	1:B:305:ASP:C	2.44	0.56
1:B:331:ASP:O	1:B:334:ARG:HB3	2.06	0.56
1:B:357:ALA:HB3	1:B:358:PRO:HD3	1.87	0.56
1:A:329:PHE:N	1:A:330:PRO:HD3	2.20	0.56
1:A:390:TYR:OH	1:A:399:LYS:HA	2.06	0.56
1:B:39:GLY:H	1:B:42:HIS:HE1	1.53	0.56
1:B:285:ARG:HD2	1:B:329:PHE:CD2	2.41	0.56
1:A:354:CYS:HB2	2:A:1407:HEM:C4A	2.40	0.56
1:B:270:ARG:NH1	1:B:270:ARG:HG2	2.21	0.56
1:A:58:TYR:HE1	1:A:343:GLY:O	1.89	0.56
1:B:281:GLU:OE2	1:B:361:ARG:NE	2.39	0.56
1:A:146:GLU:HA	1:A:146:GLU:OE2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ARG:HG3	1:A:296:ARG:HH11	1.70	0.56
1:A:406:ARG:HH11	1:A:406:ARG:HB2	1.70	0.55
1:B:261:SER:C	1:B:263:PRO:HD3	2.27	0.55
1:A:144:LEU:HD23	1:A:256:MET:HG3	1.86	0.55
1:A:152:LEU:HB3	1:A:153:PRO:CD	2.31	0.55
1:B:242:VAL:O	1:B:243:ALA:C	2.45	0.55
1:B:276:LEU:O	1:B:276:LEU:HD22	2.06	0.55
1:A:405:TRP:O	1:A:406:ARG:HG3	2.07	0.55
1:B:135:LEU:HD21	1:B:375:CYS:SG	2.45	0.55
1:B:231:GLU:HG3	4:B:2018:HOH:O	2.06	0.55
1:B:129:GLY:HA2	1:B:132:ASP:OD2	2.07	0.55
1:B:261:SER:O	1:B:263:PRO:HD3	2.07	0.55
1:A:331:ASP:OD2	1:A:334:ARG:HB2	2.07	0.55
1:B:201:LEU:HD11	1:B:205:LYS:HE2	1.88	0.55
1:A:256:MET:O	1:A:260:LEU:HG	2.07	0.55
1:B:93:LEU:HD23	3:B:1408:PXI:H6C2	1.89	0.55
1:B:340:ASP:C	1:B:342:ALA:H	2.10	0.55
1:B:282:GLU:CD	1:B:285:ARG:NH1	2.60	0.55
1:B:344:HIS:CD2	1:B:346:ALA:HB3	2.42	0.55
1:B:35:LEU:O	1:B:38:GLU:HB2	2.07	0.54
1:B:138:PRO:HD2	1:B:139:ASP:OD1	2.08	0.54
1:A:171:PHE:CE2	1:A:241:LEU:HD13	2.43	0.54
1:A:293:ALA:O	1:A:316:LEU:HD22	2.07	0.54
1:B:285:ARG:HH11	1:B:285:ARG:CB	2.11	0.54
1:A:247:THR:O	1:A:289:PRO:HG3	2.07	0.54
1:B:142:ALA:O	1:B:403:ILE:HG12	2.06	0.54
1:A:127:VAL:HG22	1:A:152:LEU:HD13	1.88	0.54
1:A:164:PRO:HB2	4:A:2015:HOH:O	2.07	0.54
1:B:125:GLU:O	1:B:126:ILE:C	2.45	0.54
1:B:236:MET:HA	1:B:239:ILE:HG22	1.89	0.54
1:B:281:GLU:O	1:B:284:LEU:HB2	2.08	0.54
1:B:327:GLU:O	1:B:330:PRO:HD3	2.08	0.54
1:A:171:PHE:HA	1:A:174:TRP:CE3	2.42	0.54
1:A:148:LEU:O	1:A:149:ALA:C	2.46	0.54
1:B:60:ARG:O	1:B:64:VAL:HG23	2.08	0.54
1:B:14:VAL:HG12	1:B:15:LEU:N	2.23	0.54
1:B:17:LEU:HD12	1:B:46:THR:HA	1.90	0.54
1:A:93:LEU:HD23	1:A:239:ILE:HD11	1.90	0.54
1:B:178:PHE:HD2	1:B:178:PHE:H	1.55	0.54
1:B:245:HIS:HB3	1:B:246:GLU:OE1	2.06	0.54
1:B:82:THR:HG21	1:B:188:GLN:OE1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:ALA:HB3	1:B:188:GLN:HE22	1.73	0.53
1:B:109:ARG:O	1:B:112:THR:HG23	2.08	0.53
1:B:151:PRO:O	1:B:152:LEU:C	2.46	0.53
1:B:157:ILE:HG23	1:B:158:SER:N	2.23	0.53
1:A:58:TYR:HA	1:A:322:ALA:HB1	1.90	0.53
1:A:112:THR:O	1:A:116:VAL:HG23	2.08	0.53
1:B:151:PRO:O	1:B:154:ILE:HG22	2.09	0.53
1:A:70:PHE:HB2	4:A:2005:HOH:O	2.09	0.53
1:A:149:ALA:HB1	1:A:249:VAL:HG13	1.91	0.53
1:B:259:LEU:HD12	1:B:335:PHE:CE2	2.43	0.53
1:B:406:ARG:CB	1:B:406:ARG:NH1	2.72	0.53
1:A:171:PHE:HA	1:A:174:TRP:HE3	1.72	0.53
1:B:281:GLU:O	1:B:284:LEU:N	2.40	0.53
1:A:382:VAL:CG2	1:A:383:SER:H	2.21	0.53
1:A:351:ILE:HG13	1:A:352:HIS:N	2.23	0.53
1:B:227:ARG:O	1:B:227:ARG:HG2	2.09	0.53
1:B:267:ALA:HA	1:B:270:ARG:HB2	1.91	0.53
1:A:45:ARG:HE	1:A:49:GLY:C	2.13	0.53
1:B:344:HIS:HD2	1:B:346:ALA:CB	2.22	0.52
1:A:33:ALA:O	1:A:34:ARG:C	2.47	0.52
1:A:81:LEU:HD12	1:A:86:ALA:HB2	1.90	0.52
1:B:92:MET:HE1	1:B:104:ARG:HA	1.92	0.52
1:B:298:PRO:HB2	1:B:300:GLU:O	2.10	0.52
1:B:29:TYR:HB2	1:B:30:PRO:HD3	1.91	0.52
1:A:60:ARG:O	1:A:64:VAL:HG23	2.08	0.52
1:B:272:ASP:OD1	1:B:273:MET:N	2.42	0.52
1:A:144:LEU:HD21	1:A:371:LEU:CD1	2.39	0.52
1:B:310:PRO:HD2	1:B:313:ASP:OD2	2.10	0.52
1:B:92:MET:HE1	1:B:107:VAL:HG22	1.92	0.52
1:B:273:MET:C	1:B:275:LEU:H	2.12	0.52
1:B:331:ASP:CG	1:B:334:ARG:HB2	2.30	0.52
1:A:181:PRO:HA	1:A:186:GLN:OE1	2.09	0.52
1:B:197:TYR:CD2	1:B:198:LEU:HD23	2.45	0.52
1:B:77:SER:HB2	1:B:297:PHE:CD2	2.45	0.51
1:A:325:THR:HG22	1:A:327:GLU:H	1.76	0.51
1:A:99:ARG:C	1:A:101:THR:H	2.14	0.51
1:A:242:VAL:HG12	1:A:243:ALA:N	2.26	0.51
1:B:116:VAL:HG21	1:B:358:PRO:HB2	1.92	0.51
1:B:272:ASP:OD1	1:B:274:THR:HG23	2.10	0.51
1:A:330:PRO:O	1:A:331:ASP:HB3	2.11	0.51
1:B:61:ALA:HA	1:B:64:VAL:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:VAL:O	1:B:300:GLU:CB	2.59	0.51
1:A:150:TRP:CE2	1:A:172:ARG:HD2	2.46	0.51
1:B:53:TRP:NE1	1:B:313:ASP:OD2	2.44	0.51
1:A:53:TRP:CD2	1:A:309:ILE:HG12	2.45	0.51
1:A:214:LEU:O	1:A:217:LEU:N	2.43	0.51
1:B:24:PHE:O	1:B:28:PRO:HB3	2.10	0.51
1:A:25:ALA:O	1:A:28:PRO:HD3	2.11	0.50
1:A:298:PRO:HD2	1:A:313:ASP:O	2.11	0.50
1:A:15:LEU:HD12	1:A:16:ASP:O	2.11	0.50
1:A:276:LEU:CD1	1:A:365:ARG:HB3	2.41	0.50
1:B:388:VAL:CG1	1:B:399:LYS:HD2	2.38	0.50
1:A:145:MET:HA	1:A:149:ALA:HB3	1.94	0.50
1:A:165:GLU:CB	1:A:166:PRO:HD3	2.41	0.50
1:A:225:GLY:HA2	1:A:228:LEU:O	2.11	0.50
1:A:260:LEU:HD21	1:A:378:LEU:HD21	1.93	0.50
1:A:282:GLU:HG3	1:A:335:PHE:CE1	2.46	0.50
1:B:243:ALA:O	1:B:247:THR:OG1	2.27	0.50
1:A:252:ILE:O	1:A:256:MET:HG2	2.11	0.50
1:A:364:ALA:O	1:A:367:ALA:HB3	2.11	0.50
1:A:382:VAL:CG2	1:A:383:SER:N	2.73	0.50
1:B:83:GLU:HA	4:B:2004:HOH:O	2.11	0.50
1:B:127:VAL:O	1:B:130:LEU:N	2.44	0.50
1:B:135:LEU:HD11	1:B:374:ARG:HB3	1.94	0.50
1:B:189:THR:O	1:B:193:GLU:HG3	2.11	0.50
1:B:368:VAL:O	1:B:372:LEU:HG	2.11	0.50
1:A:146:GLU:CG	1:A:146:GLU:O	2.60	0.50
1:B:115:ARG:HA	1:B:118:LEU:HG	1.92	0.50
1:B:131:VAL:O	1:B:131:VAL:CG1	2.60	0.50
1:B:244:GLY:HA2	1:B:247:THR:OG1	2.11	0.50
1:B:310:PRO:HG2	1:B:313:ASP:OD1	2.11	0.50
1:A:99:ARG:C	1:A:101:THR:N	2.65	0.50
1:A:99:ARG:HG2	1:A:103:LEU:HD11	1.94	0.50
1:B:165:GLU:N	1:B:166:PRO:CD	2.74	0.50
1:B:150:TRP:HA	1:B:249:VAL:HG13	1.93	0.50
1:A:161:LEU:O	1:A:214:LEU:HB2	2.12	0.49
1:A:336:ASP:O	1:A:339:ARG:HB3	2.12	0.49
1:B:273:MET:HE3	1:B:276:LEU:HB2	1.94	0.49
1:A:74:TRP:CE2	1:A:81:LEU:HD21	2.47	0.49
1:A:287:GLU:CD	1:A:396:ARG:HH21	2.16	0.49
1:A:66:ALA:CB	1:A:350:GLY:HA3	2.42	0.49
1:B:247:THR:HB	2:B:1407:HEM:CAB	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ALA:N	1:B:358:PRO:CD	2.75	0.49
1:A:331:ASP:OD2	1:A:334:ARG:HD2	2.12	0.49
1:A:356:GLY:O	1:A:357:ALA:C	2.51	0.49
1:B:66:ALA:HB2	1:B:349:HIS:HD2	1.77	0.49
1:B:131:VAL:O	1:B:131:VAL:HG12	2.12	0.49
1:B:286:TYR:CD1	1:B:324:ARG:NH2	2.81	0.49
1:B:227:ARG:NH2	4:B:2017:HOH:O	2.45	0.49
1:B:395:ILE:CG2	1:B:396:ARG:N	2.76	0.49
1:A:140:GLY:O	1:A:404:ARG:HA	2.13	0.49
1:B:203:ASP:OD1	1:B:203:ASP:N	2.46	0.49
1:B:243:ALA:HB1	3:B:1408:PXI:H1C2	1.94	0.49
1:A:406:ARG:NH1	1:A:406:ARG:CB	2.75	0.49
1:B:43:ARG:HG3	1:B:53:TRP:CE2	2.47	0.49
1:B:148:LEU:O	1:B:151:PRO:HD2	2.13	0.49
1:B:337:ILE:O	1:B:337:ILE:HG13	2.13	0.49
1:A:15:LEU:O	1:A:15:LEU:HG	2.13	0.49
1:B:132:ASP:O	1:B:136:ALA:N	2.46	0.49
1:B:74:TRP:HD1	1:B:89:ASN:HD22	1.61	0.49
1:B:162:GLY:O	1:B:164:PRO:HD3	2.12	0.49
1:B:247:THR:O	1:B:289:PRO:HG3	2.12	0.49
1:B:277:ASP:HB3	1:B:365:ARG:HE	1.78	0.49
1:A:141:ARG:HH11	1:A:141:ARG:CB	2.15	0.48
1:A:205:LYS:HE2	1:A:214:LEU:HD23	1.95	0.48
1:B:123:VAL:O	1:B:127:VAL:HG23	2.12	0.48
1:B:201:LEU:O	1:B:205:LYS:HG2	2.13	0.48
1:A:114:ARG:HG3	1:A:114:ARG:NH1	2.27	0.48
1:B:149:ALA:O	1:B:249:VAL:HA	2.13	0.48
1:A:144:LEU:HD21	1:A:256:MET:HG3	1.92	0.48
1:A:182:ASP:CB	1:A:186:GLN:NE2	2.77	0.48
1:A:45:ARG:HH11	1:A:45:ARG:CG	2.22	0.48
1:A:88:LEU:C	1:A:90:HIS:H	2.17	0.48
1:A:329:PHE:HB3	1:A:339:ARG:NH1	2.29	0.48
1:A:336:ASP:C	1:A:338:ARG:N	2.64	0.48
1:B:179:VAL:HG13	1:B:395:ILE:HD12	1.95	0.48
1:B:246:GLU:HG3	3:B:1408:PXI:O6	2.13	0.48
1:A:58:TYR:CE1	1:A:343:GLY:O	2.67	0.48
1:A:108:ALA:O	1:A:110:GLU:N	2.46	0.48
1:B:259:LEU:HD12	1:B:335:PHE:HE2	1.78	0.48
1:A:91:ASN:CG	1:A:94:GLU:HG3	2.33	0.48
1:B:36:ARG:NH2	1:B:325:THR:HA	2.27	0.48
1:A:69:ARG:O	1:A:298:PRO:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:O	1:B:181:PRO:HB3	2.14	0.48
1:A:30:PRO:O	1:A:33:ALA:HB3	2.14	0.47
1:A:60:ARG:N	4:A:2003:HOH:O	2.46	0.47
1:B:238:HIS:CD2	3:B:1408:PXI:H102	2.49	0.47
1:B:380:LEU:HD21	1:B:401:LEU:CD1	2.36	0.47
1:A:93:LEU:O	1:A:93:LEU:HD12	2.15	0.47
1:B:244:GLY:HA3	2:B:1407:HEM:C2C	2.49	0.47
1:B:295:TYR:CD1	1:B:314:THR:CG2	2.96	0.47
1:B:389:TRP:CE2	1:B:398:LEU:HD21	2.49	0.47
1:A:98:PRO:HA	1:A:101:THR:OG1	2.14	0.47
1:A:239:ILE:O	1:A:243:ALA:HB3	2.14	0.47
1:B:270:ARG:HH22	1:B:372:LEU:HA	1.79	0.47
1:A:147:SER:O	1:A:151:PRO:HG2	2.14	0.47
1:B:144:LEU:HB2	1:B:403:ILE:HD13	1.96	0.47
1:B:369:ARG:NH1	1:B:369:ARG:CG	2.77	0.47
1:B:153:PRO:O	1:B:155:THR:N	2.48	0.47
1:B:259:LEU:CD2	1:B:266:LEU:HD13	2.45	0.47
1:B:278:GLY:C	4:B:2022:HOH:O	2.51	0.47
1:B:344:HIS:C	1:B:345:LEU:HD23	2.35	0.47
1:A:179:VAL:HG11	1:A:390:TYR:CD1	2.49	0.47
1:B:251:LEU:HD13	1:B:284:LEU:HD21	1.97	0.47
1:A:64:VAL:HG13	1:A:70:PHE:CD1	2.50	0.47
1:A:203:ASP:O	1:A:204:SER:C	2.53	0.47
1:A:344:HIS:HD2	1:A:346:ALA:HB3	1.78	0.47
1:A:24:PHE:O	1:A:28:PRO:CD	2.63	0.47
1:A:174:TRP:NE1	1:A:193:GLU:HB2	2.30	0.47
1:A:177:ALA:O	1:A:181:PRO:HB3	2.14	0.47
1:B:273:MET:CE	1:B:276:LEU:HB2	2.45	0.47
1:B:72:LYS:HE3	1:B:294:THR:OG1	2.15	0.47
1:B:270:ARG:HH12	1:B:372:LEU:CD2	2.23	0.47
1:A:41:ALA:HB3	1:A:307:THR:HG21	1.98	0.46
1:B:147:SER:O	1:B:151:PRO:CD	2.63	0.46
1:B:269:LEU:O	1:B:270:ARG:C	2.52	0.46
1:A:139:ASP:CG	1:A:140:GLY:H	2.19	0.46
1:A:324:ARG:HG3	1:A:324:ARG:HH11	1.79	0.46
1:B:101:THR:O	1:B:102:ARG:C	2.52	0.46
1:B:123:VAL:O	1:B:123:VAL:HG12	2.15	0.46
1:B:144:LEU:HD11	1:B:148:LEU:HD23	1.97	0.46
