



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 PM UTC

PDB ID : 3KDN / pdb_00003kdn
Title : Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-10-23
Resolution : 2.09 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

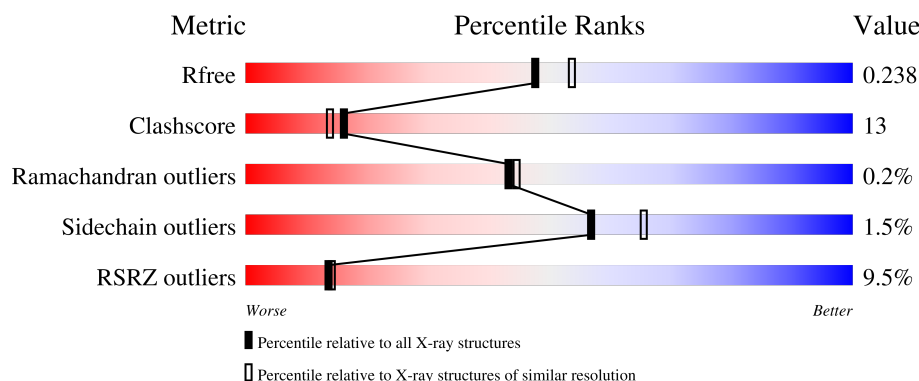
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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.



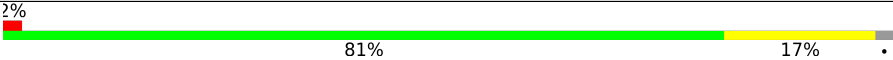
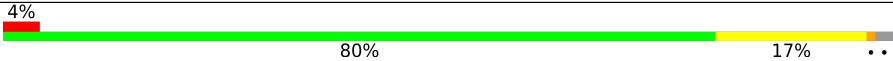
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	444	42% 56% 41% ..
1	B	444	% 79% 19% .
1	C	444	3% 78% 20% .
1	D	444	2% 79% 19% .
1	E	444	7% 78% 20% .

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Mol	Chain	Length	Quality of chain
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36999 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 Ribulose biphosphate carboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	0	0
			3349	2145	577	617	10			
1	B	437	Total	C	N	O	S	0	0	0
			3430	2201	588	631	10			
1	C	437	Total	C	N	O	S	0	0	0
			3417	2195	585	627	10			
1	D	437	Total	C	N	O	S	0	0	0
			3421	2196	586	629	10			
1	E	438	Total	C	N	O	S	0	0	0
			3428	2197	586	635	10			
1	F	437	Total	C	N	O	S	0	0	0
			3404	2185	586	623	10			
1	G	437	Total	C	N	O	S	0	0	0
			3433	2204	588	631	10			
1	H	438	Total	C	N	O	S	0	0	0
			3396	2182	584	620	10			
1	I	436	Total	C	N	O	S	0	0	0
			3421	2195	586	630	10			
1	J	437	Total	C	N	O	S	0	0	0
			3428	2199	586	633	10			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	GLU	GLY	engineered mutation	UNP O93627
A	327	ARG	LYS	engineered mutation	UNP O93627
A	328	ASP	TRP	engineered mutation	UNP O93627
A	329	ILE	ASP	engineered mutation	UNP O93627
A	330	THR	VAL	engineered mutation	UNP O93627
B	326	GLU	GLY	engineered mutation	UNP O93627
B	327	ARG	LYS	engineered mutation	UNP O93627
B	328	ASP	TRP	engineered mutation	UNP O93627
B	329	ILE	ASP	engineered mutation	UNP O93627

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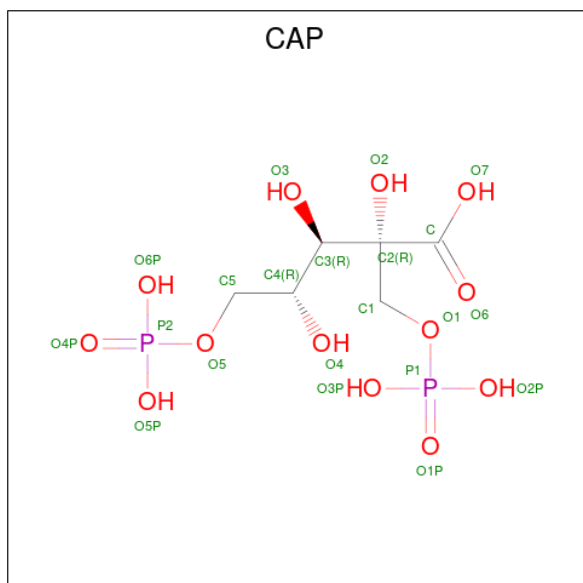
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Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	engineered mutation	UNP O93627
C	326	GLU	GLY	engineered mutation	UNP O93627
C	327	ARG	LYS	engineered mutation	UNP O93627
C	328	ASP	TRP	engineered mutation	UNP O93627
C	329	ILE	ASP	engineered mutation	UNP O93627
C	330	THR	VAL	engineered mutation	UNP O93627
D	326	GLU	GLY	engineered mutation	UNP O93627
D	327	ARG	LYS	engineered mutation	UNP O93627
D	328	ASP	TRP	engineered mutation	UNP O93627
D	329	ILE	ASP	engineered mutation	UNP O93627
D	330	THR	VAL	engineered mutation	UNP O93627
E	326	GLU	GLY	engineered mutation	UNP O93627
E	327	ARG	LYS	engineered mutation	UNP O93627
E	328	ASP	TRP	engineered mutation	UNP O93627
E	329	ILE	ASP	engineered mutation	UNP O93627
E	330	THR	VAL	engineered mutation	UNP O93627
F	326	GLU	GLY	engineered mutation	UNP O93627
F	327	ARG	LYS	engineered mutation	UNP O93627
F	328	ASP	TRP	engineered mutation	UNP O93627
F	329	ILE	ASP	engineered mutation	UNP O93627
F	330	THR	VAL	engineered mutation	UNP O93627
G	326	GLU	GLY	engineered mutation	UNP O93627
G	327	ARG	LYS	engineered mutation	UNP O93627
G	328	ASP	TRP	engineered mutation	UNP O93627
G	329	ILE	ASP	engineered mutation	UNP O93627
G	330	THR	VAL	engineered mutation	UNP O93627
H	326	GLU	GLY	engineered mutation	UNP O93627
H	327	ARG	LYS	engineered mutation	UNP O93627
H	328	ASP	TRP	engineered mutation	UNP O93627
H	329	ILE	ASP	engineered mutation	UNP O93627
H	330	THR	VAL	engineered mutation	UNP O93627
I	326	GLU	GLY	engineered mutation	UNP O93627
I	327	ARG	LYS	engineered mutation	UNP O93627
I	328	ASP	TRP	engineered mutation	UNP O93627
I	329	ILE	ASP	engineered mutation	UNP O93627
I	330	THR	VAL	engineered mutation	UNP O93627
J	326	GLU	GLY	engineered mutation	UNP O93627
J	327	ARG	LYS	engineered mutation	UNP O93627
J	328	ASP	TRP	engineered mutation	UNP O93627
J	329	ILE	ASP	engineered mutation	UNP O93627
J	330	THR	VAL	engineered mutation	UNP O93627

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	I	1	Total Mg 1 1	0	0
2	J	1	Total Mg 1 1	0	0

- Molecule 3 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (CCD ID: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O P 21 6 13 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	O	P	0	0
			21	6	13	2		
3	C	1	Total	C	O	P	0	0
			21	6	13	2		
3	D	1	Total	C	O	P	0	0
			21	6	13	2		
3	E	1	Total	C	O	P	0	0
			21	6	13	2		
3	F	1	Total	C	O	P	0	0
			21	6	13	2		
3	G	1	Total	C	O	P	0	0
			21	6	13	2		
3	H	1	Total	C	O	P	0	0
			21	6	13	2		
3	I	1	Total	C	O	P	0	0
			21	6	13	2		
3	J	1	Total	C	O	P	0	0
			21	6	13	2		

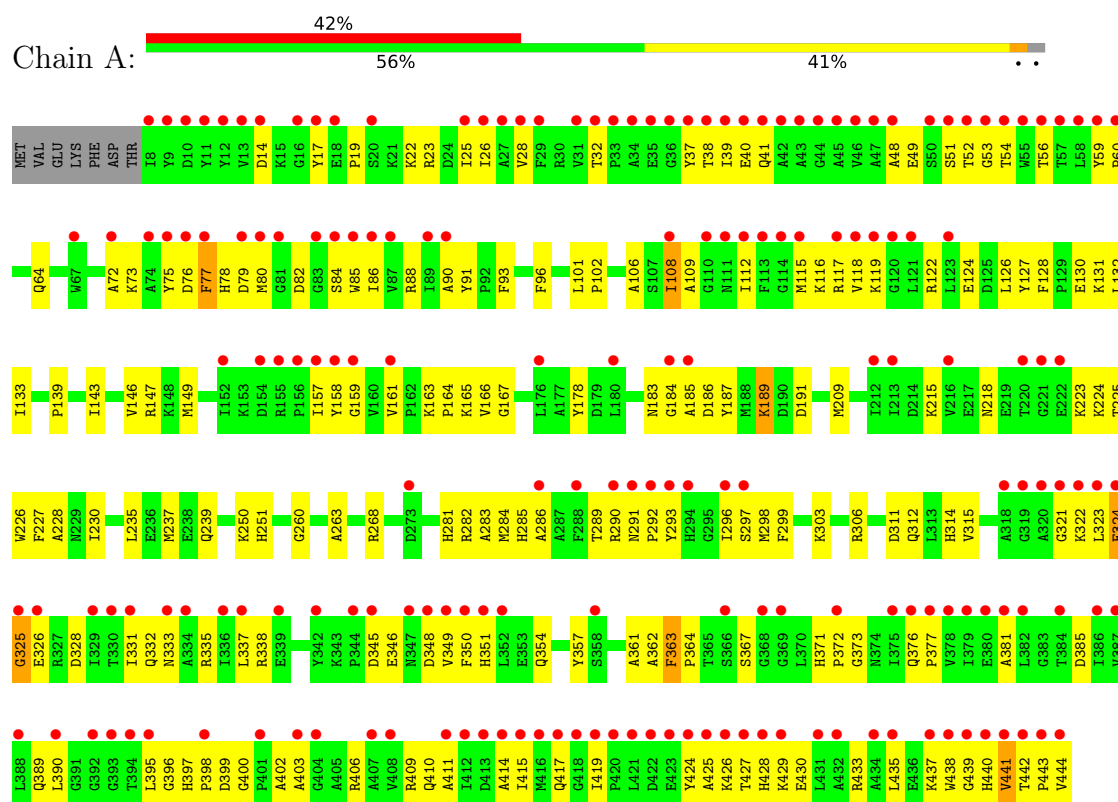
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	173	Total	O	0	0
			173	173		
4	B	290	Total	O	0	0
			290	290		
4	C	311	Total	O	0	0
			311	311		
4	D	308	Total	O	0	0
			308	308		
4	E	258	Total	O	0	0
			258	258		
4	F	268	Total	O	0	0
			268	268		
4	G	267	Total	O	0	0
			267	267		
4	H	185	Total	O	0	0
			185	185		
4	I	291	Total	O	0	0
			291	291		
4	J	301	Total	O	0	0
			301	301		

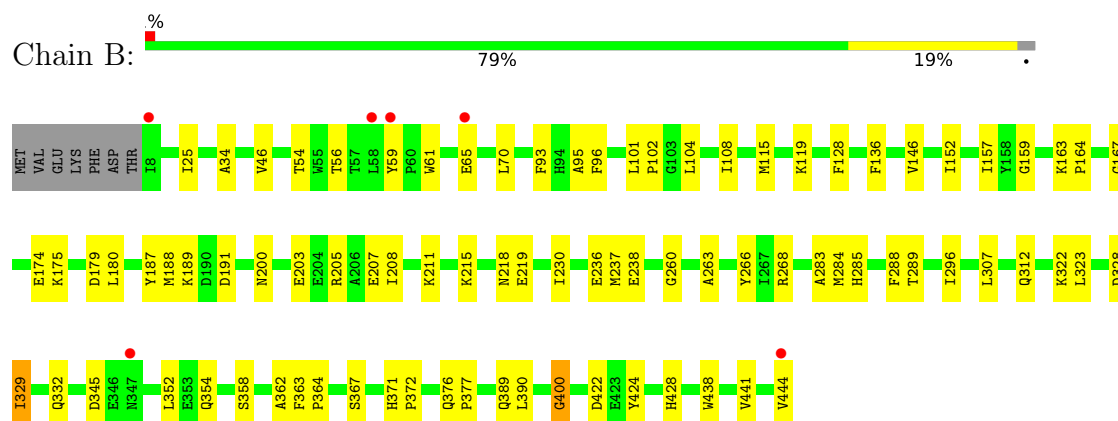
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

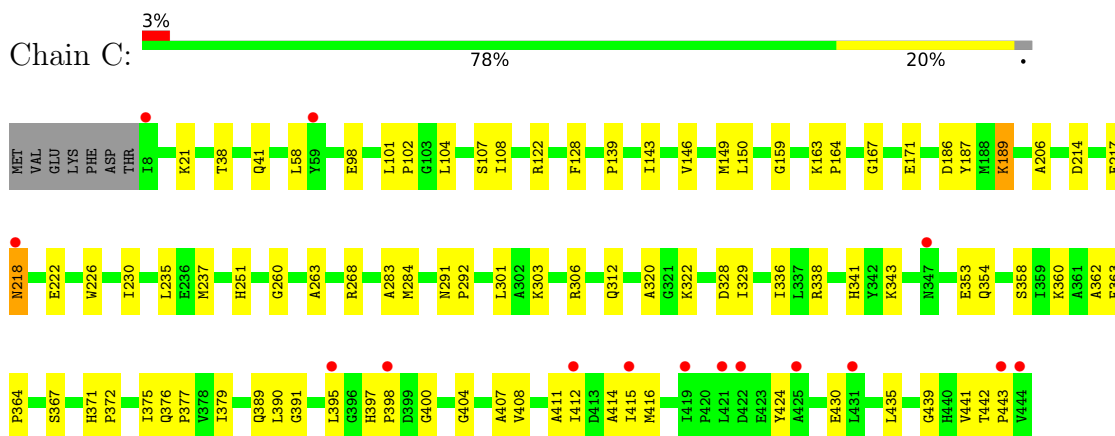
• Molecule 1: Ribulose biphosphate carboxylase



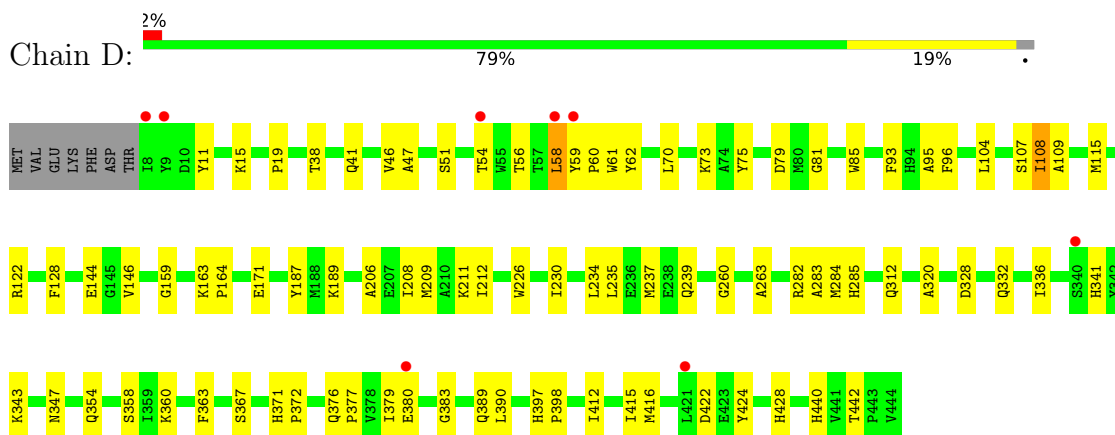
• Molecule 1: Ribulose biphosphate carboxylase



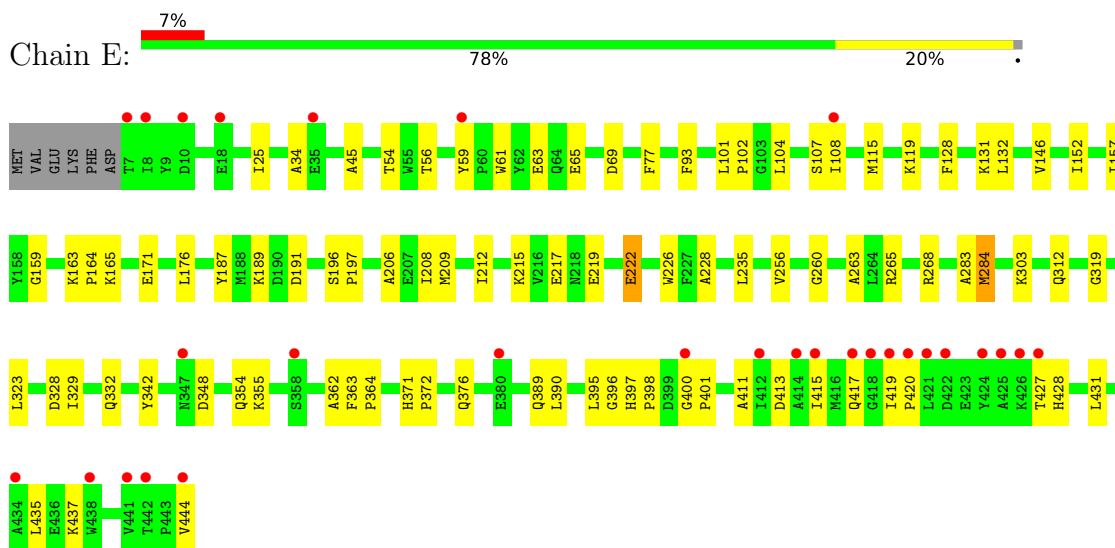
- Molecule 1: Ribulose biphosphate carboxylase