1:B:148:LEU:O	1:B:150:TRP:N	2.49	0.46
1:B:382:VAL:HG11	1:B:402:PRO:HD2	1.97	0.46
1:A:158:SER:CB	1:A:163:VAL:HB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:LEU:HD23	1:A:234:LEU:HD21	1.97	0.46
1:A:150:TRP:HE1	1:A:172:ARG:HB2	1.78	0.46
1:B:249:VAL:O	1:B:249:VAL:CG1	2.60	0.46
1:B:269:LEU:O	1:B:272:ASP:O	2.34	0.46
1:B:270:ARG:O	1:B:270:ARG:HD3	2.16	0.46
1:A:53:TRP:CE2	1:A:309:ILE:HG12	2.51	0.46
1:B:228:LEU:HD12	1:B:232:GLU:CB	2.45	0.46
1:B:282:GLU:HA	1:B:282:GLU:OE1	2.14	0.46
1:B:323:HIS:HE1	1:B:346:ALA:HB2	1.80	0.46
1:A:205:LYS:O	1:A:206:ARG:C	2.52	0.46
1:A:360:ALA:HB1	2:A:1407:HEM:CBB	2.45	0.46
1:B:70:PHE:HB3	1:B:296:ARG:HB3	1.97	0.46
1:B:233:LEU:HD12	1:B:233:LEU:C	2.36	0.46
1:A:64:VAL:HG13	1:A:70:PHE:CE1	2.51	0.46
1:A:100:HIS:CD2	1:A:352:HIS:CE1	3.03	0.46
1:A:280:VAL:HG21	1:A:365:ARG:HG3	1.96	0.46
1:B:22:GLN:O	1:B:22:GLN:HG3	2.14	0.46
1:B:197:TYR:HD2	1:B:198:LEU:HD23	1.80	0.46
1:B:269:LEU:HD12	1:B:272:ASP:O	2.15	0.46
1:B:381:ASP:O	1:B:382:VAL:HB	2.16	0.46
1:A:91:ASN:OD1	1:A:94:GLU:HG3	2.15	0.46
1:B:291:GLU:HB3	1:B:393:PRO:O	2.16	0.46
1:B:388:VAL:HG11	1:B:399:LYS:CD	2.40	0.46
1:A:139:ASP:OD1	1:A:139:ASP:N	2.49	0.46
1:B:388:VAL:HB	1:B:399:LYS:HB2	1.98	0.46
1:A:24:PHE:O	1:A:28:PRO:HB3	2.16	0.45
1:A:91:ASN:HD21	1:A:94:GLU:CG	2.16	0.45
1:A:249:VAL:O	1:A:252:ILE:HB	2.16	0.45
1:B:287:GLU:HA	4:B:2024:HOH:O	2.15	0.45
1:A:45:ARG:CG	1:A:45:ARG:NH1	2.79	0.45
1:A:114:ARG:O	1:A:115:ARG:C	2.54	0.45
1:B:92:MET:CE	1:B:104:ARG:HA	2.45	0.45
1:B:157:ILE:HD13	4:B:2019:HOH:O	2.15	0.45
1:B:247:THR:HB	2:B:1407:HEM:C3B	2.51	0.45
1:B:248:THR:C	1:B:250:ASN:H	2.19	0.45
1:B:340:ASP:OD2	1:B:342:ALA:CB	2.64	0.45
1:A:123:VAL:O	1:A:366:ILE:HG21	2.16	0.45
1:A:259:LEU:HD21	1:A:269:LEU:HD23	1.97	0.45
1:A:291:GLU:HB2	1:A:395:ILE:O	2.15	0.45
1:A:390:TYR:CE2	1:A:399:LYS:HA	2.52	0.45
1:B:82:THR:HG1	1:B:85:GLU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:VAL:HG11	1:B:390:TYR:CD1	2.52	0.45
1:B:205:LYS:HE3	1:B:214:LEU:HD23	1.98	0.45
1:B:267:ALA:HA	1:B:270:ARG:CB	2.45	0.45
1:A:45:ARG:CZ	1:A:49:GLY:HA2	2.47	0.45
1:B:120:ARG:HB3	1:B:121:PRO:HD3	1.98	0.45
1:B:383:SER:O	1:B:385:GLY:N	2.49	0.45
1:A:56:VAL:HG12	1:A:318:VAL:HB	1.98	0.45
1:A:62:ARG:HB2	1:A:345:LEU:HD11	1.98	0.45
1:A:78:THR:O	1:A:80:PRO:HD3	2.17	0.45
1:A:24:PHE:HE1	1:A:31:THR:CB	2.29	0.45
1:A:328:ARG:HG2	1:A:328:ARG:HH11	1.82	0.45
1:B:74:TRP:CE3	1:B:81:LEU:HD21	2.51	0.45
1:B:127:VAL:O	1:B:128:ASP:C	2.54	0.45
1:B:380:LEU:HD22	1:B:382:VAL:HG12	1.99	0.45
1:A:14:VAL:N	4:A:2001:HOH:O	2.50	0.45
1:A:224:ASP:OD2	1:A:227:ARG:HG3	2.16	0.45
1:A:324:ARG:HG3	1:A:324:ARG:NH1	2.32	0.45
1:A:329:PHE:N	1:A:330:PRO:CD	2.79	0.45
1:B:126:ILE:HD13	1:B:155:THR:CG2	2.46	0.45
1:B:150:TRP:HA	1:B:249:VAL:HG22	1.98	0.45
1:A:20:LEU:HB3	1:A:24:PHE:HB2	1.98	0.45
1:A:32:TYR:HB3	1:A:321:ASP:HB2	1.98	0.45
1:A:139:ASP:CG	1:A:140:GLY:N	2.71	0.45
1:B:77:SER:HB2	1:B:297:PHE:CE2	2.51	0.45
1:B:175:THR:HG23	1:B:246:GLU:OE2	2.17	0.45
1:B:177:ALA:O	1:B:181:PRO:HD3	2.17	0.45
1:B:371:LEU:O	1:B:375:CYS:HB2	2.17	0.45
1:A:150:TRP:HB3	1:A:151:PRO:CD	2.44	0.44
1:A:331:ASP:O	1:A:334:ARG:HB2	2.18	0.44
1:A:150:TRP:CD2	1:A:172:ARG:HD2	2.52	0.44
1:A:90:HIS:ND1	1:A:99:ARG:NH2	2.64	0.44
1:A:188:GLN:HA	1:A:191:MET:HE3	1.99	0.44
1:A:344:HIS:HD2	1:A:346:ALA:CB	2.30	0.44
1:B:174:TRP:O	1:B:176:ASP:N	2.51	0.44
1:B:183:ASP:O	1:B:185:ALA:N	2.47	0.44
1:B:285:ARG:HH12	1:B:286:TYR:HB2	1.83	0.44
1:B:360:ALA:O	1:B:362:LEU:N	2.50	0.44
1:A:148:LEU:O	1:A:151:PRO:CD	2.64	0.44
1:B:161:LEU:HD23	1:B:213:LEU:HB3	1.99	0.44
1:A:370:ALA:O	1:A:373:GLU:N	2.49	0.44
1:B:296:ARG:NH1	1:B:296:ARG:CG	2.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ARG:O	1:B:365:ARG:HG3	2.17	0.44
1:B:380:LEU:HD23	1:B:402:PRO:O	2.17	0.44
1:B:141:ARG:HG2	1:B:404:ARG:HB3	1.99	0.44
1:A:36:ARG:HH12	1:A:326:PRO:HD2	1.83	0.44
1:A:122:ARG:C	1:A:124:GLN:N	2.69	0.44
1:A:143:ASP:HA	1:A:402:PRO:HA	2.00	0.44
1:A:282:GLU:OE1	1:A:282:GLU:CA	2.66	0.44
1:B:108:ALA:HA	1:B:355:ILE:HD11	1.99	0.44
1:B:284:LEU:O	1:B:346:ALA:HB2	2.17	0.44
1:A:171:PHE:HE2	1:A:241:LEU:HD13	1.80	0.44
1:A:265:GLN:HE21	1:A:336:ASP:HA	1.82	0.44
1:A:333:HIS:CE1	4:A:2023:HOH:O	2.70	0.44
1:A:174:TRP:CD1	1:A:190:ALA:HB1	2.51	0.43
1:A:359:LEU:O	1:A:363:GLU:HG3	2.17	0.43
1:A:319:LEU:HD22	1:A:345:LEU:HB2	2.00	0.43
1:B:14:VAL:HA	1:B:43:ARG:O	2.18	0.43
1:A:146:GLU:OE2	1:A:146:GLU:CA	2.64	0.43
1:A:146:GLU:O	1:A:146:GLU:HG3	2.18	0.43
1:A:158:SER:HB3	1:A:163:VAL:HB	2.01	0.43
1:A:282:GLU:CD	1:A:339:ARG:HD2	2.38	0.43
1:B:45:ARG:HH11	1:B:45:ARG:CB	2.32	0.43
1:B:156:VAL:HG11	1:B:359:LEU:HD11	1.99	0.43
1:B:331:ASP:O	1:B:339:ARG:NH2	2.48	0.43
1:A:82:THR:O	1:A:83:GLU:C	2.55	0.43
1:B:242:VAL:O	1:B:244:GLY:N	2.52	0.43
1:B:270:ARG:NH1	1:B:372:LEU:HD22	2.26	0.43
1:A:161:LEU:HD13	1:A:241:LEU:HG	2.01	0.43
1:A:357:ALA:N	1:A:358:PRO:CD	2.81	0.43
1:B:186:GLN:O	1:B:190:ALA:N	2.42	0.43
1:A:351:ILE:CG1	1:A:352:HIS:N	2.82	0.43
1:A:150:TRP:CE2	1:A:172:ARG:HB2	2.53	0.43
1:A:344:HIS:CD2	1:A:346:ALA:HB3	2.52	0.43
1:B:90:HIS:O	1:B:232:GLU:HA	2.19	0.43
1:B:227:ARG:O	1:B:227:ARG:CG	2.67	0.43
1:B:390:TYR:HA	1:B:391:PRO:HD3	1.86	0.43
1:B:44:VAL:HG21	1:B:54:LEU:HD11	2.00	0.43
1:B:55:VAL:HB	1:B:317:VAL:HA	2.01	0.43
1:A:24:PHE:O	1:A:28:PRO:N	2.51	0.42
1:A:96:ASP:HB3	1:A:97:PRO:HD2	2.00	0.42
1:B:106:LEU:HD23	1:B:228:LEU:HD22	2.01	0.42
1:B:348:GLY:O	1:B:349:HIS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LEU:C	1:A:162:GLY:H	2.23	0.42
1:A:250:ASN:CB	1:A:289:PRO:HB3	2.45	0.42
1:A:279:ALA:HA	1:A:337:ILE:CG2	2.49	0.42
1:B:382:VAL:HG23	1:B:386:GLU:OE1	2.19	0.42
1:A:280:VAL:HG21	1:A:365:ARG:CG	2.49	0.42
1:B:273:MET:C	1:B:275:LEU:N	2.72	0.42
1:A:126:ILE:HD13	1:A:155:THR:CG2	2.49	0.42
1:B:150:TRP:O	1:B:151:PRO:O	2.38	0.42
1:B:179:VAL:HG22	1:B:395:ILE:HD11	1.99	0.42
1:A:265:GLN:O	1:A:268:ALA:N	2.53	0.42
1:A:398:LEU:CD1	1:A:401:LEU:HB2	2.44	0.42
1:A:149:ALA:O	1:A:153:PRO:HD2	2.20	0.42
1:A:228:LEU:CD1	1:A:232:GLU:HB3	2.49	0.42
1:A:326:PRO:O	1:A:330:PRO:HG3	2.20	0.42
1:B:303:ASP:C	1:B:303:ASP:OD1	2.57	0.42
2:B:1407:HEM:HMA2	2:B:1407:HEM:HAA1	1.90	0.42
1:A:224:ASP:C	1:A:226:SER:H	2.22	0.42
1:B:45:ARG:HH11	1:B:45:ARG:HB3	1.85	0.42
1:B:336:ASP:OD1	1:B:338:ARG:HB2	2.19	0.42
1:B:389:TRP:CZ3	1:B:396:ARG:NE	2.88	0.42
1:A:22:GLN:HE22	1:A:389:TRP:H	1.67	0.42
1:A:384:PRO:HA	1:A:387:LEU:CD1	2.50	0.42
1:B:43:ARG:HG2	1:B:43:ARG:HH11	1.85	0.42
1:A:24:PHE:O	1:A:28:PRO:HD3	2.20	0.41
1:A:130:LEU:CD1	1:A:151:PRO:HB2	2.50	0.41
1:A:285:ARG:HD3	1:A:339:ARG:CD	2.46	0.41
1:B:26:ALA:HB2	1:B:389:TRP:CD1	2.55	0.41
1:B:122:ARG:O	1:B:122:ARG:HG3	2.19	0.41
1:B:239:ILE:HD12	1:B:239:ILE:HA	1.90	0.41
1:B:304:LEU:O	1:B:307:THR:N	2.53	0.41
1:A:149:ALA:HA	1:A:252:ILE:HG21	2.03	0.41
1:B:276:LEU:O	1:B:276:LEU:CD1	2.64	0.41
1:A:24:PHE:O	1:A:25:ALA:C	2.58	0.41
1:A:377:ASP:HB2	1:A:406:ARG:HA	2.02	0.41
1:B:102:ARG:HH12	1:B:232:GLU:CD	2.24	0.41
1:B:225:GLY:O	1:B:228:LEU:N	2.35	0.41
1:A:259:LEU:HG	1:A:266:LEU:HD13	2.03	0.41
1:A:265:GLN:O	1:A:268:ALA:HB3	2.20	0.41
1:A:24:PHE:CZ	1:A:28:PRO:HB2	2.55	0.41
1:A:155:THR:HG23	1:A:168:ARG:NH1	2.36	0.41
1:B:375:CYS:HB3	1:B:378:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:THR:H	1:A:85:GLU:HB2	1.86	0.41
1:A:395:ILE:CG2	1:A:396:ARG:H	2.18	0.41
1:B:17:LEU:HD11	1:B:44:VAL:HG21	2.02	0.41
1:B:134:MET:C	1:B:136:ALA:H	2.24	0.41
1:B:269:LEU:C	1:B:271:ALA:N	2.72	0.41
1:B:282:GLU:OE2	1:B:285:ARG:NH1	2.53	0.41
1:A:127:VAL:CG2	1:A:152:LEU:HD11	2.48	0.41
1:B:174:TRP:C	1:B:176:ASP:N	2.73	0.41
1:B:225:GLY:HA2	1:B:228:LEU:O	2.21	0.41
1:B:356:GLY:O	1:B:357:ALA:C	2.59	0.41
1:A:65:LEU:HD12	1:A:345:LEU:HD13	2.02	0.41
1:A:141:ARG:HG2	1:A:381:ASP:OD1	2.21	0.41
1:A:319:LEU:CD2	1:A:345:LEU:HB2	2.50	0.41
1:B:171:PHE:HA	1:B:174:TRP:HE3	1.85	0.41
1:B:179:VAL:HG22	1:B:395:ILE:HD13	1.98	0.41
1:B:228:LEU:HD12	1:B:232:GLU:HB3	2.01	0.41
1:A:14:VAL:HA	1:A:43:ARG:O	2.21	0.41
1:A:150:TRP:O	1:A:153:PRO:HD2	2.21	0.41
1:A:156:VAL:HG12	1:A:160:LEU:HD12	2.02	0.41
1:A:191:MET:O	1:A:195:SER:HB3	2.21	0.41
2:A:1407:HEM:HMA2	2:A:1407:HEM:HAA1	1.81	0.41
1:B:32:TYR:CE2	1:B:318:VAL:HG11	2.55	0.41
1:B:43:ARG:HH12	1:B:51:GLU:CB	2.34	0.41
1:B:46:THR:HG23	1:B:52:VAL:HG22	2.03	0.41
1:B:48:GLU:N	1:B:48:GLU:CD	2.75	0.41
1:B:236:MET:O	1:B:237:ALA:C	2.60	0.41
1:A:273:MET:CE	1:A:369:ARG:HG3	2.50	0.41
1:B:254:ASN:HD21	1:B:396:ARG:HG3	1.86	0.41
1:B:340:ASP:C	1:B:342:ALA:N	2.74	0.41
1:A:406:ARG:HH11	1:A:406:ARG:CB	2.31	0.40
1:B:260:LEU:HB3	1:B:380:LEU:HG	2.03	0.40
1:A:120:ARG:CB	1:A:121:PRO:HD3	2.50	0.40
1:A:124:GLN:NE2	1:A:124:GLN:HA	2.35	0.40
1:A:45:ARG:HH21	1:A:49:GLY:CA	2.33	0.40
1:A:334:ARG:NE	1:A:334:ARG:HA	2.36	0.40
1:A:367:ALA:O	1:A:368:VAL:C	2.59	0.40
1:B:95:SER:HB2	1:B:99:ARG:HD2	2.04	0.40
1:B:198:LEU:HD13	1:B:237:ALA:HB1	2.03	0.40
1:A:82:THR:HA	1:B:146:GLU:OE1	2.22	0.40
1:A:380:LEU:CD2	1:A:401:LEU:HD11	2.51	0.40
1:B:132:ASP:O	1:B:135:LEU:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:CG2	1:B:158:SER:N	2.85	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	391/436 (90%)	285 (73%)	77 (20%)	29 (7%)	1	2
1	B	391/436 (90%)	277 (71%)	78 (20%)	36 (9%)	1	1
All	All	782/872 (90%)	562 (72%)	155 (20%)	65 (8%)	1	1