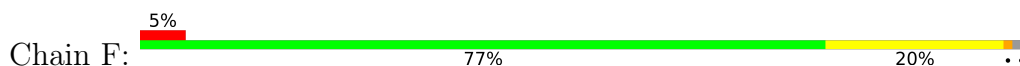
- Molecule 1: Ribulose biphosphate carboxylase

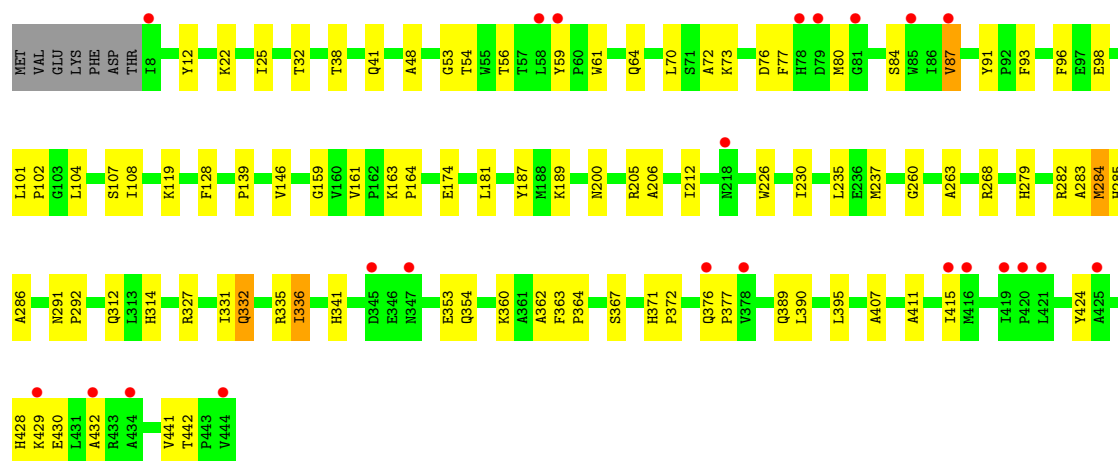


- Molecule 1: Ribulose biphosphate carboxylase

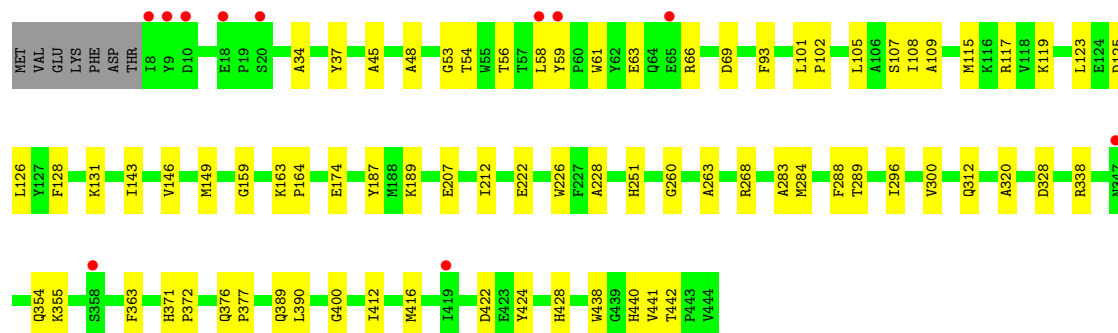
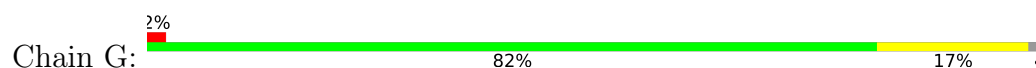


- Molecule 1: Ribulose biphosphate carboxylase

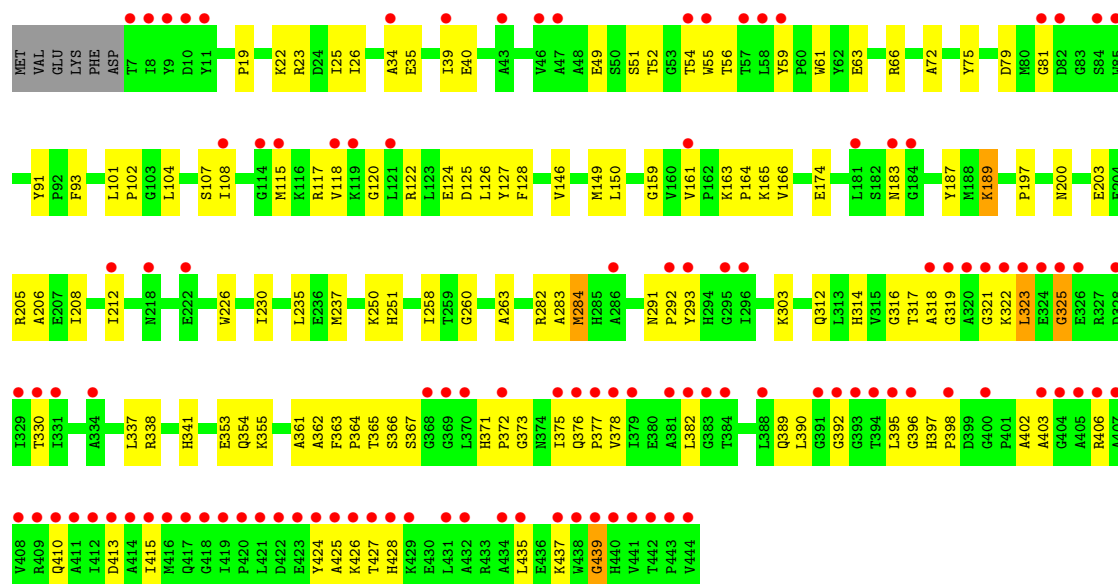




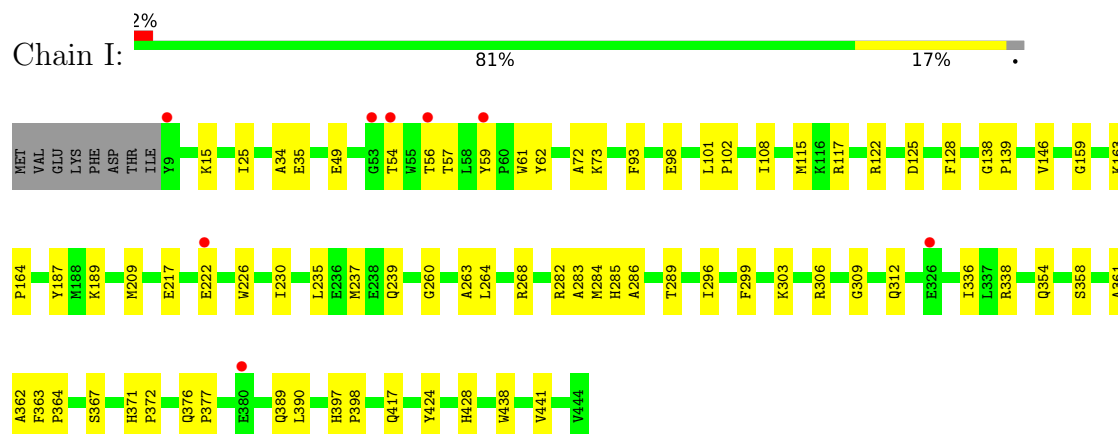
● Molecule 1: Ribulose biphosphate carboxylase



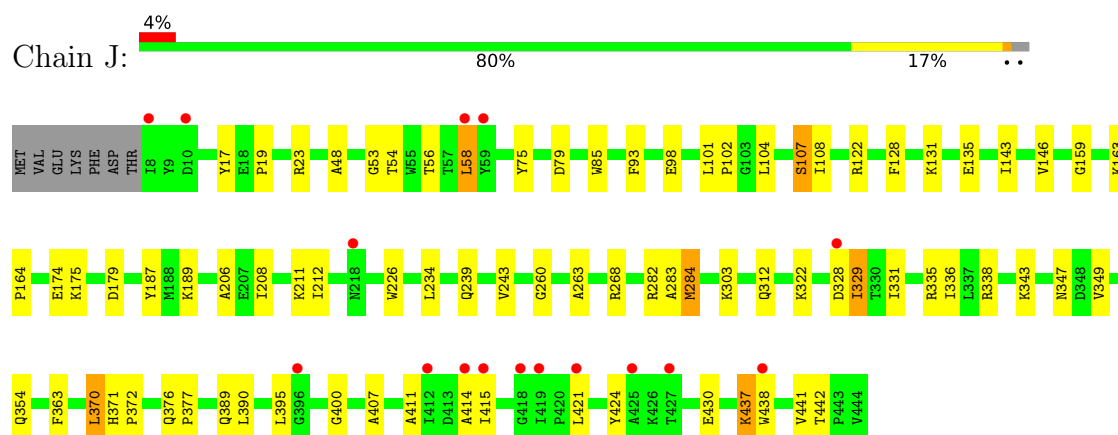
● Molecule 1: Ribulose biphosphate carboxylase



● Molecule 1: Ribulose biphosphate carboxylase



● Molecule 1: Ribulose biphosphate carboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	97.47Å 246.24Å 133.08Å 90.00° 104.10° 90.00°	Depositor
Resolution (Å)	42.86 – 2.09 42.86 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.86-2.09) 96.5 (42.86-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.213 , 0.253 (Not available) , 0.238	Depositor DCC
R_{free} test set	17388 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36999	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% 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: MG, KCX, CAP

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	0.31	0/3421	0.70	2/4652 (0.0%)
1	B	0.34	0/3505	0.68	2/4753 (0.0%)
1	C	0.35	0/3492	0.69	2/4740 (0.0%)
1	D	0.35	0/3496	0.69	0/4744
1	E	0.33	0/3503	0.68	3/4753 (0.1%)
1	F	0.33	0/3478	0.70	0/4719
1	G	0.33	0/3508	0.69	2/4757 (0.0%)
1	H	0.32	0/3471	0.68	0/4713
1	I	0.33	0/3496	0.67	0/4742
1	J	0.35	0/3503	0.68	2/4753 (0.0%)
All	All	0.33	0/34873	0.69	13/47326 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	GLY	CA-C-N	6.70	126.21	119.24
1	B	400	GLY	C-N-CA	6.70	126.21	119.24
1	A	400	GLY	CA-C-N	5.95	125.42	119.24
1	A	400	GLY	C-N-CA	5.95	125.42	119.24
1	C	400	GLY	CA-C-N	5.93	125.41	119.24
1	C	400	GLY	C-N-CA	5.93	125.41	119.24
1	G	400	GLY	CA-C-N	5.38	125.02	119.05
1	G	400	GLY	C-N-CA	5.38	125.02	119.05
1	E	400	GLY	CA-C-N	5.33	124.51	118.97
1	E	400	GLY	C-N-CA	5.33	124.51	118.97
1	E	256	VAL	N-CA-C	5.18	115.95	110.72
1	J	400	GLY	CA-C-N	5.16	124.60	119.24
1	J	400	GLY	C-N-CA	5.16	124.60	119.24

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	3349	0	3204	212	0
1	B	3430	0	3346	71	0
1	C	3417	0	3325	80	0
1	D	3421	0	3329	76	0
1	E	3428	0	3319	81	0
1	F	3404	0	3312	73	0
1	G	3433	0	3355	61	0
1	H	3396	0	3282	126	0
1	I	3421	0	3333	60	0
1	J	3428	0	3335	84	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	21	0	7	3	0
3	B	21	0	7	0	0
3	C	21	0	8	1	0
3	D	21	0	8	0	0
3	E	21	0	7	0	0
3	F	21	0	8	0	0
3	G	21	0	8	0	0
3	H	21	0	8	1	0
3	I	21	0	7	0	0
3	J	21	0	7	1	0
4	A	173	0	0	9	0
4	B	290	0	0	6	0
4	C	311	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	308	0	0	6	0
4	E	258	0	0	8	0
4	F	268	0	0	10	0
4	G	267	0	0	4	0
4	H	185	0	0	10	0
4	I	291	0	0	8	0
4	J	301	0	0	9	0
All	All	36999	0	33215	886	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 13.