All (65) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	PRO
1	A	99	ARG
1	A	149	ALA
1	A	242	VAL
1	A	243	ALA
1	A	351	ILE
1	A	376	PRO
1	B	38	GLU
1	B	127	VAL
1	B	149	ALA
1	B	151	PRO
1	B	152	LEU
1	B	228	LEU
1	B	243	ALA
1	B	270	ARG
1	B	300	GLU
1	B	384	PRO

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	114	ARG
1	A	311	ALA
1	A	337	ILE
1	A	339	ARG
1	A	370	ALA
1	B	126	ILE
1	B	148	LEU
1	B	305	ASP
1	B	327	GLU
1	B	382	VAL
1	A	47	PRO
1	A	144	LEU
1	A	184	PRO
1	A	305	ASP
1	A	377	ASP
1	B	125	GLU
1	B	139	ASP
1	B	175	THR
1	B	245	HIS
1	B	341	THR
1	B	354	CYS
1	B	361	ARG
1	A	85	GLU
1	A	193	GLU
1	A	293	ALA
1	A	364	ALA
1	A	382	VAL
1	B	69	ARG
1	B	168	ARG
1	B	358	PRO
1	B	376	PRO
1	A	106	LEU
1	A	244	GLY
1	A	371	LEU
1	B	40	PRO
1	B	80	PRO
1	B	144	LEU
1	B	164	PRO
1	B	268	ALA
1	A	330	PRO
1	B	153	PRO