All (886) 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:149:MET:HE3	1:A:250:LYS:CD	1.59	1.29
1:A:38:THR:HG23	1:A:41:GLN:OE1	1.53	1.07
1:G:45:ALA:HB1	1:G:115:MET:HE1	1.36	1.05
1:E:45:ALA:HB1	1:E:115:MET:HE1	1.35	1.04
1:A:149:MET:HE3	1:A:250:LYS:HD2	1.09	1.03
1:A:438:TRP:O	1:A:441:VAL:HG12	1.58	1.03
1:A:424:TYR:CE2	1:A:428:HIS:CE1	2.46	1.03
1:G:174:GLU:HG3	1:G:212:ILE:HD11	1.37	1.03
1:J:328:ASP:OD1	1:J:329:ILE:CD1	2.08	1.02
1:F:376:GLN:HG3	4:F:2817:HOH:O	1.61	1.00
1:J:347:ASN:HB2	4:J:2614:HOH:O	1.59	0.99
1:A:149:MET:CE	1:A:250:LYS:HD2	1.94	0.98
1:A:108:ILE:HD12	1:A:109:ALA:N	1.80	0.97
1:E:159:GLY:HA3	1:E:187:TYR:CZ	1.99	0.97
1:H:159:GLY:HA3	1:H:187:TYR:CZ	1.98	0.96
1:B:328:ASP:OD2	1:B:329:ILE:HD12	1.64	0.96
1:C:149:MET:HE1	1:C:251:HIS:CE1	2.01	0.95
1:A:338:ARG:HA	1:A:361:ALA:HB1	1.47	0.94
1:A:424:TYR:CZ	1:A:428:HIS:CE1	2.55	0.94
1:D:15:LYS:HD2	4:D:2868:HOH:O	1.67	0.94
1:J:175:LYS:HE2	4:J:2582:HOH:O	1.68	0.91
1:A:149:MET:HE3	1:A:250:LYS:CE	1.99	0.91
1:A:290:ARG:HE	1:A:324:GLU:HG3	1.34	0.91
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.06	0.90
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.07	0.88
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:54:THR:HG21	1:J:58:LEU:CD1	2.05	0.87
1:J:329:ILE:HD12	1:J:329:ILE:N	1.89	0.86
1:D:263:ALA:HB2	1:J:263:ALA:HB2	1.56	0.86
1:D:128:PHE:H	1:D:354:GLN:HE22	1.22	0.86
1:G:149:MET:HE1	1:G:251:HIS:CE1	2.10	0.86
1:G:128:PHE:H	1:G:354:GLN:HE22	1.22	0.85
1:A:178:TYR:CE1	1:A:215:LYS:NZ	2.45	0.84
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.12	0.84
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.13	0.84
1:E:376:GLN:CB	4:E:2871:HOH:O	2.25	0.84
1:F:98:GLU:CD	4:F:2195:HOH:O	2.21	0.84
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.59	0.83
1:A:39:ILE:HD13	1:A:85:TRP:CE3	2.13	0.83
1:A:332:GLN:OE1	1:A:351:HIS:CE1	2.32	0.82
1:A:389:GLN:NE2	3:A:600:CAP:H11	1.95	0.82
1:H:317:THR:HG21	4:H:2909:HOH:O	1.79	0.82
1:G:45:ALA:CB	1:G:115:MET:HE1	2.09	0.81
1:J:328:ASP:CG	1:J:329:ILE:HD12	2.05	0.81
1:B:328:ASP:OD2	1:B:329:ILE:CD1	2.28	0.81
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.15	0.81
1:B:203:GLU:O	1:B:207:GLU:HG2	1.81	0.81
1:C:263:ALA:HB2	1:F:263:ALA:HB2	1.61	0.81
1:J:328:ASP:OD1	1:J:329:ILE:HD12	1.78	0.80
1:H:317:THR:CG2	4:H:2909:HOH:O	2.30	0.80
1:D:341:HIS:CE1	1:D:343:LYS:HZ2	1.98	0.80
1:B:263:ALA:HB2	1:G:263:ALA:HB2	1.63	0.79
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.18	0.78
1:A:324:GLU:OE2	1:A:325:GLY:N	2.16	0.78
1:H:322:LYS:HG2	1:H:323:LEU:HD12	1.65	0.77
1:B:128:PHE:H	1:B:354:GLN:HE22	1.31	0.77
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.20	0.77
1:C:358:SER:HB2	4:C:2464:HOH:O	1.85	0.77
1:A:149:MET:CE	1:A:250:LYS:CE	2.62	0.76
1:H:128:PHE:H	1:H:354:GLN:HE22	1.31	0.76
1:A:143:ILE:HD11	1:A:338:ARG:HG2	1.68	0.76
1:A:38:THR:CG2	1:A:41:GLN:OE1	2.32	0.76
1:A:149:MET:CE	1:A:250:LYS:CD	2.54	0.76
1:H:149:MET:HE1	1:H:251:HIS:CE1	2.21	0.76
1:H:397:HIS:CG	1:H:398:PRO:HD2	2.21	0.76
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.20	0.76
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:GLN:HA	1:A:415:ILE:HD13	1.69	0.75
1:A:32:THR:HG21	1:A:119:LYS:HE2	1.69	0.74
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.22	0.74
1:A:108:ILE:HD12	1:A:108:ILE:C	2.12	0.74
1:F:332:GLN:HE21	1:F:332:GLN:HA	1.50	0.74
1:A:396:GLY:O	1:A:437:LYS:NZ	2.20	0.74
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.21	0.74
1:B:215:LYS:NZ	1:B:219:GLU:OE2	2.21	0.74
1:H:293:TYR:CE2	4:H:2342:HOH:O	2.39	0.73
1:I:358:SER:HB2	4:I:2433:HOH:O	1.87	0.73
1:A:376:GLN:CB	4:A:2304:HOH:O	2.35	0.73
1:E:427:THR:HG23	1:E:428:HIS:ND1	2.03	0.73
1:J:174:GLU:OE1	1:J:211:LYS:NZ	2.22	0.73
1:J:411:ALA:O	1:J:415:ILE:HG13	1.89	0.73
1:J:329:ILE:CD1	1:J:329:ILE:N	2.52	0.72
1:J:329:ILE:CD1	1:J:329:ILE:H	2.02	0.72
1:H:376:GLN:HB3	4:H:2840:HOH:O	1.89	0.72
1:J:389:GLN:C	1:J:390:LEU:HD12	2.14	0.72
1:A:108:ILE:C	1:A:108:ILE:CD1	2.63	0.72
1:B:59:TYR:O	1:B:61:TRP:HD1	1.71	0.72
1:A:376:GLN:HA	1:A:415:ILE:CD1	2.20	0.71
1:G:54:THR:HG21	1:G:58:LEU:HG	1.70	0.71
1:G:149:MET:HE1	1:G:251:HIS:ND1	2.06	0.71
1:A:39:ILE:CD1	1:A:85:TRP:HB2	2.20	0.71
1:A:54:THR:CG2	1:A:56:THR:O	2.39	0.71
1:A:332:GLN:HE21	1:A:332:GLN:HA	1.54	0.71
1:A:281:HIS:CE1	1:A:283:ALA:HB2	2.25	0.71
1:G:54:THR:HG21	1:G:58:LEU:CG	2.21	0.70
1:H:403:ALA:HA	1:H:406:ARG:NH2	2.06	0.70
1:I:15:LYS:HD2	4:I:1867:HOH:O	1.89	0.70
1:C:128:PHE:H	1:C:354:GLN:HE22	1.39	0.70
1:C:214:ASP:O	1:C:218:ASN:HB2	1.90	0.70
1:F:200:ASN:OD1	1:F:205:ARG:HG3	1.91	0.70
1:H:108:ILE:HG22	1:H:108:ILE:O	1.91	0.70
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.27	0.69
1:E:263:ALA:HB2	1:I:263:ALA:HB2	1.73	0.69
1:H:367:SER:HB2	1:H:389:GLN:HB3	1.75	0.69
1:A:39:ILE:HD13	1:A:85:TRP:HE3	1.58	0.69
1:A:54:THR:HG23	1:A:56:THR:O	1.92	0.69
1:C:149:MET:HE1	1:C:251:HIS:ND1	2.07	0.69
1:D:341:HIS:CD2	1:D:343:LYS:HZ2	2.11	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:LEU:O	1:E:435:LEU:HD23	1.93	0.69
1:A:389:GLN:HE22	3:A:600:CAP:H11	1.58	0.68
1:C:376:GLN:HB3	1:C:377:PRO:HD3	1.74	0.68
1:E:428:HIS:NE2	4:E:2782:HOH:O	2.26	0.68
1:A:37:TYR:HA	1:A:41:GLN:NE2	2.07	0.68
1:E:65:GLU:OE1	1:E:65:GLU:N	2.25	0.68
1:G:45:ALA:HB1	1:G:115:MET:CE	2.20	0.68
1:A:149:MET:HE3	1:A:250:LYS:CB	2.23	0.68
1:D:58:LEU:HD12	1:D:58:LEU:N	2.09	0.68
1:E:427:THR:HG23	1:E:428:HIS:CE1	2.28	0.68
1:A:331:ILE:O	1:A:335:ARG:HG3	1.94	0.68
1:I:128:PHE:H	1:I:354:GLN:HE22	1.41	0.68
1:A:86:ILE:HG21	1:A:349:VAL:O	1.94	0.68
1:A:367:SER:HB2	1:A:389:GLN:HB3	1.75	0.67
1:E:119:LYS:HE2	4:E:777:HOH:O	1.94	0.67
1:I:235:LEU:O	1:I:239:GLN:HG3	1.94	0.67
1:C:303:LYS:NZ	1:C:354:GLN:HE21	1.93	0.67
1:G:93:PHE:CE1	1:G:131:LYS:HD3	2.30	0.67
1:H:283:ALA:O	1:H:284:MET:HB3	1.93	0.67
1:A:49:GLU:HG3	1:A:115:MET:SD	2.35	0.67
1:B:389:GLN:C	1:B:390:LEU:HD12	2.20	0.67
1:A:115:MET:O	1:A:118:VAL:HG12	1.94	0.67
1:H:389:GLN:C	1:H:390:LEU:HD12	2.19	0.67
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.30	0.66
1:A:38:THR:H	1:A:41:GLN:CD	2.02	0.66
1:A:332:GLN:OE1	1:A:351:HIS:ND1	2.28	0.66
1:H:149:MET:HE1	1:H:251:HIS:ND1	2.09	0.66
1:E:165:LYS:HE2	1:I:49:GLU:O	1.96	0.66
1:G:149:MET:CE	1:G:251:HIS:CE1	2.79	0.66
1:A:38:THR:OG1	1:A:41:GLN:HG3	1.95	0.66
1:F:32:THR:HG21	1:F:119:LYS:HE3	1.77	0.66
1:J:163:LYS:H	1:J:395:LEU:HD12	1.61	0.66
1:E:303:LYS:NZ	1:E:354:GLN:HE21	1.92	0.66
1:J:54:THR:HG21	1:J:58:LEU:HD11	1.78	0.66
1:B:358:SER:HB2	4:B:2811:HOH:O	1.95	0.66
1:H:183:ASN:OD1	1:H:406:ARG:NH1	2.29	0.66
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.31	0.66
1:F:163:LYS:HA	1:F:164:PRO:C	2.21	0.66
1:G:207:GLU:HG3	4:G:1811:HOH:O	1.95	0.66
1:A:72:ALA:HA	1:A:90:ALA:O	1.96	0.65
1:A:165:LYS:HB3	1:A:191:ASP:OD2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:ASP:OD1	1:D:440:HIS:HE1	1.79	0.65
1:H:125:ASP:OD1	1:H:126:LEU:N	2.30	0.65
1:H:366:SER:HA	4:H:2657:HOH:O	1.95	0.65
1:A:424:TYR:CD2	1:A:428:HIS:ND1	2.65	0.65
1:A:37:TYR:HA	1:A:41:GLN:HE22	1.61	0.65
1:A:424:TYR:CD2	1:A:428:HIS:CE1	2.85	0.65
1:C:328:ASP:OD1	1:C:329:ILE:CD1	2.44	0.65
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.32	0.65
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.78	0.65
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.32	0.65
1:F:376:GLN:CG	4:F:2817:HOH:O	2.32	0.65
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.62	0.65
1:A:178:TYR:CZ	1:A:215:LYS:NZ	2.65	0.64
1:J:54:THR:HG21	1:J:58:LEU:HD13	1.77	0.64
1:A:362:ALA:O	1:A:364:PRO:HD3	1.97	0.64
1:H:396:GLY:O	1:H:437:LYS:NZ	2.25	0.64
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.32	0.64
1:A:149:MET:CE	1:A:250:LYS:CB	2.75	0.64
1:A:39:ILE:HD13	1:A:85:TRP:HB2	1.79	0.64
1:H:330:THR:HG22	1:H:382:LEU:HD21	1.79	0.64
1:H:376:GLN:HG2	1:H:415:ILE:CD1	2.27	0.64
1:H:338:ARG:HH11	1:H:364:PRO:HG2	1.63	0.64
1:H:79:ASP:OD1	1:H:81:GLY:N	2.31	0.64
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.32	0.63
1:A:331:ILE:HG12	1:A:381:ALA:O	1.96	0.63
1:D:108:ILE:HD12	1:D:108:ILE:C	2.23	0.63
1:J:146:VAL:HG21	1:J:312:GLN:HE21	1.63	0.63
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.32	0.63
1:F:268:ARG:HD3	1:F:268:ARG:C	2.24	0.63
1:A:442:THR:O	1:A:444:VAL:HG23	1.98	0.63
1:A:268:ARG:HD3	1:A:268:ARG:C	2.23	0.63
1:A:22:LYS:CE	1:G:63:GLU:OE1	2.46	0.63
1:B:329:ILE:HD12	1:B:329:ILE:N	2.13	0.63
1:D:341:HIS:CE1	1:D:343:LYS:NZ	2.67	0.63
1:F:54:THR:HG23	1:F:56:THR:O	1.99	0.63
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.34	0.63
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.81	0.62
1:E:128:PHE:H	1:E:354:GLN:HE22	1.46	0.62
1:E:260:GLY:HA3	1:I:260:GLY:HA3	1.81	0.62
1:G:389:GLN:C	1:G:390:LEU:HD12	2.24	0.62
1:A:23:ARG:NE	1:G:69:ASP:OD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ILE:HD12	1:E:157:ILE:HD12	1.81	0.62
1:A:282:ARG:HD3	1:A:298:MET:HE2	1.80	0.62
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.34	0.62
1:G:34:ALA:HA	1:G:119:LYS:HG3	1.82	0.62
1:H:120:GLY:C	4:H:2182:HOH:O	2.43	0.62
1:H:284:MET:O	1:H:284:MET:HG2	1.98	0.62
1:A:298:MET:HE2	1:A:314:HIS:O	1.99	0.62
1:J:343:LYS:HD2	4:J:2757:HOH:O	1.98	0.62
1:F:128:PHE:H	1:F:354:GLN:HE22	1.47	0.62
1:H:322:LYS:HG2	1:H:323:LEU:CD1	2.29	0.62
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.36	0.61
1:A:26:ILE:HB	1:A:127:TYR:HB3	1.83	0.61
1:H:341:HIS:NE2	1:H:353:GLU:OE2	2.32	0.61
1:I:438:TRP:O	1:I:441:VAL:HG22	2.01	0.61
1:B:163:LYS:HA	1:B:164:PRO:C	2.25	0.61
1:A:163:LYS:HA	1:A:164:PRO:C	2.25	0.61
1:A:25:ILE:HD12	1:A:96:PHE:CE2	2.35	0.61
1:A:424:TYR:CE2	1:A:428:HIS:ND1	2.68	0.61
1:H:159:GLY:CA	1:H:187:TYR:CZ	2.80	0.61
1:F:362:ALA:O	1:F:364:PRO:HD3	2.01	0.60
1:A:157:ILE:N	1:A:157:ILE:HD12	2.15	0.60
1:H:371:HIS:HB2	1:H:372:PRO:HD2	1.83	0.60
1:A:425:ALA:C	1:A:427:THR:H	2.10	0.60
1:C:328:ASP:CG	1:C:329:ILE:HD12	2.25	0.60
1:E:159:GLY:CA	1:E:187:TYR:CZ	2.80	0.60
1:F:327:ARG:NH2	4:F:2580:HOH:O	2.31	0.60
1:B:376:GLN:N	1:B:377:PRO:HD2	2.16	0.60
1:J:79:ASP:HB2	1:J:85:TRP:CH2	2.37	0.60
1:J:163:LYS:HA	1:J:164:PRO:C	2.27	0.60
1:F:389:GLN:C	1:F:390:LEU:HD12	2.25	0.60
1:A:263:ALA:HB2	1:H:263:ALA:HB2	1.82	0.60
1:B:438:TRP:O	1:B:441:VAL:HG22	2.02	0.60
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.31	0.60
1:I:376:GLN:HB3	1:I:377:PRO:HD3	1.83	0.60
1:A:430:GLU:OE1	1:A:430:GLU:N	2.22	0.60
1:H:371:HIS:HB2	1:H:372:PRO:CD	2.32	0.60
1:A:235:LEU:O	1:A:239:GLN:HG3	2.01	0.60
1:H:283:ALA:O	1:H:284:MET:CB	2.50	0.60
1:C:98:GLU:HG3	4:C:1235:HOH:O	2.02	0.59
1:C:322:LYS:HA	1:C:443:PRO:O	2.02	0.59
1:J:79:ASP:HB2	1:J:85:TRP:CZ3	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLN:HA	1:A:332:GLN:NE2	2.17	0.59
1:H:403:ALA:HA	1:H:406:ARG:CZ	2.33	0.59
1:A:40:GLU:HB2	4:A:2245:HOH:O	2.03	0.59
1:B:59:TYR:O	1:B:61:TRP:CD1	2.55	0.59
1:D:59:TYR:O	1:D:61:TRP:HD1	1.85	0.59
1:E:59:TYR:O	1:E:61:TRP:HD1	1.84	0.59
1:G:108:ILE:C	1:G:108:ILE:HD12	2.28	0.59
1:J:328:ASP:OD1	1:J:329:ILE:HD13	1.98	0.59
1:H:338:ARG:NH1	1:H:364:PRO:HG2	2.17	0.59
1:C:328:ASP:OD1	1:C:329:ILE:HD12	2.02	0.59
1:C:441:VAL:HG12	1:C:442:THR:N	2.16	0.59
1:E:215:LYS:O	1:E:219:GLU:HG3	2.03	0.59
1:A:230:ILE:O	1:A:237:MET:HG2	2.03	0.59
1:F:38:THR:OG1	1:F:41:GLN:HG3	2.03	0.59
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.37	0.59
1:A:218:ASN:HB2	4:A:1583:HOH:O	2.03	0.59
1:C:397:HIS:CG	1:C:398:PRO:HD2	2.38	0.59
1:A:93:PHE:CE1	1:A:131:LYS:HE3	2.38	0.59
1:A:149:MET:HE3	1:A:250:LYS:CG	2.30	0.59
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.38	0.59
1:A:78:HIS:C	1:A:85:TRP:HD1	2.10	0.58
1:J:104:LEU:C	1:J:104:LEU:HD23	2.28	0.58
1:E:63:GLU:OE1	1:H:355:LYS:NZ	2.35	0.58
1:E:389:GLN:C	1:E:390:LEU:HD12	2.28	0.58
1:J:54:THR:HG21	1:J:58:LEU:CD2	2.34	0.58
1:A:126:LEU:O	1:A:303:LYS:NZ	2.36	0.58
1:F:59:TYR:O	1:F:61:TRP:HD1	1.85	0.58
1:C:149:MET:HE2	1:C:150:LEU:HD21	1.85	0.58
1:E:163:LYS:HA	1:E:164:PRO:C	2.28	0.58
1:G:163:LYS:HA	1:G:164:PRO:C	2.28	0.58
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.39	0.58
1:E:444:VAL:O	1:I:117:ARG:HG3	2.04	0.58
1:J:128:PHE:H	1:J:354:GLN:HE22	1.50	0.58
1:A:183:ASN:ND2	1:A:402:ALA:HB1	2.19	0.57
1:C:329:ILE:HD12	1:C:329:ILE:N	2.19	0.57
1:H:59:TYR:O	1:H:61:TRP:HD1	1.87	0.57
1:J:268:ARG:HD3	1:J:268:ARG:C	2.29	0.57
1:A:324:GLU:OE2	1:A:324:GLU:C	2.48	0.57
1:A:77:PHE:N	1:A:77:PHE:CD2	2.72	0.57
1:C:149:MET:CE	1:C:251:HIS:CE1	2.82	0.57
1:E:396:GLY:O	1:E:437:LYS:NZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:329:ILE:HD12	1:J:329:ILE:H	1.59	0.57
1:A:282:ARG:HD3	1:A:298:MET:CE	2.35	0.56
1:A:131:LYS:NZ	4:A:1992:HOH:O	2.35	0.56
1:A:149:MET:CE	1:A:250:LYS:HB3	2.35	0.56
1:I:282:ARG:HG3	1:I:285:HIS:CD2	2.40	0.56
1:C:149:MET:HE1	1:C:251:HIS:HE1	1.63	0.56
1:D:54:THR:HG23	1:D:56:THR:O	2.04	0.56
1:D:376:GLN:NE2	1:D:380:GLU:OE1	2.34	0.56
1:B:152:ILE:HD12	1:B:157:ILE:HD12	1.87	0.56
1:C:441:VAL:CG1	1:C:442:THR:N	2.68	0.56
1:H:93:PHE:CD1	1:H:93:PHE:C	2.84	0.56
1:C:389:GLN:C	1:C:390:LEU:HD12	2.30	0.56
1:E:427:THR:HG23	1:E:428:HIS:HD1	1.68	0.56
1:F:108:ILE:C	1:F:108:ILE:HD12	2.30	0.56
1:A:39:ILE:HD11	1:A:85:TRP:HB2	1.87	0.56
1:A:282:ARG:O	1:A:283:ALA:C	2.49	0.56
1:C:341:HIS:NE2	1:C:353:GLU:OE2	2.31	0.56
1:H:149:MET:HE1	1:H:251:HIS:HD1	1.69	0.56
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.71	0.56
1:J:328:ASP:CG	1:J:329:ILE:CD1	2.70	0.56
1:H:323:LEU:HD12	1:H:323:LEU:N	2.20	0.56
1:I:209:MET:HE2	1:I:226:TRP:HB2	1.88	0.56
1:J:437:LYS:HG3	1:J:438:TRP:CG	2.41	0.56
1:B:108:ILE:HD12	1:B:108:ILE:C	2.30	0.56
1:A:76:ASP:C	1:A:77:PHE:CD2	2.84	0.55
1:A:130:GLU:HG3	1:A:357:TYR:CE2	2.41	0.55
1:C:362:ALA:O	1:C:364:PRO:HD3	2.06	0.55
1:A:293:TYR:CE1	4:A:2523:HOH:O	2.59	0.55
1:B:260:GLY:HA3	1:G:260:GLY:HA3	1.88	0.55
1:E:332:GLN:NE2	1:E:342:TYR:OH	2.40	0.55
1:A:442:THR:O	1:A:442:THR:HG22	2.07	0.55
1:F:230:ILE:O	1:F:237:MET:HG2	2.07	0.55
1:H:163:LYS:H	1:H:395:LEU:CD2	2.20	0.55
1:H:208:ILE:O	1:H:212:ILE:HG13	2.06	0.55
1:A:64:GLN:HG2	4:A:1148:HOH:O	2.05	0.55
1:C:411:ALA:O	1:C:415:ILE:HG13	2.05	0.55
1:J:56:THR:O	1:J:58:LEU:HD13	2.07	0.55
1:B:167:GLY:O	1:G:66:ARG:HD2	2.07	0.55
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.41	0.55
1:D:230:ILE:O	1:D:237:MET:HG2	2.06	0.55
1:E:431:LEU:O	1:E:435:LEU:CD2	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:424:TYR:CZ	1:I:428:HIS:CE1	2.93	0.55
1:C:412:ILE:O	1:C:416:MET:HG2	2.07	0.55
1:F:72:ALA:HB2	1:F:91:TYR:CD1	2.41	0.54
1:F:376:GLN:NE2	4:F:2525:HOH:O	2.28	0.54
1:E:427:THR:HG21	4:E:2735:HOH:O	2.08	0.54
1:G:105:LEU:HD23	1:G:108:ILE:HD11	1.89	0.54
1:H:316:GLY:O	1:H:366:SER:CB	2.56	0.54
1:D:260:GLY:HA3	1:J:260:GLY:HA3	1.89	0.54
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.37	0.54
1:F:73:LYS:HG3	4:F:2809:HOH:O	2.07	0.54
1:H:39:ILE:HG23	1:H:40:GLU:N	2.21	0.54
1:A:328:ASP:OD1	1:A:328:ASP:N	2.37	0.54
1:J:54:THR:HG23	1:J:56:THR:O	2.08	0.54
1:J:108:ILE:CG2	1:J:108:ILE:O	2.55	0.54
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.06	0.54
1:A:48:ALA:HB1	1:A:53:GLY:HA3	1.89	0.54
1:A:260:GLY:HA3	1:H:260:GLY:HA3	1.89	0.54
1:B:25:ILE:HD12	1:B:96:PHE:CE2	2.43	0.54
1:D:389:GLN:C	1:D:390:LEU:HD12	2.33	0.54
1:D:108:ILE:C	1:D:108:ILE:CD1	2.80	0.54
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.89	0.53
1:H:375:ILE:O	1:H:378:VAL:N	2.39	0.53
1:J:407:ALA:HB2	1:J:430:GLU:HB3	1.90	0.53
1:A:376:GLN:N	1:A:377:PRO:HD2	2.24	0.53
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.73	0.53
1:G:149:MET:HE1	1:G:251:HIS:HD1	1.74	0.53
1:H:403:ALA:CA	1:H:406:ARG:NH2	2.71	0.53
1:J:19:PRO:HG3	1:J:75:TYR:CZ	2.44	0.53
1:A:165:LYS:CB	1:A:191:ASP:OD2	2.56	0.53
1:B:329:ILE:HD12	1:B:329:ILE:H	1.72	0.53
1:C:21:LYS:HE3	4:C:892:HOH:O	2.08	0.53
1:D:360:LYS:HE3	4:D:508:HOH:O	2.07	0.53
1:D:376:GLN:HB3	1:D:377:PRO:HD3	1.90	0.53
1:C:341:HIS:CE1	1:C:343:LYS:HZ2	2.25	0.53
1:E:159:GLY:HA3	1:E:187:TYR:CD1	2.43	0.53
1:H:435:LEU:O	1:H:439:GLY:N	2.41	0.53
1:I:268:ARG:HD3	1:I:268:ARG:C	2.33	0.53
1:J:376:GLN:HB3	1:J:377:PRO:HD3	1.91	0.53
1:B:175:LYS:HE3	1:B:179:ASP:OD2	2.09	0.53
1:E:165:LYS:HG2	1:E:191:ASP:OD2	2.09	0.53
1:H:338:ARG:HA	1:H:361:ALA:HB1	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:CD1	1:A:338:ARG:HG2	2.38	0.52
1:D:208:ILE:O	1:D:212:ILE:HG12	2.09	0.52
1:H:406:ARG:O	1:H:410:GLN:HG3	2.09	0.52
1:I:163:LYS:HA	1:I:164:PRO:C	2.34	0.52
1:C:149:MET:CE	1:C:251:HIS:HE1	2.21	0.52
1:A:76:ASP:OD1	1:A:77:PHE:N	2.42	0.52
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.40	0.52
1:D:424:TYR:CE1	1:D:428:HIS:CE1	2.97	0.52
1:A:78:HIS:C	1:A:85:TRP:CD1	2.87	0.52
1:A:78:HIS:O	1:A:85:TRP:CD1	2.62	0.52
1:E:159:GLY:CA	1:E:187:TYR:CE2	2.92	0.52
1:A:52:THR:HG22	1:H:166:VAL:O	2.10	0.52
1:F:206:ALA:HA	1:F:226:TRP:CZ3	2.45	0.52
1:A:424:TYR:CZ	1:A:428:HIS:HE1	2.22	0.52
1:F:32:THR:CG2	1:F:119:LYS:HE3	2.39	0.52
1:J:23:ARG:HD3	4:J:485:HOH:O	2.09	0.52
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.73	0.52
1:E:176:LEU:HD11	1:E:395:LEU:HD11	1.91	0.52
1:G:268:ARG:HD3	1:G:268:ARG:C	2.34	0.52
1:A:185:ALA:O	1:A:224:LYS:NZ	2.27	0.52
1:A:338:ARG:HA	1:A:361:ALA:CB	2.30	0.52
1:G:371:HIS:HB2	1:G:372:PRO:HD2	1.92	0.52
1:I:93:PHE:CD1	1:I:93:PHE:C	2.87	0.52
1:A:290:ARG:NE	1:A:324:GLU:HG3	2.14	0.52
1:D:163:LYS:HA	1:D:164:PRO:C	2.34	0.52
1:D:422:ASP:OD1	1:D:440:HIS:CE1	2.60	0.52
1:I:283:ALA:O	1:I:284:MET:HB3	2.10	0.52
1:A:163:LYS:H	1:A:395:LEU:HD22	1.75	0.52
1:A:285:HIS:CG	1:A:286:ALA:N	2.78	0.52
1:G:54:THR:HG23	1:G:56:THR:O	2.10	0.52
1:G:376:GLN:HB3	1:G:377:PRO:HD3	1.92	0.52
1:J:163:LYS:H	1:J:395:LEU:CD1	2.23	0.52
1:H:159:GLY:HA3	1:H:187:TYR:CD1	2.45	0.51
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.75	0.51
1:A:82:ASP:OD1	1:A:82:ASP:C	2.53	0.51
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.92	0.51
1:I:230:ILE:O	1:I:237:MET:HG2	2.11	0.51
1:A:283:ALA:O	1:A:284:MET:HB3	2.10	0.51
1:B:34:ALA:HA	1:B:119:LYS:HG3	1.91	0.51
1:D:59:TYR:O	1:D:61:TRP:CD1	2.63	0.51
1:J:108:ILE:O	1:J:108:ILE:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:343:LYS:CD	4:J:2757:HOH:O	2.57	0.51
1:A:424:TYR:CE1	1:A:428:HIS:HE1	2.28	0.51
1:D:282:ARG:HG3	1:D:285:HIS:CD2	2.46	0.51
1:G:54:THR:HA	4:G:466:HOH:O	2.11	0.51
1:H:397:HIS:ND1	1:H:398:PRO:HD2	2.25	0.51
1:A:78:HIS:O	1:A:85:TRP:HD1	1.93	0.51
1:H:34:ALA:O	1:H:35:GLU:C	2.54	0.51
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.93	0.51
1:E:108:ILE:CG2	1:E:108:ILE:O	2.58	0.51
1:G:149:MET:CE	1:G:251:HIS:HE1	2.23	0.51
1:A:289:THR:HA	1:A:296:ILE:O	2.10	0.50
1:A:406:ARG:O	1:A:410:GLN:HG3	2.11	0.50
1:I:424:TYR:CE1	1:I:428:HIS:CE1	2.99	0.50
1:J:414:ALA:HB2	1:J:424:TYR:CD2	2.46	0.50
1:D:96:PHE:CE1	1:D:104:LEU:CD1	2.94	0.50
1:D:96:PHE:CE1	1:D:104:LEU:HD13	2.46	0.50
1:D:58:LEU:N	1:D:58:LEU:CD1	2.75	0.50
1:E:283:ALA:O	1:E:284:MET:HB3	2.11	0.50
1:G:59:TYR:O	1:G:61:TRP:HD1	1.95	0.50
1:H:403:ALA:CB	1:H:406:ARG:NH2	2.75	0.50
1:A:157:ILE:HD13	1:A:363:PHE:CZ	2.46	0.50
1:B:236:GLU:N	1:B:236:GLU:OE1	2.43	0.50
1:D:412:ILE:O	1:D:416:MET:HG2	2.12	0.50
1:E:419:ILE:O	1:E:420:PRO:C	2.54	0.50
1:H:163:LYS:HA	1:H:164:PRO:C	2.36	0.50
1:J:107:SER:HB3	1:J:108:ILE:HD12	1.93	0.50
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.94	0.50
1:G:424:TYR:CE2	1:G:428:HIS:CE1	3.00	0.50
1:A:116:LYS:C	1:A:118:VAL:H	2.19	0.50
1:C:376:GLN:N	1:C:377:PRO:CD	2.74	0.50
1:D:341:HIS:CG	1:D:343:LYS:NZ	2.80	0.50
1:E:131:LYS:NZ	4:E:1899:HOH:O	2.27	0.50
1:H:25:ILE:HD13	1:H:93:PHE:HA	1.94	0.50
1:H:51:SER:OG	1:H:52:THR:N	2.45	0.50
1:H:149:MET:CE	1:H:251:HIS:CE1	2.95	0.50
1:C:303:LYS:HZ2	1:C:354:GLN:HE21	1.59	0.50
1:H:316:GLY:O	1:H:366:SER:HB2	2.12	0.50
1:H:337:LEU:HD22	1:H:362:ALA:HB3	1.94	0.50
1:I:25:ILE:CD1	1:I:93:PHE:HA	2.41	0.50
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.47	0.50
1:C:397:HIS:ND1	1:C:398:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:265:ARG:HD3	4:I:2459:HOH:O	2.11	0.50
1:F:59:TYR:O	1:F:61:TRP:CD1	2.65	0.50
1:H:292:PRO:O	4:H:2255:HOH:O	2.20	0.50
1:A:56:THR:HG21	1:H:392:GLY:O	2.12	0.49
1:D:96:PHE:CD1	1:D:104:LEU:HD13	2.47	0.49
1:E:303:LYS:HZ1	1:E:354:GLN:HE21	1.59	0.49
1:F:73:LYS:CG	4:F:2809:HOH:O	2.60	0.49
1:H:104:LEU:C	1:H:104:LEU:HD23	2.37	0.49
1:A:86:ILE:HD11	1:A:350:PHE:CE1	2.47	0.49
1:D:19:PRO:HG3	1:D:75:TYR:CZ	2.47	0.49
1:F:441:VAL:HG22	1:F:442:THR:N	2.28	0.49
1:H:203:GLU:OE1	1:H:203:GLU:N	2.31	0.49
1:J:206:ALA:HA	1:J:226:TRP:CZ3	2.48	0.49
1:A:72:ALA:CA	1:A:90:ALA:O	2.60	0.49
1:B:367:SER:HB2	1:B:389:GLN:HB3	1.93	0.49
1:H:403:ALA:HB2	1:H:406:ARG:NH2	2.28	0.49
1:J:159:GLY:CA	1:J:187:TYR:CZ	2.89	0.49
1:J:349:VAL:HG22	4:J:461:HOH:O	2.12	0.49
1:A:411:ALA:O	1:A:414:ALA:HB3	2.13	0.49
1:C:397:HIS:CE1	1:C:398:PRO:HD2	2.47	0.49
1:G:48:ALA:HB1	1:G:53:GLY:HA3	1.93	0.49
1:H:26:ILE:HB	1:H:127:TYR:HB3	1.93	0.49
1:H:319:GLY:N	1:H:325:GLY:O	2.44	0.49
1:B:322:LYS:HG3	1:B:323:LEU:HG	1.94	0.49
1:C:328:ASP:OD1	1:C:329:ILE:HD13	2.12	0.49
1:D:159:GLY:CA	1:D:187:TYR:CZ	2.90	0.49
1:D:341:HIS:CD2	1:D:343:LYS:NZ	2.80	0.49
1:E:25:ILE:HD11	1:E:132:LEU:HD21	1.94	0.49
1:A:32:THR:CG2	1:A:119:LYS:HE2	2.38	0.49
1:A:417:GLN:C	1:A:419:ILE:H	2.21	0.49
1:J:208:ILE:O	1:J:212:ILE:HG12	2.13	0.49
1:B:54:THR:HG23	1:B:56:THR:O	2.12	0.49
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.47	0.49
1:H:108:ILE:O	1:H:108:ILE:CG2	2.58	0.49
1:I:25:ILE:HD13	1:I:93:PHE:HA	1.93	0.49
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.49
1:C:407:ALA:HB2	1:C:430:GLU:HB3	1.95	0.49
1:I:72:ALA:O	1:I:73:LYS:HD3	2.13	0.49
1:I:303:LYS:NZ	1:I:354:GLN:HE21	2.11	0.49
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.78	0.49
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.42	0.49
1:H:376:GLN:N	1:H:377:PRO:CD	2.75	0.49
1:I:25:ILE:N	1:I:25:ILE:HD12	2.28	0.49
1:J:414:ALA:HB2	1:J:424:TYR:CG	2.48	0.49
1:A:184:GLY:HA3	1:A:409:ARG:HG3	1.95	0.48
1:D:46:VAL:HG22	1:D:115:MET:HE1	1.95	0.48
1:J:93:PHE:CD1	1:J:93:PHE:C	2.91	0.48
1:J:175:LYS:NZ	1:J:179:ASP:OD2	2.31	0.48
1:A:299:PHE:CE2	1:A:351:HIS:CD2	3.00	0.48
1:D:397:HIS:CG	1:D:398:PRO:HD2	2.48	0.48
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.60	0.48
1:G:412:ILE:O	1:G:416:MET:HG2	2.13	0.48
1:A:116:LYS:C	1:A:118:VAL:N	2.69	0.48
1:C:341:HIS:CD2	1:C:343:LYS:HZ2	2.32	0.48
1:D:283:ALA:O	1:D:284:MET:HB3	2.13	0.48
1:F:48:ALA:HB1	1:F:53:GLY:HA3	1.95	0.48
1:H:117:ARG:HB2	4:H:1642:HOH:O	2.11	0.48
1:C:303:LYS:HZ3	1:C:354:GLN:HE21	1.60	0.48
1:H:149:MET:HE2	1:H:150:LEU:HD21	1.94	0.48
1:A:22:LYS:NZ	1:G:63:GLU:OE1	2.45	0.48
1:A:149:MET:CE	1:A:250:LYS:HE2	2.43	0.48
1:J:98:GLU:HG3	1:J:135:GLU:OE2	2.13	0.48
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.43	0.48
1:C:159:GLY:CA	1:C:187:TYR:CE2	2.95	0.48
1:C:283:ALA:O	1:C:284:MET:HB3	2.13	0.48
1:C:375:ILE:O	1:C:379:ILE:HG13	2.13	0.48
1:H:101:LEU:N	1:H:102:PRO:CD	2.75	0.48
1:H:203:GLU:H	1:H:203:GLU:CD	2.18	0.48
1:A:22:LYS:NZ	1:A:130:GLU:OE1	2.44	0.48
1:A:51:SER:OG	1:A:52:THR:N	2.45	0.48
1:C:38:THR:OG1	1:C:41:GLN:HG3	2.14	0.48
1:E:208:ILE:O	1:E:212:ILE:HG12	2.14	0.48
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.95	0.48
1:H:376:GLN:HG2	1:H:415:ILE:HD13	1.96	0.48
1:I:235:LEU:HB3	4:I:2572:HOH:O	2.13	0.48
1:A:106:ALA:HA	1:H:258:ILE:CD1	2.44	0.47
1:B:65:GLU:CG	1:F:22:LYS:HD3	2.44	0.47
1:G:438:TRP:O	1:G:441:VAL:HG12	2.14	0.47
1:H:161:VAL:CG2	1:H:189:KCX:HD2	2.43	0.47
1:I:122:ARG:HD2	4:I:455:HOH:O	2.13	0.47
1:J:159:GLY:CA	1:J:187:TYR:CE2	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:MET:HE2	1:A:226:TRP:HB2	1.96	0.47
1:F:80:MET:HE3	4:F:2035:HOH:O	2.12	0.47
1:A:283:ALA:O	1:A:284:MET:CB	2.62	0.47
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.94	0.47
1:C:139:PRO:HD3	1:C:306:ARG:O	2.15	0.47
1:D:376:GLN:N	1:D:377:PRO:CD	2.77	0.47
1:E:54:THR:HG23	1:E:56:THR:O	2.14	0.47
1:E:226:TRP:CZ3	1:E:228:ALA:HB2	2.50	0.47
1:H:163:LYS:HE3	3:H:600:CAP:O2P	2.13	0.47
1:A:128:PHE:H	1:A:354:GLN:HE22	1.61	0.47
1:A:328:ASP:HB2	4:A:445:HOH:O	2.13	0.47
1:E:108:ILE:O	1:E:108:ILE:HG22	2.14	0.47
1:F:283:ALA:O	1:F:284:MET:HB3	2.14	0.47
1:J:283:ALA:O	1:J:284:MET:HB3	2.15	0.47
1:J:331:ILE:O	1:J:335:ARG:HG3	2.14	0.47
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.95	0.47
1:J:441:VAL:HG13	4:J:677:HOH:O	2.13	0.47
1:A:147:ARG:HH21	1:A:385:ASP:HA	1.79	0.47
1:C:230:ILE:O	1:C:237:MET:HG2	2.13	0.47
1:D:397:HIS:CE1	1:D:398:PRO:HD2	2.50	0.47
1:I:389:GLN:C	1:I:390:LEU:HD12	2.40	0.47
1:J:143:ILE:HD11	1:J:338:ARG:HG2	1.97	0.47
1:A:116:LYS:O	1:A:118:VAL:N	2.47	0.47
1:G:422:ASP:OD1	1:G:440:HIS:HE1	1.97	0.47
1:A:72:ALA:O	1:A:73:LYS:HD3	2.15	0.47
1:A:425:ALA:O	1:A:427:THR:N	2.48	0.47
1:C:268:ARG:HD3	1:C:268:ARG:C	2.40	0.47
1:A:80:MET:HB2	1:A:84:SER:O	2.15	0.47
1:B:329:ILE:CD1	1:B:329:ILE:H	2.28	0.47
1:B:444:VAL:HB	1:G:37:TYR:OH	2.15	0.47
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.13	0.47
1:B:70:LEU:HD22	1:B:95:ALA:HA	1.98	0.46
1:B:400:GLY:HA2	1:G:59:TYR:CD1	2.50	0.46
1:F:96:PHE:CE1	1:F:104:LEU:HD13	2.50	0.46
1:H:291:ASN:OD1	1:H:292:PRO:HD2	2.15	0.46
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.97	0.46
1:B:175:LYS:CE	4:B:2916:HOH:O	2.63	0.46
1:A:297:SER:C	1:A:299:PHE:N	2.72	0.46
1:B:283:ALA:O	1:B:284:MET:HB3	2.15	0.46
1:E:159:GLY:HA3	1:E:187:TYR:CD2	2.50	0.46
1:E:413:ASP:O	1:E:417:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:320:ALA:O	1:G:442:THR:HG23	2.15	0.46
1:A:165:LYS:HZ2	1:A:191:ASP:CG	2.21	0.46
1:B:211:LYS:HE3	1:B:211:LYS:HB2	1.81	0.46
1:C:260:GLY:HA3	1:F:260:GLY:HA3	1.97	0.46
1:E:268:ARG:HD3	1:E:268:ARG:C	2.41	0.46
1:F:279:HIS:NE2	1:F:314:HIS:NE2	2.61	0.46
1:A:263:ALA:HB2	1:H:263:ALA:CB	2.46	0.46
1:C:108:ILE:HG22	1:C:108:ILE:O	2.15	0.46
1:C:149:MET:HE1	1:C:251:HIS:HD1	1.77	0.46
1:C:404:GLY:O	1:C:408:VAL:HG23	2.16	0.46
1:E:59:TYR:O	1:E:61:TRP:CD1	2.66	0.46
1:A:79:ASP:HA	1:A:85:TRP:CD1	2.50	0.46
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.51	0.46
1:D:144:GLU:CD	4:D:1914:HOH:O	2.58	0.46
1:J:441:VAL:HG12	1:J:442:THR:N	2.30	0.46
1:A:326:GLU:HG2	4:A:2331:HOH:O	2.14	0.46
1:A:443:PRO:C	1:A:444:VAL:HG23	2.40	0.46
1:B:191:ASP:HB2	4:B:473:HOH:O	2.15	0.46
1:D:234:LEU:HD21	1:J:234:LEU:HD21	1.98	0.46
1:E:319:GLY:HA2	4:E:995:HOH:O	2.14	0.46
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.46	0.46
1:F:376:GLN:CB	1:F:377:PRO:CD	2.93	0.46
1:J:370:LEU:HB2	4:J:1892:HOH:O	2.15	0.46
1:D:47:ALA:O	1:D:51:SER:HB2	2.16	0.46
1:E:93:PHE:CD1	1:E:93:PHE:C	2.94	0.46
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.81	0.46
1:F:336:ILE:HD12	1:F:336:ILE:HA	1.83	0.46
1:H:174:GLU:HG3	1:H:212:ILE:HD11	1.98	0.46
1:J:303:LYS:HZ3	1:J:354:GLN:HE21	1.63	0.46
1:J:322:LYS:NZ	3:J:600:CAP:O3P	2.49	0.46
1:B:283:ALA:O	1:B:284:MET:CB	2.65	0.45
1:C:320:ALA:O	1:C:442:THR:HG23	2.15	0.45
1:D:397:HIS:ND1	1:D:398:PRO:HD2	2.30	0.45
1:H:410:GLN:O	1:H:413:ASP:HB2	2.16	0.45
1:C:104:LEU:C	1:C:104:LEU:HD23	2.41	0.45
1:D:108:ILE:HD12	1:D:109:ALA:N	2.30	0.45
1:F:424:TYR:CZ	1:F:428:HIS:CE1	3.04	0.45
1:G:283:ALA:O	1:G:284:MET:HB3	2.16	0.45
1:I:101:LEU:N	1:I:102:PRO:CD	2.79	0.45
1:I:125:ASP:OD1	1:I:299:PHE:HE2	1.99	0.45
1:A:166:VAL:HG23	1:H:52:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:VAL:O	1:A:443:PRO:HD3	2.15	0.45
1:B:180:LEU:HD12	1:B:188:MET:HE1	1.98	0.45
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.97	0.45
1:E:355:LYS:NZ	1:H:63:GLU:OE1	2.38	0.45
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.97	0.45
1:I:289:THR:HG22	1:I:296:ILE:O	2.16	0.45
1:F:360:LYS:CE	4:F:452:HOH:O	2.65	0.45
1:H:376:GLN:HB2	1:H:377:PRO:HD3	1.99	0.45
1:I:283:ALA:O	1:I:284:MET:CB	2.64	0.45
1:I:338:ARG:HA	1:I:361:ALA:HB1	1.98	0.45
1:A:76:ASP:C	1:A:76:ASP:OD1	2.57	0.45
1:A:122:ARG:HG2	1:A:124:GLU:OE2	2.16	0.45
1:B:104:LEU:HD23	1:B:104:LEU:C	2.41	0.45
1:E:209:MET:HE2	1:E:226:TRP:HB2	1.98	0.45
1:F:283:ALA:O	1:F:284:MET:CB	2.65	0.45
1:H:314:HIS:HA	1:H:365:THR:O	2.15	0.45
1:C:189:KCX:OQ1	3:C:600:CAP:O3	2.35	0.45
1:C:397:HIS:CG	1:C:398:PRO:CD	2.99	0.45
1:D:383:GLY:HA3	4:D:872:HOH:O	2.15	0.45
1:H:424:TYR:CZ	1:H:428:HIS:CE1	3.04	0.45
1:A:59:TYR:CG	1:A:60:PRO:HD2	2.51	0.45
1:A:165:LYS:NZ	1:A:191:ASP:OD2	2.38	0.45
1:A:337:LEU:HD22	1:A:362:ALA:HB3	1.98	0.45
1:A:429:LYS:O	1:A:433:ARG:HG2	2.16	0.45
1:B:174:GLU:HB2	1:B:208:ILE:HD13	1.98	0.45
1:B:362:ALA:O	1:B:364:PRO:HD3	2.17	0.45
1:G:143:ILE:HD11	1:G:338:ARG:HG2	1.98	0.45
1:B:268:ARG:HD3	1:B:268:ARG:C	2.42	0.45
1:B:424:TYR:CZ	1:B:428:HIS:CE1	3.05	0.45
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.82	0.45
1:E:217:GLU:HG2	1:E:222:GLU:O	2.15	0.45
1:F:76:ASP:O	1:F:87:VAL:HA	2.17	0.45
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.61	0.45
1:H:200:ASN:OD1	1:H:205:ARG:HD3	2.16	0.45
1:B:230:ILE:O	1:B:237:MET:HG2	2.16	0.45
1:C:143:ILE:HD11	1:C:338:ARG:HG2	1.98	0.45
1:D:79:ASP:HB2	1:D:85:TRP:CH2	2.51	0.45
1:F:139:PRO:O	1:F:360:LYS:HD3	2.17	0.45
1:H:321:GLY:HA3	4:H:2909:HOH:O	2.15	0.45
1:I:62:TYR:OH	4:I:1237:HOH:O	2.21	0.45
1:C:360:LYS:HE3	4:C:2743:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:ALA:O	1:D:442:THR:HG23	2.17	0.45
1:F:331:ILE:O	1:F:335:ARG:HG3	2.16	0.45
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.52	0.45
1:H:282:ARG:O	1:H:283:ALA:C	2.59	0.45
1:A:158:TYR:O	1:A:186:ASP:HB2	2.18	0.44
1:B:329:ILE:CD1	1:B:329:ILE:N	2.79	0.44
1:H:323:LEU:HD12	1:H:323:LEU:H	1.82	0.44
1:A:14:ASP:OD1	1:A:17:TYR:N	2.44	0.44
1:A:226:TRP:CZ3	1:A:228:ALA:HB2	2.51	0.44
1:E:63:GLU:OE2	1:H:22:LYS:NZ	2.42	0.44
1:I:101:LEU:HB3	1:I:102:PRO:HD3	1.99	0.44
1:B:101:LEU:N	1:B:102:PRO:CD	2.80	0.44
1:G:355:LYS:HB3	4:G:788:HOH:O	2.16	0.44
1:H:425:ALA:O	1:H:427:THR:N	2.50	0.44
1:I:367:SER:HB2	1:I:389:GLN:HB3	1.99	0.44
1:J:159:GLY:HA3	1:J:187:TYR:CD2	2.50	0.44
1:J:376:GLN:N	1:J:377:PRO:CD	2.80	0.44
1:A:184:GLY:O	1:A:409:ARG:HD3	2.17	0.44
1:A:424:TYR:O	1:A:428:HIS:ND1	2.48	0.44
1:D:59:TYR:HA	1:D:60:PRO:HD3	1.80	0.44
1:G:376:GLN:N	1:G:377:PRO:CD	2.80	0.44
1:I:59:TYR:O	1:I:61:TRP:HD1	2.00	0.44
1:C:186:ASP:OD1	4:C:1387:HOH:O	2.21	0.44
1:J:347:ASN:CB	4:J:2614:HOH:O	2.39	0.44
1:C:329:ILE:CD1	1:C:329:ILE:N	2.81	0.44
1:D:159:GLY:CA	1:D:187:TYR:CE2	2.95	0.44
1:G:108:ILE:HD12	1:G:109:ALA:N	2.33	0.44
1:H:19:PRO:HG3	1:H:75:TYR:CZ	2.52	0.44
1:A:322:LYS:HG2	1:A:323:LEU:HG	2.00	0.44
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.98	0.44
1:B:332:GLN:CD	4:B:984:HOH:O	2.61	0.44
1:C:360:LYS:CE	4:C:2743:HOH:O	2.66	0.44
1:D:79:ASP:HB2	1:D:85:TRP:CZ3	2.52	0.44
1:E:69:ASP:OD1	1:H:23:ARG:NE	2.36	0.44
1:E:283:ALA:O	1:E:284:MET:CB	2.65	0.44
1:F:77:PHE:N	1:F:77:PHE:CD2	2.85	0.44
1:I:138:GLY:C	1:I:309:GLY:HA2	2.43	0.44
1:A:72:ALA:HB2	1:A:91:TYR:CD1	2.52	0.44
1:A:149:MET:HE1	1:A:250:LYS:HB2	1.99	0.44
1:D:336:ILE:HD12	1:D:336:ILE:HA	1.83	0.44
1:E:376:GLN:HA	1:E:415:ILE:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.52	0.44
1:G:45:ALA:CB	1:G:117:ARG:HD2	2.48	0.44
1:A:149:MET:CE	1:A:250:LYS:HB2	2.47	0.44
1:B:159:GLY:CA	1:B:187:TYR:CZ	2.97	0.44
1:C:122:ARG:HD2	4:C:475:HOH:O	2.18	0.44
1:G:424:TYR:CZ	1:G:428:HIS:CE1	3.06	0.44
1:H:183:ASN:OD1	1:H:402:ALA:HB1	2.18	0.44
1:H:371:HIS:C	1:H:373:GLY:H	2.25	0.44
1:H:425:ALA:C	1:H:427:THR:N	2.75	0.44
1:J:239:GLN:O	1:J:243:VAL:HG23	2.18	0.44
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.48	0.43
1:J:283:ALA:O	1:J:284:MET:CB	2.65	0.43
1:A:389:GLN:C	1:A:390:LEU:HD12	2.43	0.43
1:E:104:LEU:C	1:E:104:LEU:HD23	2.44	0.43
1:H:230:ILE:O	1:H:237:MET:HG2	2.18	0.43
1:A:115:MET:O	1:A:118:VAL:CG1	2.65	0.43
1:B:93:PHE:CD1	1:B:93:PHE:C	2.96	0.43
1:D:347:ASN:HA	4:D:2652:HOH:O	2.18	0.43
1:H:389:GLN:C	1:H:389:GLN:CD	2.85	0.43
1:I:108:ILE:HD12	1:I:108:ILE:C	2.44	0.43
1:A:19:PRO:HG3	1:A:75:TYR:CZ	2.53	0.43
1:B:288:PHE:HB3	1:G:288:PHE:HB3	2.00	0.43
1:E:348:ASP:C	1:E:348:ASP:OD1	2.61	0.43
1:F:73:LYS:HA	1:F:73:LYS:HD3	1.85	0.43
1:G:125:ASP:OD1	1:G:126:LEU:N	2.51	0.43
1:A:38:THR:H	1:A:41:GLN:NE2	2.16	0.43
1:A:282:ARG:HD3	1:A:314:HIS:O	2.19	0.43
1:C:283:ALA:O	1:C:284:MET:CB	2.66	0.43
1:H:317:THR:O	1:H:318:ALA:HB3	2.18	0.43
1:J:48:ALA:HB1	1:J:53:GLY:HA3	2.00	0.43
1:A:425:ALA:C	1:A:427:THR:N	2.73	0.43
1:D:38:THR:OG1	1:D:41:GLN:HG3	2.18	0.43
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.99	0.43
1:G:226:TRP:CZ3	1:G:228:ALA:HB2	2.53	0.43
1:A:78:HIS:CE1	1:A:349:VAL:HG11	2.54	0.43
1:A:161:VAL:CG2	1:A:189:KCX:HD2	2.48	0.43
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.80	0.43
1:A:299:PHE:CZ	1:A:351:HIS:CD2	3.07	0.43
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.49	0.43
1:B:136:PHE:HB3	1:B:307:LEU:O	2.18	0.43
1:B:174:GLU:HB2	1:B:208:ILE:HG21	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:GLU:OE2	1:B:266:TYR:OH	2.24	0.43
1:D:206:ALA:HA	1:D:226:TRP:CZ3	2.54	0.43
1:F:282:ARG:O	1:F:285:HIS:HB3	2.19	0.43
1:A:149:MET:HE1	1:A:250:LYS:CB	2.48	0.43
1:A:443:PRO:O	1:A:444:VAL:CG2	2.65	0.43
1:H:397:HIS:CD2	1:H:398:PRO:HD2	2.53	0.43
1:I:54:THR:HG23	1:I:56:THR:O	2.18	0.43
1:B:358:SER:OG	1:C:171:GLU:HG2	2.19	0.43
1:D:341:HIS:CG	1:D:343:LYS:HZ2	2.37	0.43
1:E:34:ALA:HA	1:E:119:LYS:HG3	2.01	0.43
1:E:390:LEU:HD12	1:E:390:LEU:N	2.33	0.43
1:H:49:GLU:HG3	1:H:115:MET:SD	2.59	0.43
1:H:54:THR:HG23	1:H:56:THR:H	1.84	0.43
1:H:59:TYR:O	1:H:61:TRP:CD1	2.70	0.43
1:A:225:THR:OG1	1:A:251:HIS:ND1	2.50	0.42
1:A:435:LEU:O	1:A:439:GLY:N	2.52	0.42
1:C:167:GLY:HA2	1:F:70:LEU:HD12	2.01	0.42
1:D:62:TYR:N	1:D:62:TYR:CD2	2.87	0.42
1:G:283:ALA:O	1:G:284:MET:CB	2.67	0.42
1:I:362:ALA:O	1:I:364:PRO:HD3	2.19	0.42
1:A:227:PHE:N	1:A:227:PHE:CD1	2.83	0.42
1:A:315:VAL:HG12	1:A:333:ASN:HB3	2.01	0.42
1:D:146:VAL:HG21	1:D:312:GLN:HE21	1.84	0.42
1:H:362:ALA:O	1:H:364:PRO:HD3	2.19	0.42
1:H:435:LEU:O	1:H:439:GLY:HA2	2.19	0.42
1:J:390:LEU:HD12	1:J:390:LEU:N	2.34	0.42
1:C:391:GLY:O	1:C:395:LEU:HD22	2.20	0.42
1:G:54:THR:HG21	1:G:58:LEU:CD2	2.49	0.42
1:I:159:GLY:HA3	1:I:187:TYR:CD1	2.55	0.42
1:I:217:GLU:HG2	1:I:222:GLU:O	2.19	0.42
1:A:49:GLU:O	1:H:165:LYS:HE2	2.18	0.42
1:A:167:GLY:O	1:H:66:ARG:HD2	2.20	0.42
1:A:415:ILE:C	1:A:417:GLN:H	2.26	0.42
1:E:319:GLY:CA	4:E:995:HOH:O	2.67	0.42
1:H:25:ILE:HD12	1:H:25:ILE:N	2.35	0.42
1:A:348:ASP:OD1	1:A:348:ASP:C	2.63	0.42
1:D:332:GLN:NE2	4:D:450:HOH:O	2.32	0.42
1:E:435:LEU:HD22	1:E:435:LEU:N	2.34	0.42
1:C:217:GLU:HG2	1:C:222:GLU:O	2.19	0.42
1:D:211:LYS:HG3	1:D:212:ILE:N	2.35	0.42
1:D:424:TYR:CZ	1:D:428:HIS:CE1	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:MET:HB2	1:F:84:SER:O	2.19	0.42
1:F:376:GLN:HB3	1:F:377:PRO:CD	2.48	0.42
1:F:407:ALA:HB2	1:F:430:GLU:HB3	2.01	0.42
1:I:34:ALA:O	1:I:35:GLU:C	2.63	0.42
1:I:56:THR:O	1:I:57:THR:C	2.62	0.42
1:A:299:PHE:CD2	1:A:351:HIS:HD2	2.38	0.42
1:A:311:ASP:C	1:A:312:GLN:HG3	2.44	0.42
1:B:46:VAL:HG22	1:B:115:MET:HE1	2.01	0.42
1:F:12:TYR:CD2	1:F:48:ALA:HB2	2.54	0.42
1:F:101:LEU:HB3	1:F:102:PRO:HD3	2.01	0.42
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.94	0.42
1:B:289:THR:HG22	1:B:296:ILE:O	2.20	0.42
1:D:11:TYR:CE2	1:D:73:LYS:NZ	2.87	0.42
1:E:77:PHE:N	1:E:77:PHE:CD2	2.87	0.42
1:F:101:LEU:N	1:F:102:PRO:CD	2.83	0.42
1:F:429:LYS:O	1:F:432:ALA:HB3	2.20	0.42
1:A:285:HIS:ND1	1:A:286:ALA:N	2.68	0.42
1:C:291:ASN:HA	1:C:292:PRO:HD3	1.81	0.42
1:D:79:ASP:OD1	1:D:81:GLY:N	2.51	0.42
1:G:440:HIS:CD2	4:G:712:HOH:O	2.72	0.42
1:H:54:THR:HG23	1:H:55:TRP:N	2.35	0.42
1:A:28:VAL:HG22	1:A:88:ARG:HG2	2.02	0.41
1:A:345:ASP:O	1:A:346:GLU:C	2.63	0.41
1:A:373:GLY:O	1:A:440:HIS:HA	2.20	0.41
1:B:65:GLU:HG3	1:F:22:LYS:HD3	2.01	0.41
1:C:367:SER:HB2	1:C:389:GLN:HB3	2.01	0.41
1:B:285:HIS:ND1	1:B:289:THR:OG1	2.49	0.41
1:D:70:LEU:HD22	1:D:95:ALA:HA	2.01	0.41
1:F:327:ARG:HB3	4:F:1943:HOH:O	2.20	0.41
1:A:443:PRO:C	1:A:444:VAL:CG2	2.94	0.41
1:C:159:GLY:CA	1:C:187:TYR:CZ	2.93	0.41
1:E:362:ALA:O	1:E:364:PRO:HD3	2.19	0.41
1:F:163:LYS:O	1:F:395:LEU:HD22	2.21	0.41
1:F:291:ASN:HA	1:F:292:PRO:HD3	1.87	0.41
1:I:159:GLY:CA	1:I:187:TYR:CZ	3.00	0.41
1:I:376:GLN:N	1:I:377:PRO:CD	2.83	0.41
1:A:139:PRO:HD3	1:A:306:ARG:O	2.21	0.41
1:D:235:LEU:O	1:D:239:GLN:HG3	2.20	0.41
1:F:424:TYR:CE2	1:F:428:HIS:CE1	3.08	0.41
1:A:25:ILE:HD12	1:A:96:PHE:HE2	1.84	0.41
1:B:376:GLN:N	1:B:377:PRO:CD	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:LEU:HD12	1:D:58:LEU:H	1.85	0.41
1:H:197:PRO:HD2	1:H:200:ASN:O	2.20	0.41
1:H:375:ILE:C	1:H:377:PRO:HD2	2.45	0.41
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.56	0.41
1:A:112:ILE:HA	1:A:115:MET:HE2	2.03	0.41
1:A:417:GLN:O	1:A:419:ILE:N	2.46	0.41
1:F:411:ALA:O	1:F:415:ILE:HG13	2.20	0.41
1:H:371:HIS:C	1:H:373:GLY:N	2.77	0.41
1:I:417:GLN:HG3	4:I:686:HOH:O	2.21	0.41
1:J:175:LYS:HD3	1:J:179:ASP:OD2	2.20	0.41
1:A:39:ILE:HB	1:A:85:TRP:CE3	2.56	0.41
1:A:77:PHE:N	1:A:77:PHE:HD2	2.16	0.41
1:A:149:MET:CE	1:A:250:LYS:HE3	2.49	0.41
1:D:283:ALA:O	1:D:284:MET:CB	2.69	0.41
1:E:101:LEU:HB3	1:E:102:PRO:HD3	2.01	0.41
1:J:336:ILE:HD12	1:J:336:ILE:HA	1.96	0.41
1:A:433:ARG:HG2	1:A:433:ARG:H	1.72	0.41
1:B:345:ASP:OD2	4:B:1444:HOH:O	2.21	0.41
1:D:93:PHE:CD1	1:D:93:PHE:C	2.98	0.41
1:E:196:SER:N	1:E:197:PRO:CD	2.84	0.41
1:E:323:LEU:HD23	1:I:115:MET:HA	2.02	0.41
1:E:329:ILE:HG23	4:E:827:HOH:O	2.20	0.41
1:F:108:ILE:C	1:F:108:ILE:CD1	2.94	0.41
1:F:341:HIS:NE2	1:F:353:GLU:OE2	2.37	0.41
1:H:122:ARG:HG2	1:H:124:GLU:OE2	2.21	0.41
1:J:54:THR:CG2	1:J:58:LEU:CD2	2.98	0.41
1:J:414:ALA:HB3	1:J:421:LEU:CD2	2.50	0.41
1:J:437:LYS:HG3	1:J:438:TRP:N	2.33	0.41
1:A:321:GLY:HA3	4:A:573:HOH:O	2.21	0.41
1:A:399:ASP:HB2	1:A:403:ALA:HB3	2.03	0.41
1:A:415:ILE:C	1:A:417:GLN:N	2.78	0.41
1:B:422:ASP:O	4:B:2564:HOH:O	2.21	0.41
1:C:58:LEU:HD13	1:F:163:LYS:C	2.45	0.41
1:F:25:ILE:CD1	1:F:93:PHE:HA	2.51	0.41
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.51	0.41
1:G:101:LEU:N	1:G:102:PRO:CD	2.83	0.41
1:G:289:THR:HG22	1:G:296:ILE:O	2.21	0.41
1:I:98:GLU:HG3	4:I:2591:HOH:O	2.21	0.41
1:J:93:PHE:CE1	1:J:131:LYS:HE3	2.55	0.41
1:A:223:LYS:O	1:A:224:LYS:HD3	2.21	0.41
1:D:379:ILE:HD12	1:D:415:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:GLY:N	1:E:187:TYR:CE2	2.89	0.41
1:E:395:LEU:HD13	1:E:401:PRO:HB3	2.02	0.41
1:E:411:ALA:O	1:E:415:ILE:HG13	2.20	0.41
1:H:115:MET:O	1:H:118:VAL:HG12	2.20	0.41
1:H:322:LYS:HE2	1:H:323:LEU:HD11	2.03	0.41
1:B:34:ALA:HA	1:B:119:LYS:CG	2.50	0.40
1:C:101:LEU:HB3	1:C:102:PRO:HD3	2.03	0.40
1:C:336:ILE:HD12	1:C:336:ILE:HA	1.89	0.40
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.56	0.40
1:J:159:GLY:HA3	1:J:187:TYR:CD1	2.56	0.40
1:C:435:LEU:O	1:C:439:GLY:N	2.53	0.40
1:D:159:GLY:HA3	1:D:187:TYR:CD2	2.56	0.40
1:D:358:SER:HB2	1:E:171:GLU:OE2	2.21	0.40
1:E:176:LEU:HD11	1:E:395:LEU:CD1	2.51	0.40
1:E:206:ALA:HA	1:E:226:TRP:CZ3	2.57	0.40
1:F:285:HIS:CG	1:F:286:ALA:N	2.89	0.40
1:J:101:LEU:N	1:J:102:PRO:CD	2.84	0.40
1:A:72:ALA:CB	1:A:90:ALA:O	2.70	0.40
1:E:34:ALA:HA	1:E:119:LYS:CG	2.51	0.40
1:F:174:GLU:HG3	1:F:212:ILE:HD11	2.02	0.40
1:H:403:ALA:HB2	1:H:406:ARG:HH22	1.87	0.40
1:I:285:HIS:CG	1:I:286:ALA:N	2.89	0.40
1:A:14:ASP:CG	1:A:17:TYR:H	2.30	0.40
1:A:132:LEU:O	1:A:133:ILE:C	2.64	0.40
1:B:25:ILE:HD12	1:B:96:PHE:HE2	1.86	0.40
1:B:200:ASN:OD1	1:B:205:ARG:HD3	2.22	0.40
1:C:358:SER:OG	1:D:171:GLU:OE2	2.23	0.40
1:D:209:MET:HE2	1:D:226:TRP:HB2	2.03	0.40
1:F:161:VAL:HG23	1:F:389:GLN:CD	2.46	0.40
1:H:390:LEU:HD12	1:H:390:LEU:N	2.36	0.40
1:J:437:LYS:HG2	1:J:438:TRP:CE2	2.56	0.40
3:A:600:CAP:O4	3:A:600:CAP:H12	2.22	0.40
1:C:414:ALA:HB2	1:C:424:TYR:CG	2.56	0.40
1:G:123:LEU:HG	1:G:300:VAL:HG21	2.04	0.40
1:H:303:LYS:NZ	4:H:606:HOH:O	2.52	0.40
1:I:139:PRO:HD3	1:I:306:ARG:O	2.22	0.40
1:I:264:LEU:HD12	1:I:264:LEU:HA	1.95	0.40
1:I:336:ILE:HD12	1:I:336:ILE:HA	1.86	0.40
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.56	0.40
1:J:282:ARG:O	1:J:283:ALA:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	434/444 (98%)	394 (91%)	37 (8%)	3 (1%)	18	15
1	B	434/444 (98%)	418 (96%)	16 (4%)	0	100	100
1	C	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	D	434/444 (98%)	422 (97%)	12 (3%)	0	100	100
1	E	435/444 (98%)	418 (96%)	16 (4%)	1 (0%)	43	44
1	F	434/444 (98%)	419 (96%)	14 (3%)	1 (0%)	43	44
1	G	434/444 (98%)	419 (96%)	15 (4%)	0	100	100
1	H	435/444 (98%)	399 (92%)	32 (7%)	4 (1%)	14	10
1	I	433/444 (98%)	418 (96%)	15 (4%)	0	100	100
1	J	434/444 (98%)	420 (97%)	13 (3%)	1 (0%)	43	44
All	All	4341/4440 (98%)	4146 (96%)	185 (4%)	10 (0%)	43	44