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Mol	Chain	Res	Type
1	B	185	ALA
1	B	242	VAL
1	B	299	VAL
1	A	49	GLY
1	B	184	PRO
1	A	331	ASP

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	313/355 (88%)	288 (92%)	25 (8%)	12	31
1	B	313/355 (88%)	285 (91%)	28 (9%)	9	26
All	All	626/710 (88%)	573 (92%)	53 (8%)	10	28

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
1	A	43	ARG
1	A	45	ARG
1	A	46	THR
1	A	59	ASP
1	A	77	SER
1	A	89	ASN
1	A	94	GLU
1	A	100	HIS
1	A	101	THR
1	A	104	ARG
1	A	132	ASP
1	A	159	GLU
1	A	160	LEU
1	A	164	PRO
1	A	165	GLU
1	A	215	SER

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Mol	Chain	Res	Type
1	A	270	ARG
1	A	285	ARG
1	A	313	ASP
1	A	330	PRO
1	A	334	ARG
1	A	351	ILE
1	A	384	PRO
1	A	395	ILE
1	B	45	ARG
1	B	89	ASN
1	B	101	THR
1	B	104	ARG
1	B	114	ARG
1	B	139	ASP
1	B	151	PRO
1	B	152	LEU
1	B	178	PHE
1	B	198	LEU
1	B	203	ASP
1	B	219	ARG
1	B	223	GLU
1	B	233	LEU
1	B	238	HIS
1	B	240	LEU
1	B	242	VAL
1	B	247	THR
1	B	270	ARG
1	B	272	ASP
1	B	277	ASP
1	B	285	ARG
1	B	297	PHE
1	B	334	ARG
1	B	339	ARG
1	B	369	ARG
1	B	384	PRO
1	B	406	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	76	ASN