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	LYS
1	E	284	MET
1	J	284	MET
1	A	117	ARG
1	A	325	GLY
1	F	284	MET
1	H	284	MET
1	H	426	LYS
1	H	325	GLY
1	H	439	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	323/356 (91%)	318 (98%)	5 (2%)	57	65
1	B	341/356 (96%)	337 (99%)	4 (1%)	63	72
1	C	338/356 (95%)	333 (98%)	5 (2%)	57	65
1	D	339/356 (95%)	333 (98%)	6 (2%)	51	60
1	E	339/356 (95%)	334 (98%)	5 (2%)	57	65
1	F	335/356 (94%)	327 (98%)	8 (2%)	43	49
1	G	342/356 (96%)	338 (99%)	4 (1%)	63	72
1	H	330/356 (93%)	326 (99%)	4 (1%)	63	72
1	I	340/356 (96%)	339 (100%)	1 (0%)	86	91
1	J	341/356 (96%)	334 (98%)	7 (2%)	47	54
All	All	3368/3560 (95%)	3319 (98%)	49 (2%)	57	65

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	PHE
1	A	108	ILE
1	A	324	GLU
1	A	363	PHE
1	A	441	VAL
1	B	218	ASN
1	B	329	ILE
1	B	352	LEU
1	B	363	PHE
1	C	107	SER
1	C	218	ASN
1	C	235	LEU
1	C	301	LEU
1	C	363	PHE
1	D	58	LEU
1	D	107	SER

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Mol	Chain	Res	Type
1	D	108	ILE
1	D	122	ARG
1	D	328	ASP
1	D	363	PHE
1	E	107	SER
1	E	222	GLU
1	E	235	LEU
1	E	328	ASP
1	E	363	PHE
1	F	64	GLN
1	F	87	VAL
1	F	107	SER
1	F	181	LEU
1	F	235	LEU
1	F	332	GLN
1	F	336	ILE
1	F	363	PHE
1	G	107	SER
1	G	222	GLU
1	G	328	ASP
1	G	363	PHE
1	H	107	SER
1	H	235	LEU
1	H	323	LEU
1	H	363	PHE
1	I	363	PHE
1	J	58	LEU
1	J	107	SER
1	J	122	ARG
1	J	329	ILE
1	J	363	PHE
1	J	370	LEU
1	J	437	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	78	HIS
1	A	183	ASN
1	A	312	GLN
1	A	332	GLN

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Mol	Chain	Res	Type
1	A	351	HIS
1	A	354	GLN
1	B	64	GLN
1	B	312	GLN
1	B	347	ASN
1	B	354	GLN
1	B	376	GLN
1	C	312	GLN
1	C	354	GLN
1	C	440	HIS
1	D	239	GLN
1	D	312	GLN
1	D	354	GLN
1	D	440	HIS
1	E	312	GLN
1	E	332	GLN
1	E	354	GLN
1	E	417	GLN
1	F	64	GLN
1	F	312	GLN
1	F	332	GLN
1	F	354	GLN
1	F	376	GLN
1	G	312	GLN
1	G	354	GLN
1	G	440	HIS
1	H	64	GLN
1	H	78	HIS
1	H	312	GLN
1	H	354	GLN
1	I	312	GLN
1	I	354	GLN
1	I	376	GLN
1	J	312	GLN
1	J	354	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	KCX	F	189	2,1	10,11,12	0.99	0	6,12,14	1.37	1 (16%)
1	KCX	J	189	2,1	10,11,12	0.90	0	6,12,14	1.36	1 (16%)
1	KCX	E	189	2,1	10,11,12	0.91	0	6,12,14	1.41	1 (16%)
1	KCX	B	189	2,1	10,11,12	0.95	0	6,12,14	1.18	1 (16%)
1	KCX	G	189	2,1	10,11,12	0.97	0	6,12,14	1.35	1 (16%)
1	KCX	A	189	2,1	10,11,12	0.93	0	6,12,14	1.30	1 (16%)
1	KCX	C	189	2,1	10,11,12	0.93	0	6,12,14	1.14	1 (16%)
1	KCX	H	189	2,1	10,11,12	0.87	0	6,12,14	1.29	1 (16%)
1	KCX	D	189	2,1	10,11,12	0.91	0	6,12,14	1.45	1 (16%)
1	KCX	I	189	2,1	10,11,12	0.99	0	6,12,14	1.35	1 (16%)

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
1	KCX	F	189	2,1	-	1/9/10/12	-
1	KCX	J	189	2,1	-	0/9/10/12	-
1	KCX	E	189	2,1	-	0/9/10/12	-
1	KCX	B	189	2,1	-	0/9/10/12	-
1	KCX	G	189	2,1	-	0/9/10/12	-
1	KCX	A	189	2,1	-	0/9/10/12	-
1	KCX	C	189	2,1	-	1/9/10/12	-
1	KCX	H	189	2,1	-	1/9/10/12	-
1	KCX	D	189	2,1	-	1/9/10/12	-
1	KCX	I	189	2,1	-	0/9/10/12	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	189	KCX	OQ1-CX-NZ	-3.45	119.67	124.92
1	F	189	KCX	OQ1-CX-NZ	-3.23	120.02	124.92
1	G	189	KCX	OQ1-CX-NZ	-3.21	120.05	124.92
1	E	189	KCX	OQ1-CX-NZ	-3.20	120.06	124.92
1	J	189	KCX	OQ1-CX-NZ	-3.17	120.10	124.92
1	I	189	KCX	OQ1-CX-NZ	-3.17	120.11	124.92
1	A	189	KCX	OQ1-CX-NZ	-3.00	120.36	124.92
1	H	189	KCX	OQ1-CX-NZ	-2.99	120.37	124.92
1	B	189	KCX	OQ1-CX-NZ	-2.78	120.70	124.92
1	C	189	KCX	OQ1-CX-NZ	-2.67	120.86	124.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	189	KCX	C-CA-CB-CG
1	D	189	KCX	C-CA-CB-CG
1	F	189	KCX	C-CA-CB-CG
1	H	189	KCX	C-CA-CB-CG

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	189	KCX	1	0
1	C	189	KCX	1	0
1	H	189	KCX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

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	CAP	A	600	2	18,20,20	0.97	0	23,31,31	1.04	1 (4%)
3	CAP	I	600	2	18,20,20	0.88	0	23,31,31	0.93	1 (4%)
3	CAP	J	600	2	18,20,20	0.99	0	23,31,31	0.98	1 (4%)
3	CAP	F	600	2	18,20,20	0.89	0	23,31,31	0.95	1 (4%)
3	CAP	H	600	2	18,20,20	0.89	0	23,31,31	1.06	1 (4%)
3	CAP	D	600	2	18,20,20	0.88	0	23,31,31	1.01	1 (4%)
3	CAP	B	600	2	18,20,20	0.91	0	23,31,31	1.04	1 (4%)
3	CAP	C	600	2	18,20,20	0.94	0	23,31,31	0.96	1 (4%)
3	CAP	G	600	2	18,20,20	0.85	0	23,31,31	1.00	1 (4%)
3	CAP	E	600	2	18,20,20	0.90	0	23,31,31	1.03	1 (4%)

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	CAP	A	600	2	-	6/29/29/29	-
3	CAP	I	600	2	-	6/29/29/29	-
3	CAP	J	600	2	-	6/29/29/29	-
3	CAP	F	600	2	-	6/29/29/29	-
3	CAP	H	600	2	-	11/29/29/29	-
3	CAP	D	600	2	-	9/29/29/29	-
3	CAP	B	600	2	-	8/29/29/29	-
3	CAP	C	600	2	-	6/29/29/29	-
3	CAP	G	600	2	-	6/29/29/29	-
3	CAP	E	600	2	-	6/29/29/29	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	600	CAP	O7-C-C2	3.65	120.17	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	600	CAP	O7-C-C2	3.30	119.59	114.06
3	B	600	CAP	O7-C-C2	3.30	119.59	114.06
3	G	600	CAP	O7-C-C2	3.29	119.56	114.06
3	D	600	CAP	O7-C-C2	3.28	119.55	114.06
3	E	600	CAP	O7-C-C2	3.24	119.49	114.06
3	C	600	CAP	O7-C-C2	3.13	119.30	114.06
3	J	600	CAP	O7-C-C2	3.06	119.18	114.06
3	F	600	CAP	O7-C-C2	2.81	118.77	114.06
3	I	600	CAP	O7-C-C2	2.77	118.70	114.06

There are no chirality outliers.