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Mol	Chain	Res	Type
1	A	100	HIS
1	A	124	GLN
1	A	238	HIS
1	A	344	HIS
1	B	89	ASN
1	B	188	GLN
1	B	254	ASN
1	B	265	GLN
1	B	344	HIS
1	B	349	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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
3	PXI	B	1408	-	33,33,33	1.94	6 (18%)	40,47,47	2.04	9 (22%)
3	PXI	A	1408	-	33,33,33	2.07	7 (21%)	40,47,47	1.85	10 (25%)
2	HEM	A	1407	1	41,50,50	1.56	10 (24%)	45,82,82	1.56	9 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	1407	1	41,50,50	1.59	8 (19%)	45,82,82	1.51	6 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PXI	B	1408	-	-	19/43/59/59	0/1/2/2
3	PXI	A	1408	-	-	14/43/59/59	0/1/2/2
2	HEM	A	1407	1	-	10/12/54/54	-
2	HEM	B	1407	1	-	6/12/54/54	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1408	PXI	C16-C7	6.32	1.64	1.53
3	A	1408	PXI	C19-C21	5.87	1.61	1.51
3	A	1408	PXI	C16-C7	5.44	1.63	1.53
2	A	1407	HEM	C3C-CAC	-4.19	1.39	1.47
3	B	1408	PXI	C19-C21	4.07	1.58	1.51
3	B	1408	PXI	C24-C3	3.98	1.63	1.53
3	A	1408	PXI	C15-C12	3.78	1.61	1.53
3	A	1408	PXI	C24-C3	3.69	1.62	1.53
2	B	1407	HEM	CAB-C3B	-3.61	1.37	1.47
2	B	1407	HEM	C4A-NA	3.42	1.43	1.36
2	A	1407	HEM	CBB-CAB	3.28	1.46	1.30
2	A	1407	HEM	CAB-C3B	-3.16	1.38	1.47
2	B	1407	HEM	CBB-CAB	3.05	1.45	1.30
2	B	1407	HEM	CBC-CAC	2.96	1.48	1.29
3	B	1408	PXI	C11-C9	2.95	1.57	1.51
2	A	1407	HEM	C4D-C3D	2.95	1.50	1.45
3	B	1408	PXI	C15-C12	2.91	1.59	1.53
2	B	1407	HEM	C3C-CAC	-2.68	1.42	1.47
2	B	1407	HEM	CHB-C1B	2.60	1.41	1.35
2	A	1407	HEM	CMD-C2D	2.58	1.56	1.50
2	B	1407	HEM	C2C-C1C	2.50	1.48	1.42
3	A	1408	PXI	O3-C7	2.35	1.50	1.43
2	A	1407	HEM	C2A-C3A	-2.20	1.31	1.37
3	A	1408	PXI	O4-C9	2.20	1.48	1.44
3	A	1408	PXI	O3-C8	2.17	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1407	HEM	C1A-NA	2.13	1.40	1.36
2	A	1407	HEM	C4A-NA	2.10	1.40	1.36
3	B	1408	PXI	O4-C9	2.09	1.48	1.44
2	A	1407	HEM	CBC-CAC	2.07	1.43	1.29
2	A	1407	HEM	CHA-C4D	2.01	1.40	1.35
2	A	1407	HEM	O2A-CGA	-2.01	1.24	1.30

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1408	PXI	C3-O1-C4	7.97	129.85	117.89
3	A	1408	PXI	C3-O1-C4	7.11	128.56	117.89
3	B	1408	PXI	O3-C7-C5	-4.96	102.51	111.14
2	B	1407	HEM	CBD-CAD-C3D	4.43	124.94	112.63
2	B	1407	HEM	CBA-CAA-C2A	4.30	119.95	112.62
2	A	1407	HEM	C4A-C3A-C2A	4.30	109.98	107.00
2	A	1407	HEM	CAD-C3D-C4D	4.19	131.99	124.66
3	A	1408	PXI	O3-C7-C5	-3.53	104.99	111.14
3	A	1408	PXI	O1-C3-C2	3.23	112.09	106.92
2	A	1407	HEM	C4C-CHD-C1D	3.10	126.65	122.56
2	A	1407	HEM	CAA-C2A-C3A	-3.08	118.41	127.25
2	A	1407	HEM	CAD-C3D-C2D	-3.06	122.18	127.88
3	B	1408	PXI	O1-C3-C2	3.00	111.72	106.92
3	B	1408	PXI	C10-C9-C11	-2.98	108.72	113.40
3	B	1408	PXI	C6-C5-C7	-2.84	106.48	112.92
3	A	1408	PXI	C10-C9-C11	-2.81	108.99	113.40
3	B	1408	PXI	C7-C5-C4	2.77	115.68	110.01
3	A	1408	PXI	C7-C5-C4	2.73	115.59	110.01
2	B	1407	HEM	CAA-C2A-C3A	-2.69	119.52	127.25
2	A	1407	HEM	CHD-C1D-C2D	-2.66	120.82	124.98
2	B	1407	HEM	C4B-CHC-C1C	2.59	125.98	122.56
2	B	1407	HEM	CAD-C3D-C4D	2.55	129.11	124.66
3	B	1408	PXI	C25-C24-C23	-2.34	104.33	109.99
2	B	1407	HEM	C4C-CHD-C1D	2.31	125.61	122.56
3	A	1408	PXI	C19-C21-C22	2.30	124.06	118.29
3	A	1408	PXI	C17-C16-C7	2.14	114.65	111.15
3	B	1408	PXI	C11-C12-C15	-2.12	106.91	109.97
3	A	1408	PXI	C9-C11-C12	-2.10	106.79	110.46
2	A	1407	HEM	CBD-CAD-C3D	2.09	118.44	112.63
3	A	1408	PXI	C25-C24-C23	-2.07	105.00	109.99
3	A	1408	PXI	C6-C5-C7	-2.06	108.24	112.92
2	A	1407	HEM	C2C-C3C-C4C	-2.02	105.49	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1407	HEM	CMC-C2C-C3C	2.01	128.43	124.68
3	B	1408	PXI	C13-N1-C12	-2.00	107.09	113.11

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1407	HEM	C1A-C2A-CAA-CBA
2	A	1407	HEM	C3A-C2A-CAA-CBA
2	A	1407	HEM	C2B-C3B-CAB-CBB
2	A	1407	HEM	C4B-C3B-CAB-CBB
3	A	1408	PXI	C11-C12-N1-C13
3	A	1408	PXI	C11-C12-N1-C14
3	A	1408	PXI	C7-C16-C18-C19
3	A	1408	PXI	C16-C18-C19-C20
3	A	1408	PXI	C16-C18-C19-C21
3	B	1408	PXI	C23-C24-C3-O1
3	B	1408	PXI	C18-C16-C7-O3
3	B	1408	PXI	C11-C12-N1-C13
3	B	1408	PXI	C11-C12-N1-C14
3	B	1408	PXI	C7-C16-C18-C19
3	A	1408	PXI	O4-C8-O3-C7
3	B	1408	PXI	O4-C8-O3-C7
2	A	1407	HEM	C4D-C3D-CAD-CBD
2	B	1407	HEM	C4D-C3D-CAD-CBD
3	A	1408	PXI	C22-C23-C24-C25
3	B	1408	PXI	C22-C23-C24-C25
2	A	1407	HEM	C2D-C3D-CAD-CBD
2	B	1407	HEM	C2D-C3D-CAD-CBD
3	A	1408	PXI	C15-C12-N1-C13
3	B	1408	PXI	C4-C5-C7-C16
3	B	1408	PXI	C15-C12-N1-C13
3	A	1408	PXI	O6-C21-C22-C23
3	B	1408	PXI	O6-C21-C22-C23
3	B	1408	PXI	C6-C5-C7-O3
3	B	1408	PXI	C17-C16-C18-C19
3	A	1408	PXI	C19-C21-C22-C23
3	B	1408	PXI	C19-C21-C22-C23
3	B	1408	PXI	C16-C18-C19-C21
3	B	1408	PXI	C25-C24-C3-O1
3	B	1408	PXI	C23-C24-C3-C2
3	B	1408	PXI	C17-C16-C7-O3