All (70) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	600	CAP	O6-C-C2-C1
3	A	600	CAP	O7-C-C2-C1
3	A	600	CAP	O6-C-C2-O2
3	A	600	CAP	O7-C-C2-O2
3	B	600	CAP	O6-C-C2-C1
3	B	600	CAP	O7-C-C2-C1
3	B	600	CAP	O6-C-C2-O2
3	B	600	CAP	O7-C-C2-O2
3	B	600	CAP	O3-C3-C4-O4
3	C	600	CAP	O6-C-C2-C1
3	C	600	CAP	O7-C-C2-C1
3	C	600	CAP	O6-C-C2-O2
3	C	600	CAP	O7-C-C2-O2
3	C	600	CAP	O3-C3-C4-O4
3	D	600	CAP	O1-C1-C2-C
3	D	600	CAP	O1-C1-C2-O2
3	D	600	CAP	O6-C-C2-C1
3	D	600	CAP	O7-C-C2-C1
3	D	600	CAP	O6-C-C2-O2
3	D	600	CAP	O7-C-C2-O2
3	D	600	CAP	O3-C3-C4-O4
3	E	600	CAP	O6-C-C2-C1
3	E	600	CAP	O7-C-C2-C1
3	E	600	CAP	O6-C-C2-O2
3	E	600	CAP	O7-C-C2-O2
3	F	600	CAP	O6-C-C2-C1
3	F	600	CAP	O7-C-C2-C1
3	F	600	CAP	O6-C-C2-O2

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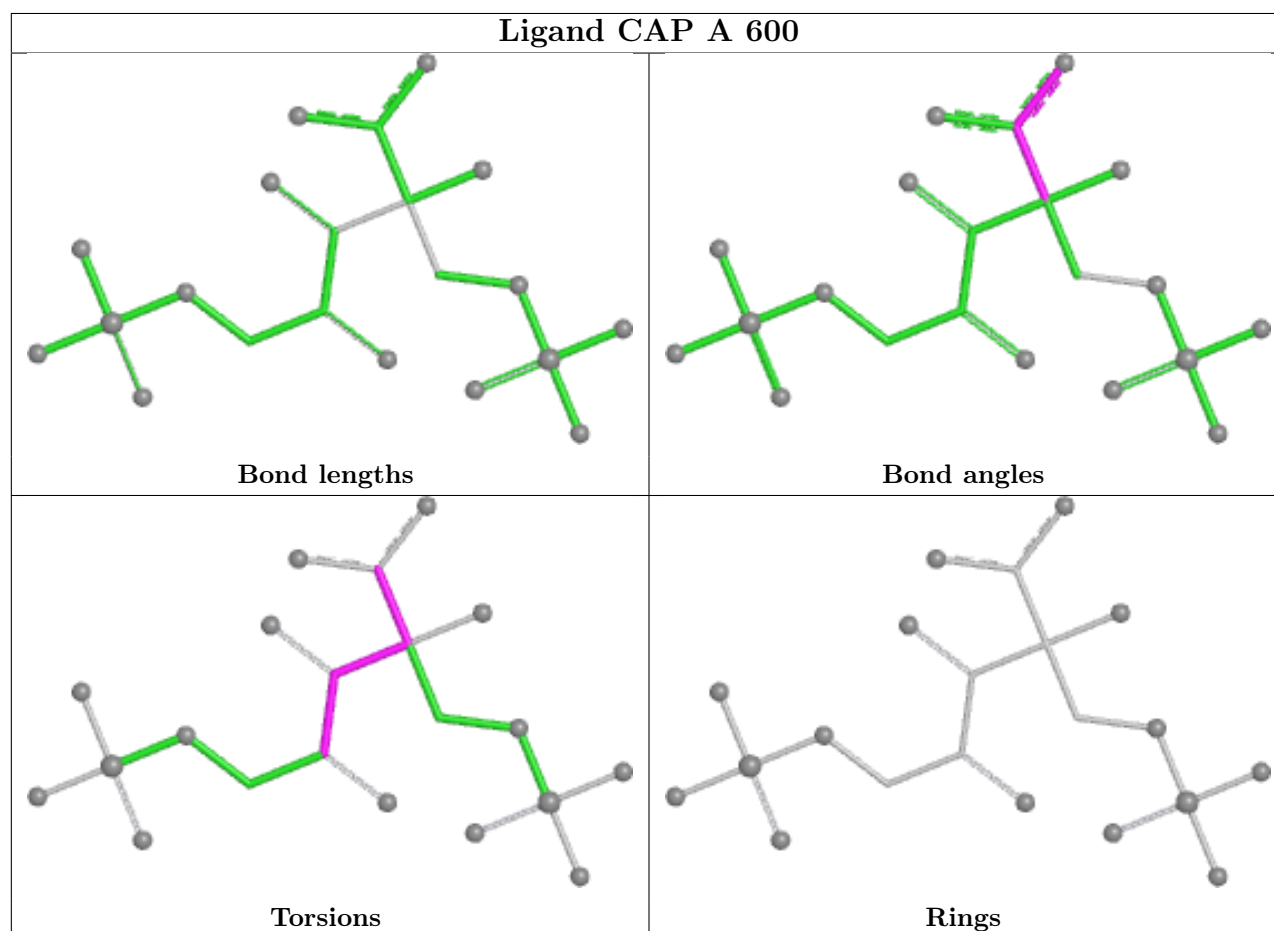
Mol	Chain	Res	Type	Atoms
3	F	600	CAP	O7-C-C2-O2
3	G	600	CAP	O6-C-C2-C1
3	G	600	CAP	O7-C-C2-C1
3	G	600	CAP	O6-C-C2-O2
3	G	600	CAP	O7-C-C2-O2
3	H	600	CAP	O1-C1-C2-C
3	H	600	CAP	O1-C1-C2-O2
3	H	600	CAP	O6-C-C2-C1
3	H	600	CAP	O7-C-C2-C1
3	H	600	CAP	O6-C-C2-O2
3	H	600	CAP	O7-C-C2-O2
3	H	600	CAP	O3-C3-C4-O4
3	I	600	CAP	O6-C-C2-C1
3	I	600	CAP	O7-C-C2-C1
3	I	600	CAP	O6-C-C2-O2
3	I	600	CAP	O7-C-C2-O2
3	I	600	CAP	O3-C3-C4-O4
3	J	600	CAP	O6-C-C2-C1
3	J	600	CAP	O7-C-C2-C1
3	J	600	CAP	O6-C-C2-O2
3	J	600	CAP	O7-C-C2-O2
3	H	600	CAP	C2-C3-C4-O4
3	H	600	CAP	C1-O1-P1-O1P
3	A	600	CAP	O2-C2-C3-C4
3	B	600	CAP	O2-C2-C3-C4
3	C	600	CAP	O2-C2-C3-C4
3	D	600	CAP	O2-C2-C3-C4
3	E	600	CAP	O2-C2-C3-C4
3	F	600	CAP	O2-C2-C3-C4
3	G	600	CAP	O2-C2-C3-C4
3	H	600	CAP	O2-C2-C3-C4
3	I	600	CAP	O2-C2-C3-C4
3	J	600	CAP	O2-C2-C3-C4
3	H	600	CAP	O1-C1-C2-C3
3	D	600	CAP	C1-O1-P1-O1P
3	E	600	CAP	C5-O5-P2-O4P
3	B	600	CAP	O7-C-C2-C3
3	A	600	CAP	O3-C3-C4-O4
3	F	600	CAP	O3-C3-C4-O4
3	G	600	CAP	O3-C3-C4-O4
3	J	600	CAP	O3-C3-C4-O4
3	B	600	CAP	C2-C3-C4-O4

There are no ring outliers.

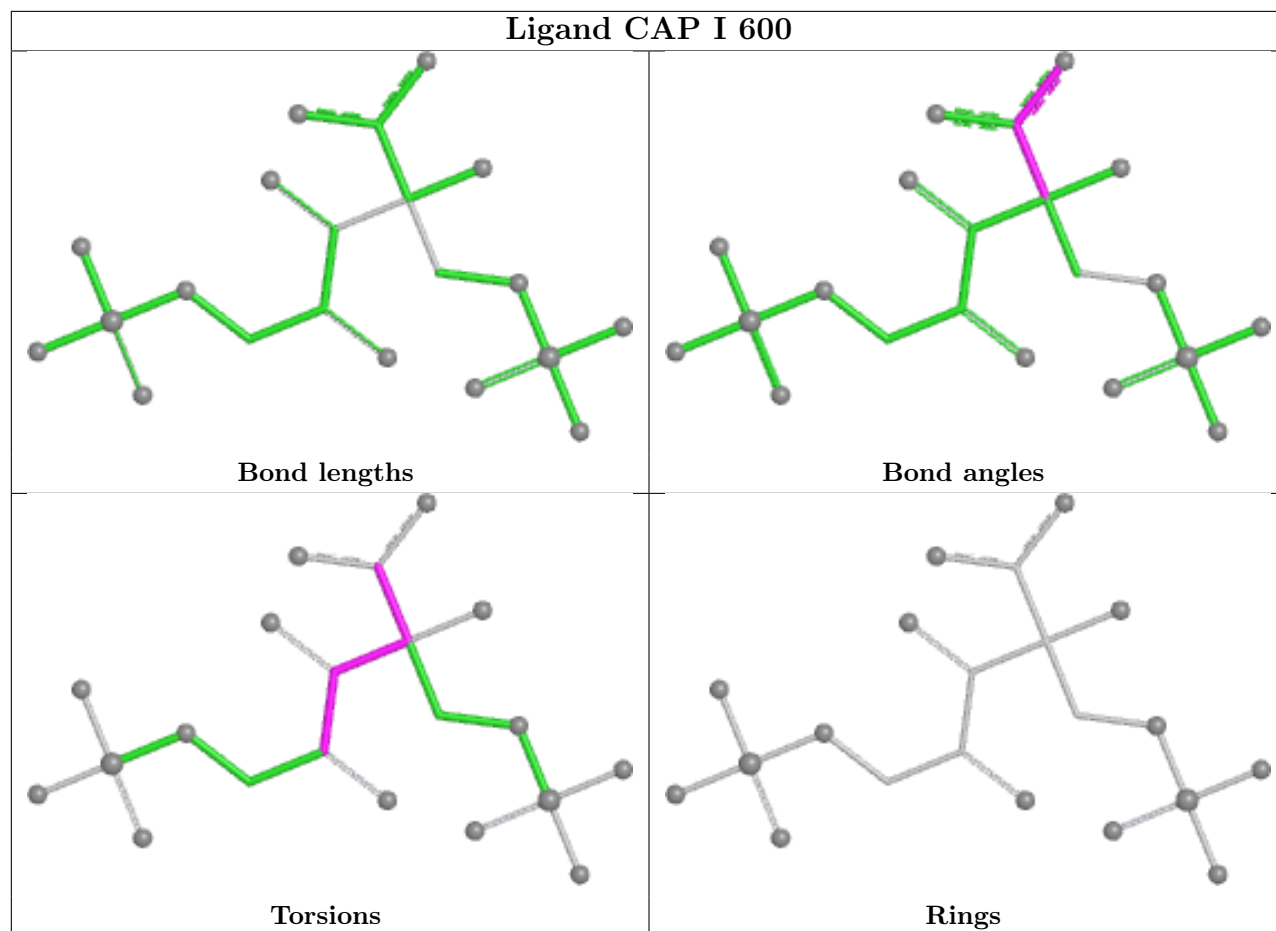
4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	600	CAP	3	0
3	J	600	CAP	1	0
3	H	600	CAP	1	0
3	C	600	CAP	1	0

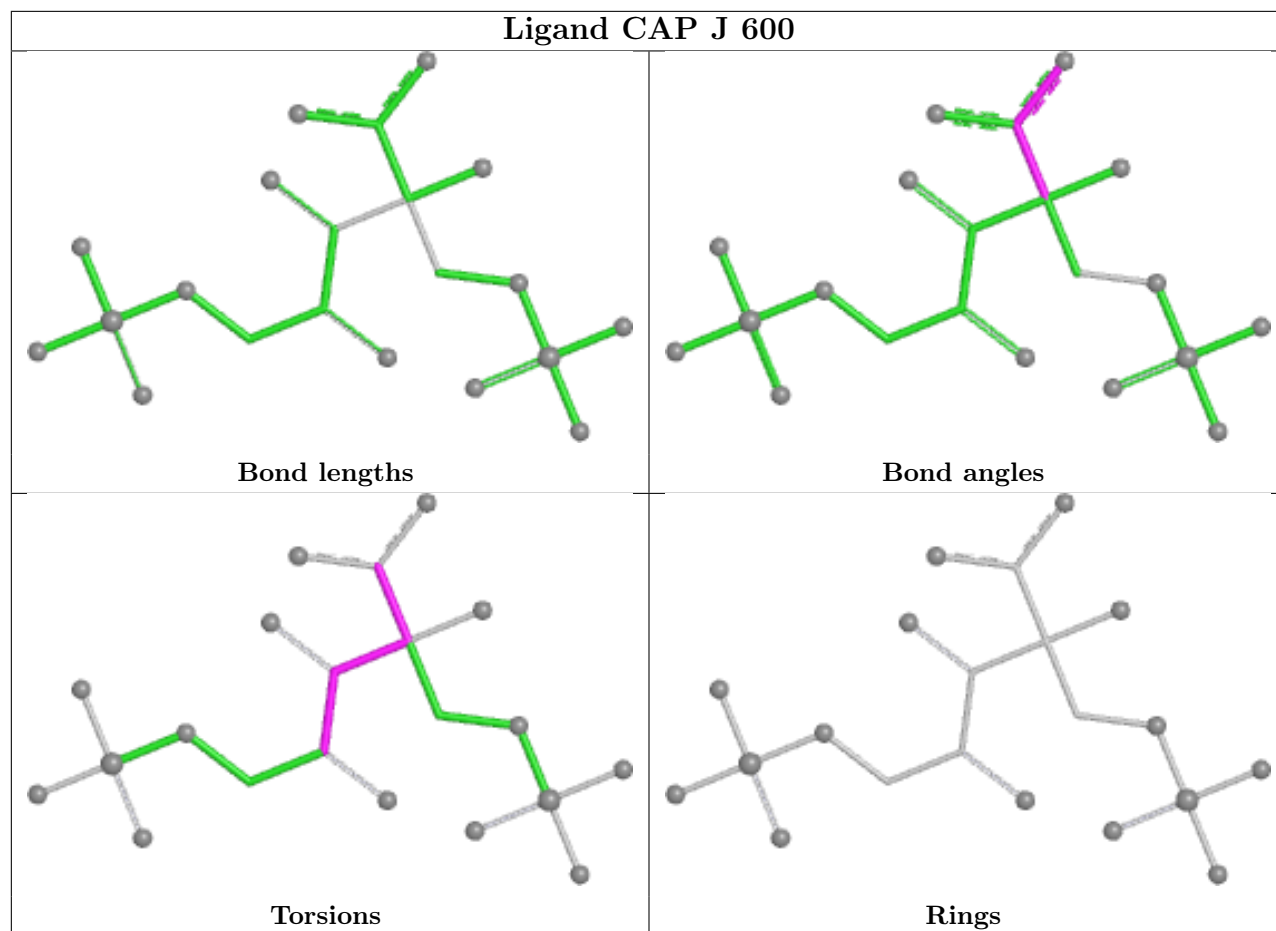
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