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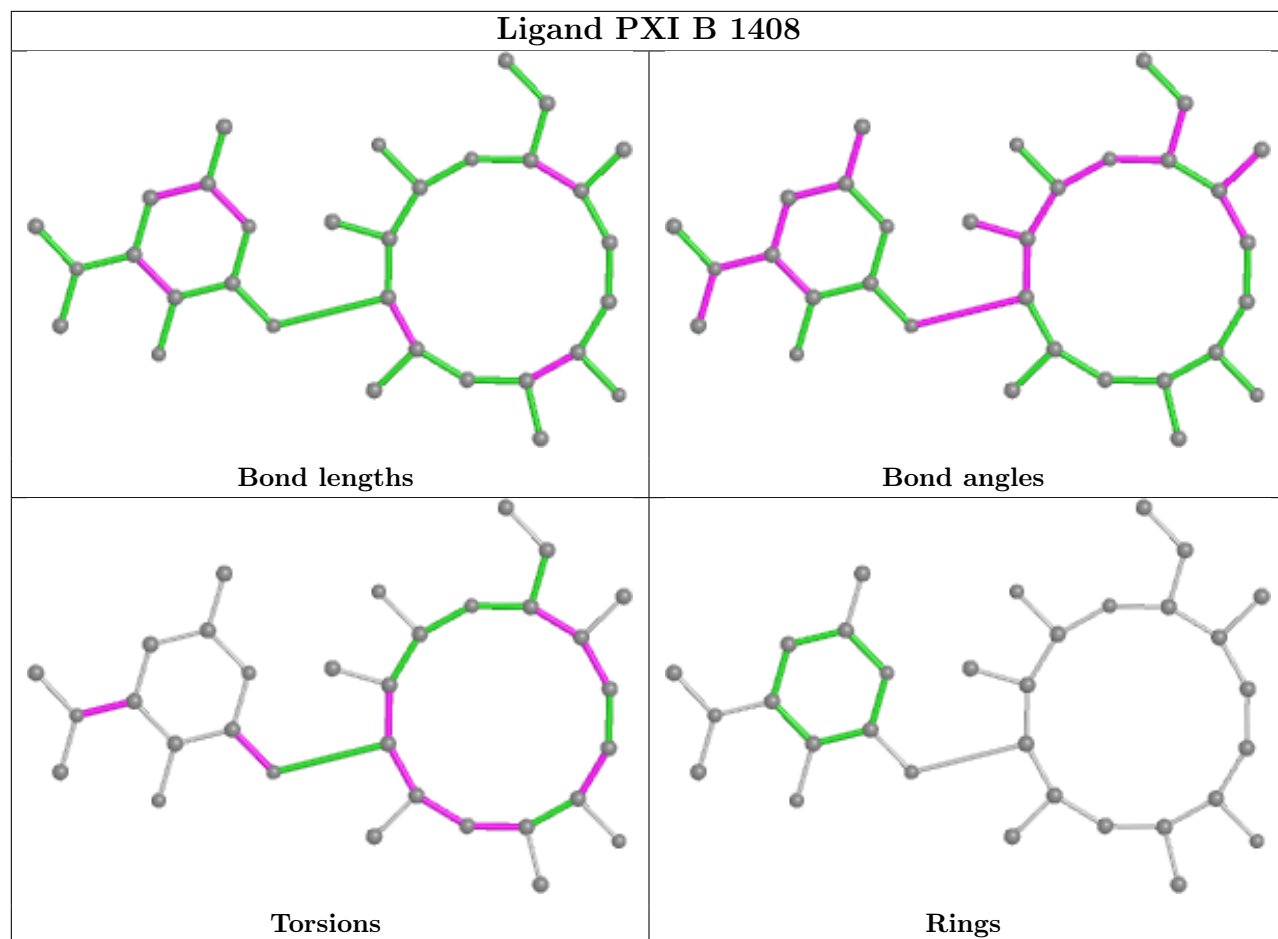
Mol	Chain	Res	Type	Atoms
3	A	1408	PXI	C25-C24-C3-O1
3	B	1408	PXI	C25-C24-C3-C2
3	B	1408	PXI	C17-C16-C7-C5
3	A	1408	PXI	C17-C16-C18-C19
3	A	1408	PXI	C15-C12-N1-C14
2	A	1407	HEM	CAD-CBD-CGD-O2D
2	A	1407	HEM	CAA-CBA-CGA-O2A
2	A	1407	HEM	CAD-CBD-CGD-O1D
3	A	1408	PXI	C5-C4-O1-C3
2	B	1407	HEM	CAD-CBD-CGD-O2D
2	A	1407	HEM	CAA-CBA-CGA-O1A
2	B	1407	HEM	CAA-CBA-CGA-O2A
2	B	1407	HEM	CAD-CBD-CGD-O1D
2	B	1407	HEM	CAA-CBA-CGA-O1A

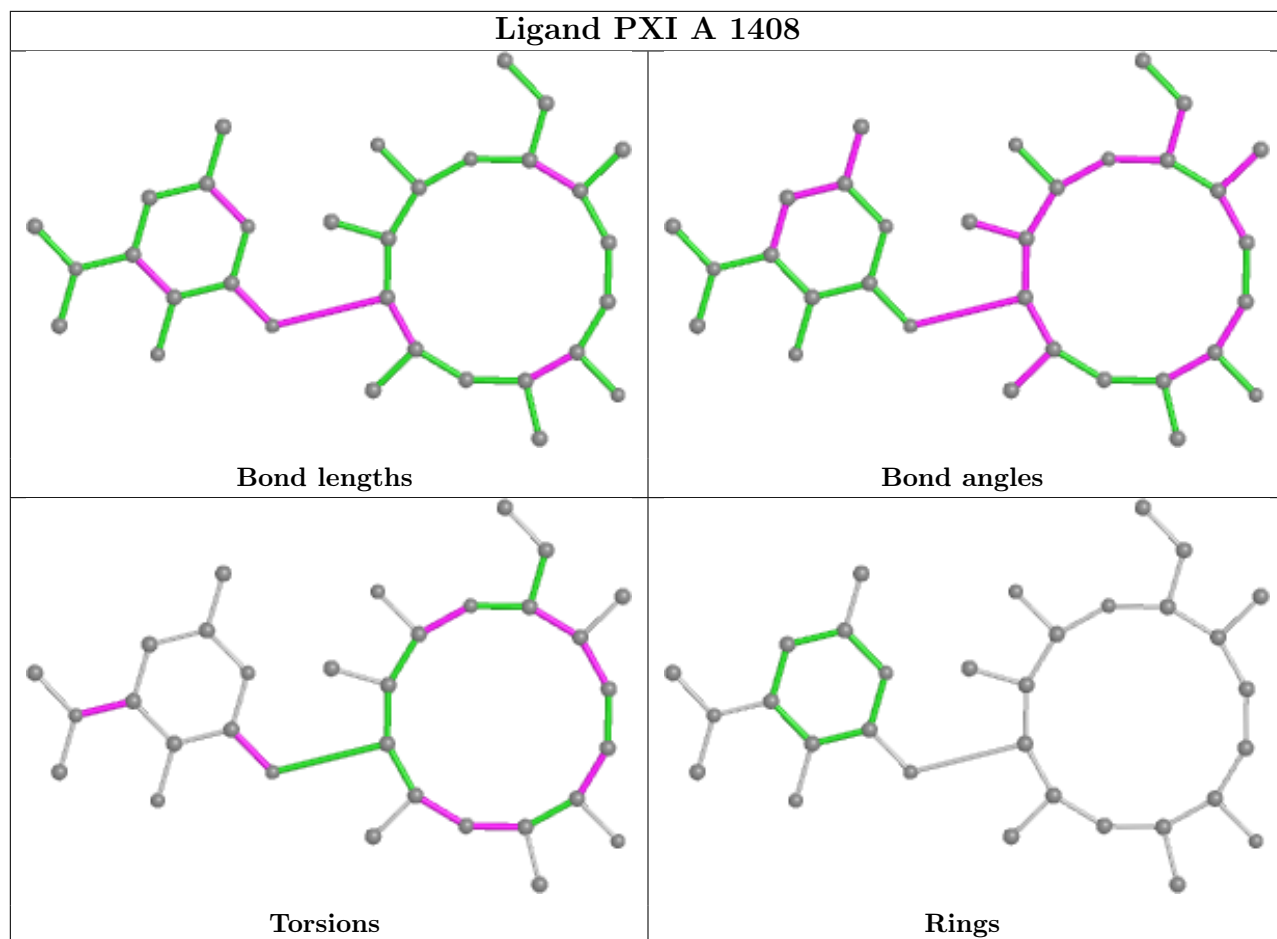
There are no ring outliers.

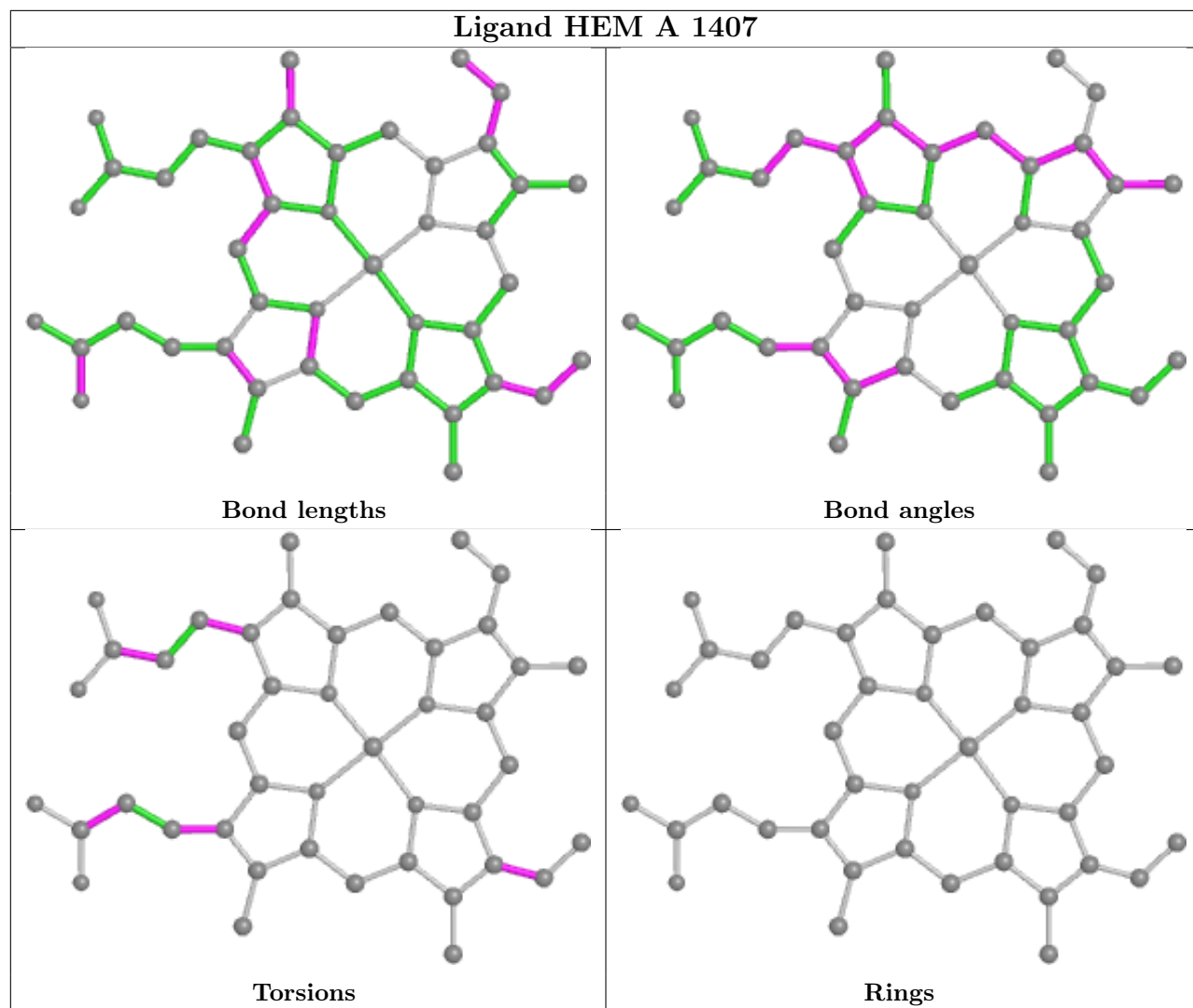
4 monomers are involved in 16 short contacts:

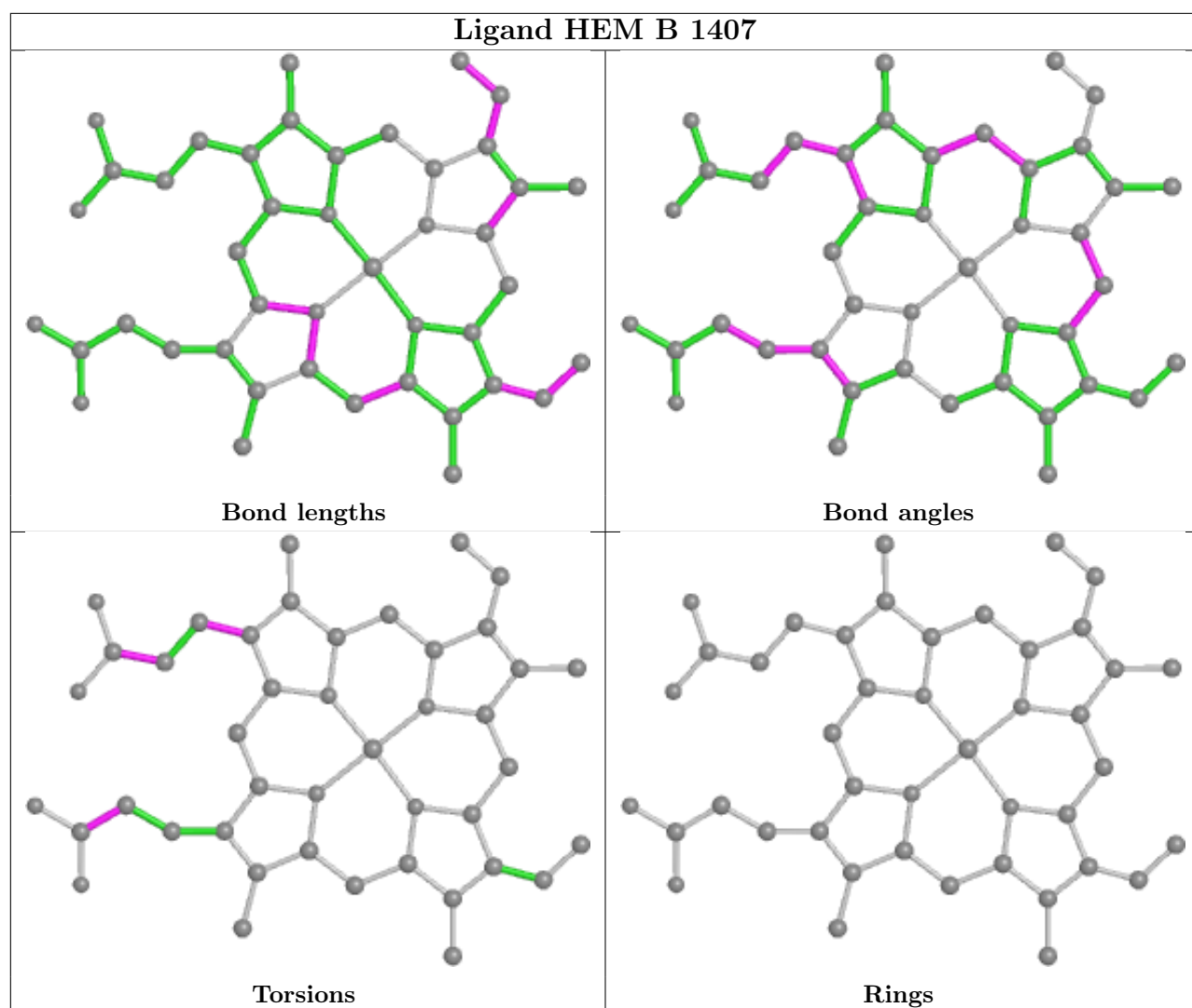
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1408	PXI	7	0
3	A	1408	PXI	1	0
2	A	1407	HEM	3	0
2	B	1407	HEM	5	0

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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/436 (90%)	0.32	6 (1%) 73 72	4, 23, 37, 48	0
1	B	393/436 (90%)	0.34	3 (0%) 86 85	5, 22, 39, 46	0
All	All	786/872 (90%)	0.33	9 (1%) 80 80	4, 23, 38, 48	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	ILE	3.2
1	B	89	ASN	3.0
1	B	384	PRO	2.5
1	A	172	ARG	2.4
1	A	207	GLY	2.4
1	A	91	ASN	2.3
1	B	270	ARG	2.2
1	A	179	VAL	2.2
1	A	375	CYS	2.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

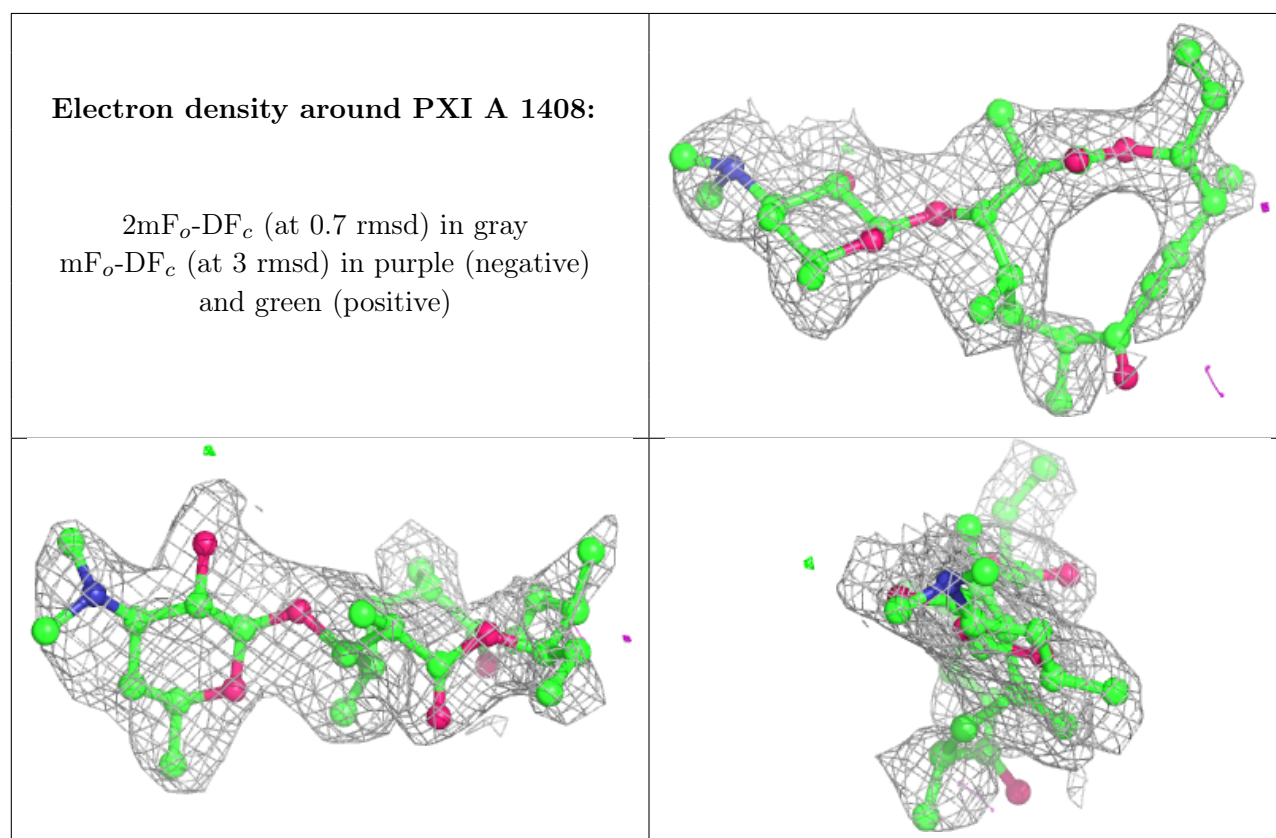
6.4 Ligands [i](#)

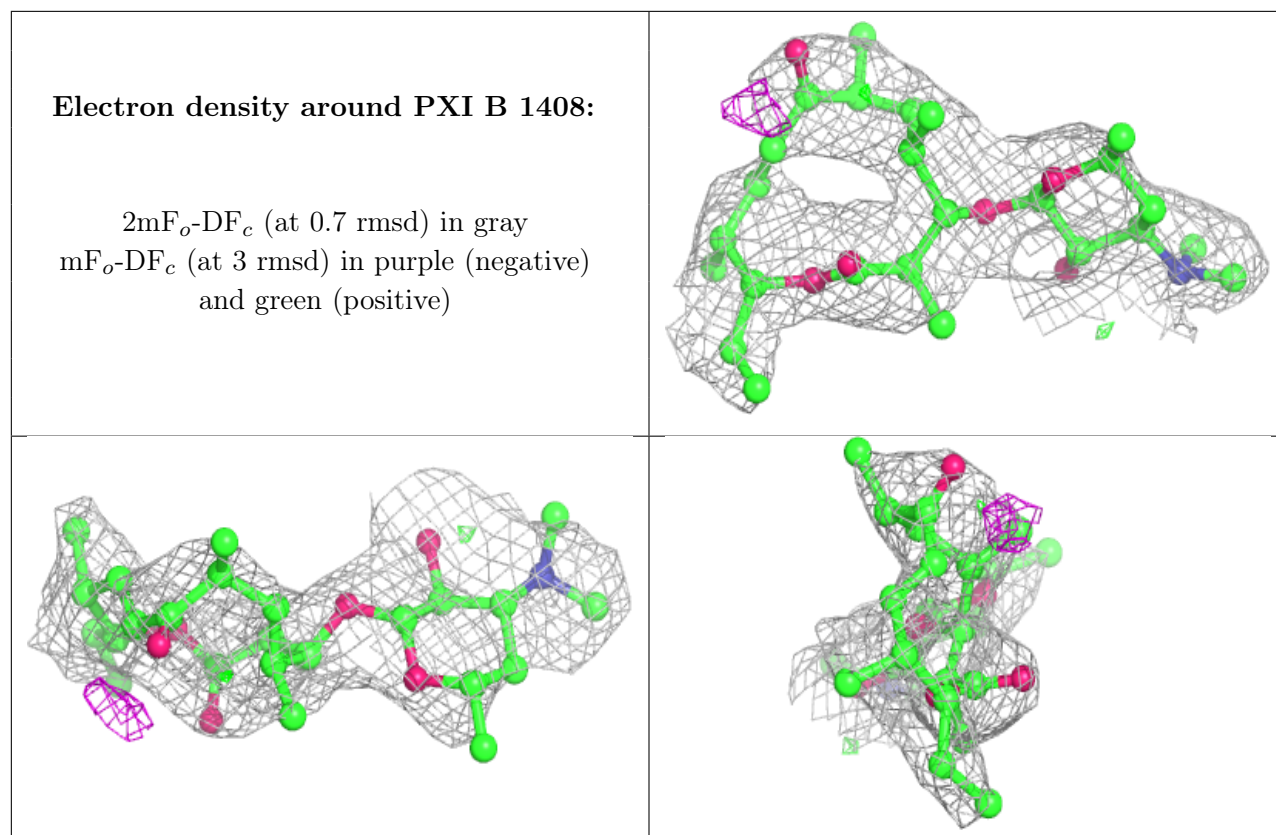
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PXI	A	1408	32/32	0.82	0.29	27,31,32,35	0
3	PXI	B	1408	32/32	0.89	0.28	28,31,33,34	0
2	HEM	A	1407	43/43	0.94	0.20	3,4,12,15	0
2	HEM	B	1407	43/43	0.94	0.19	3,6,12,19	0

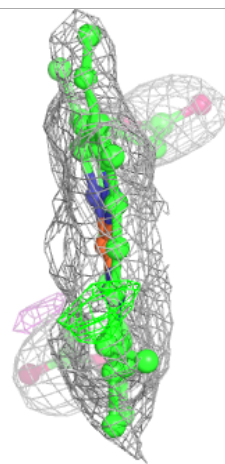
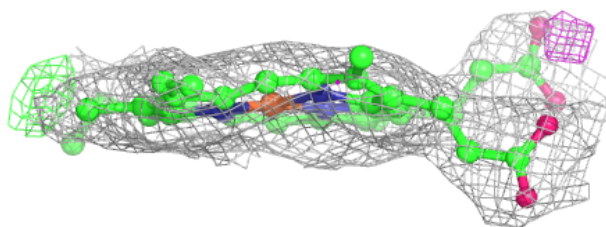
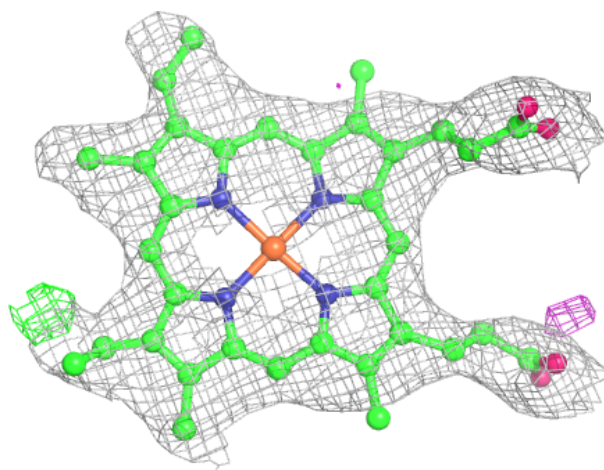
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

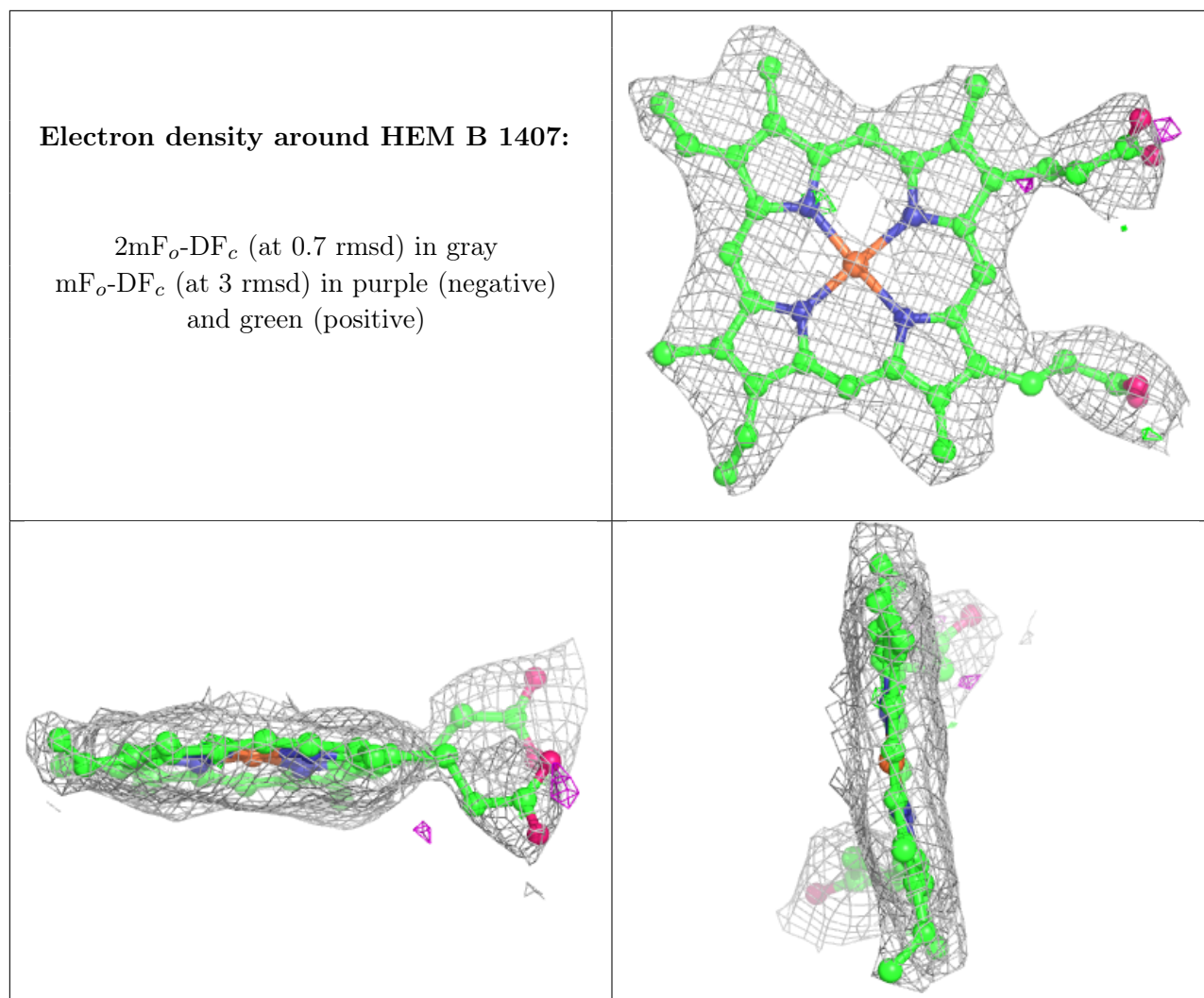




Electron density around HEM A 1407:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.