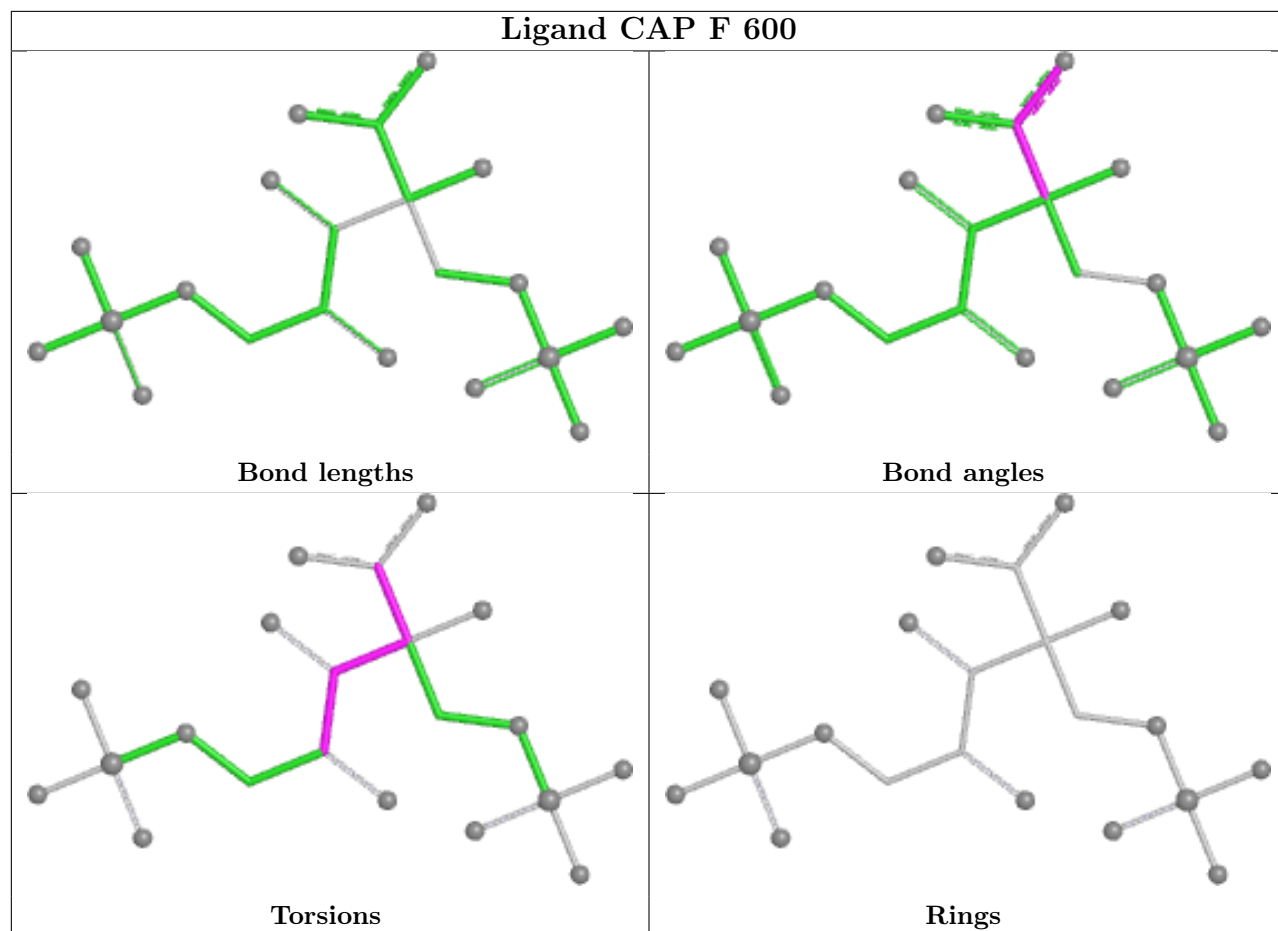


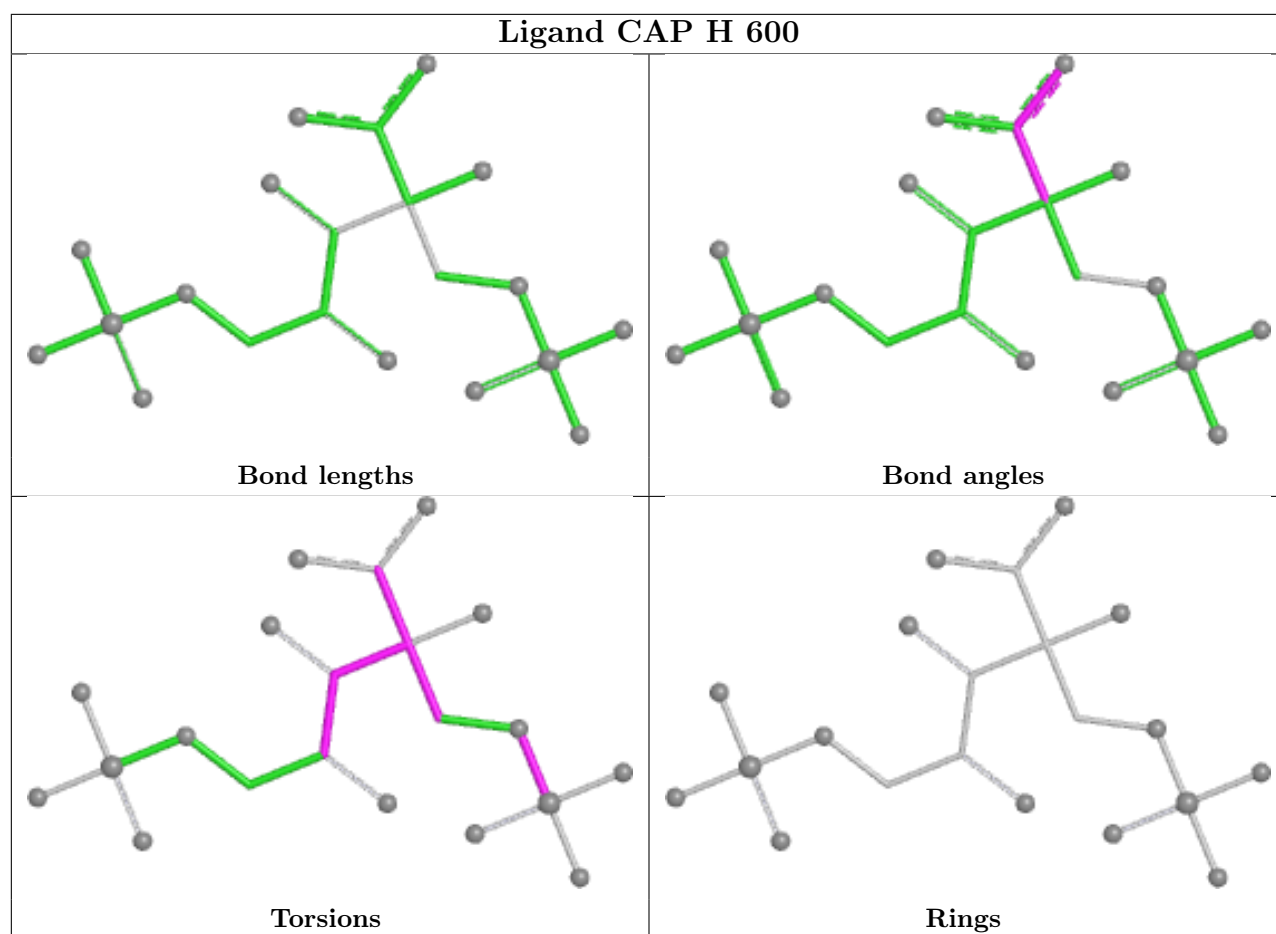
Ligand CAP I 600

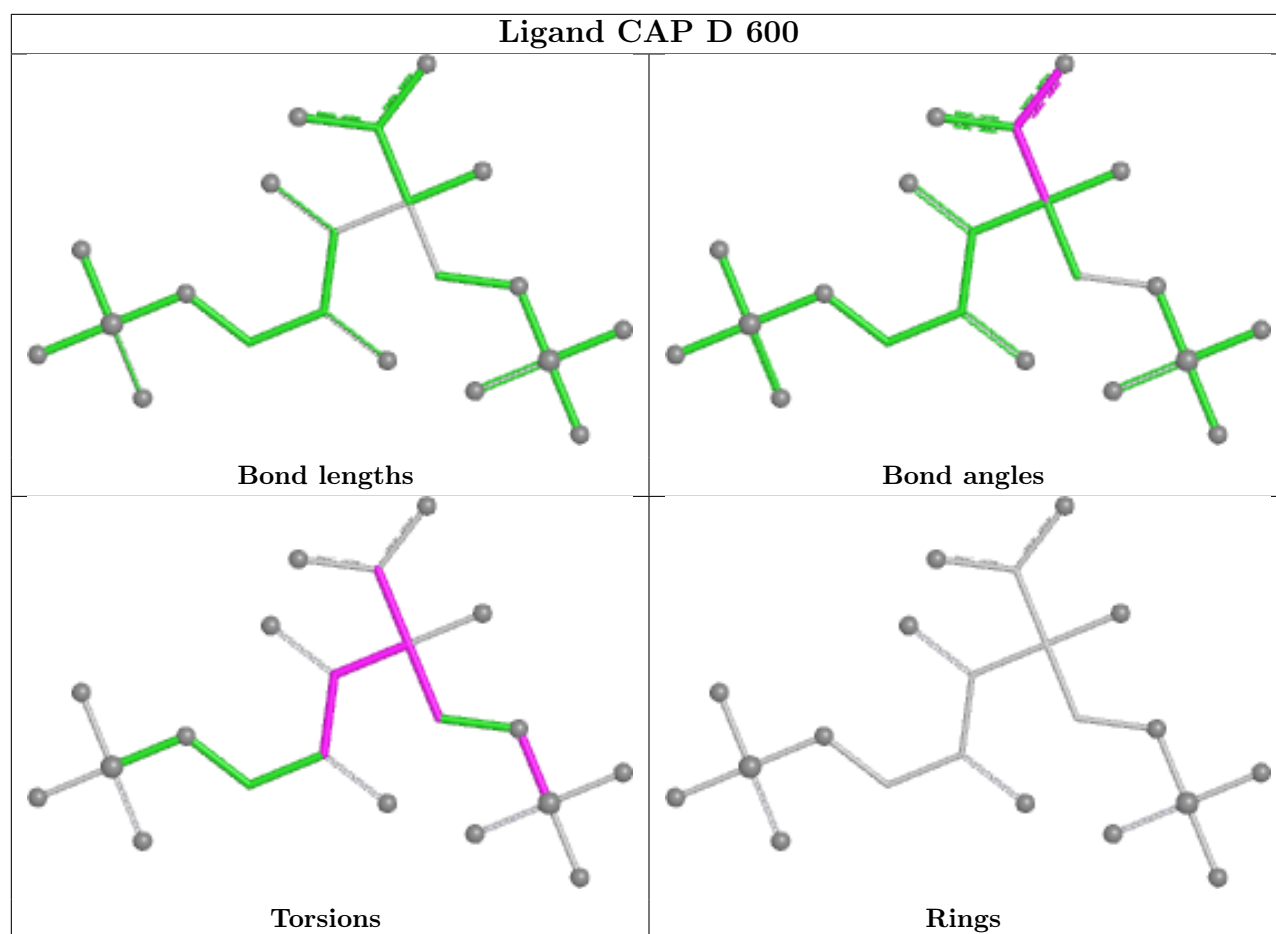


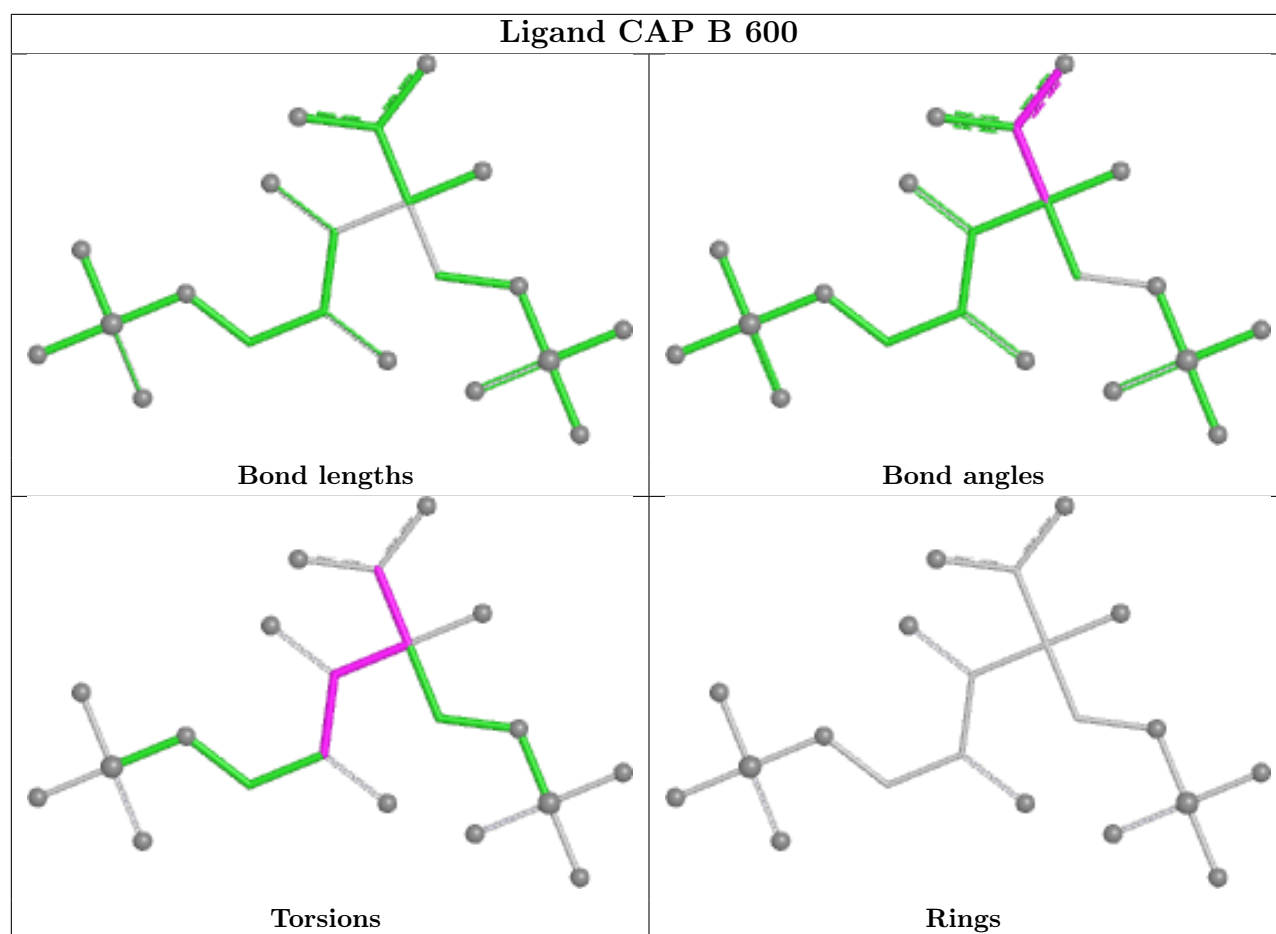
Ligand CAP J 600

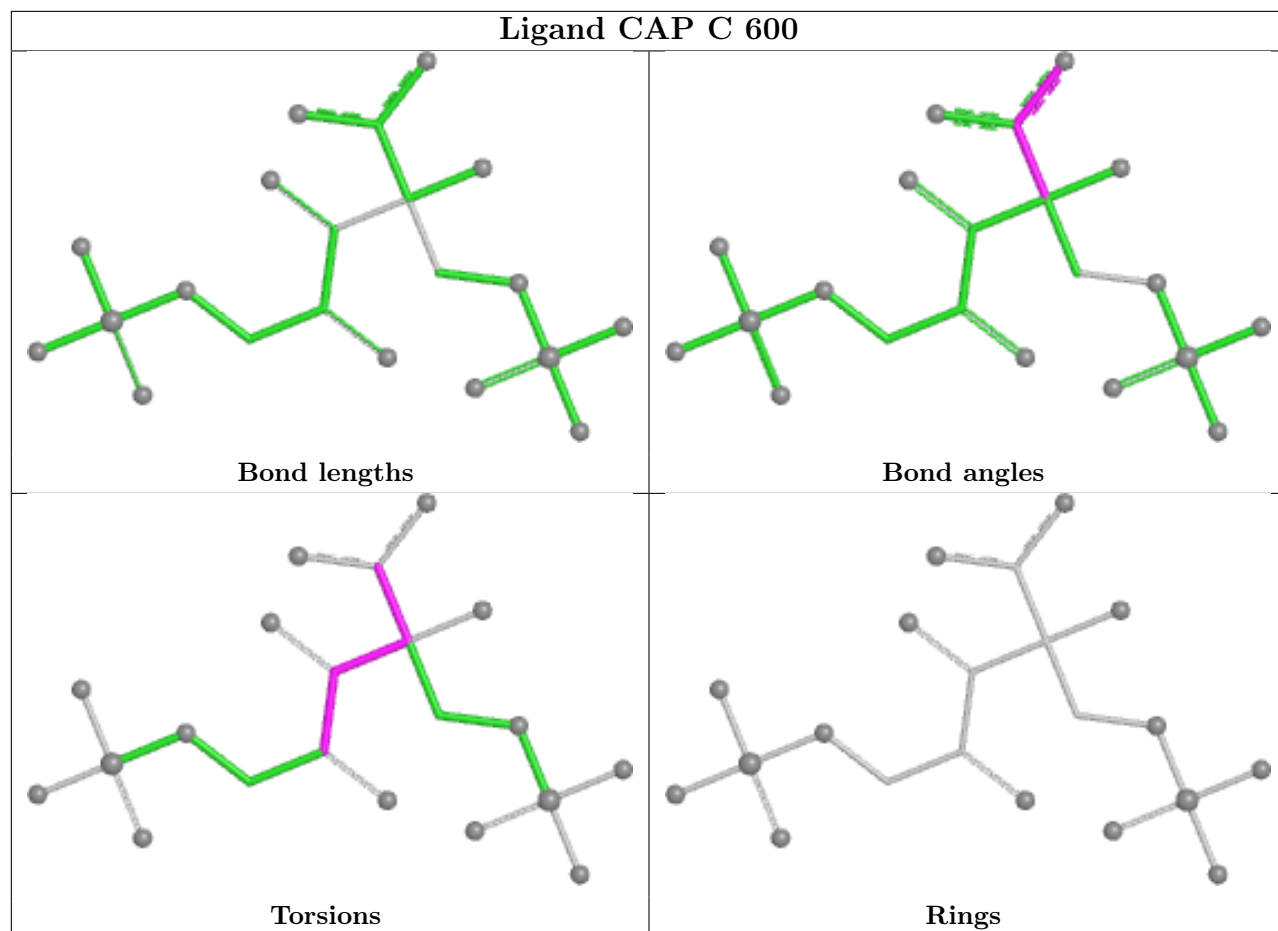


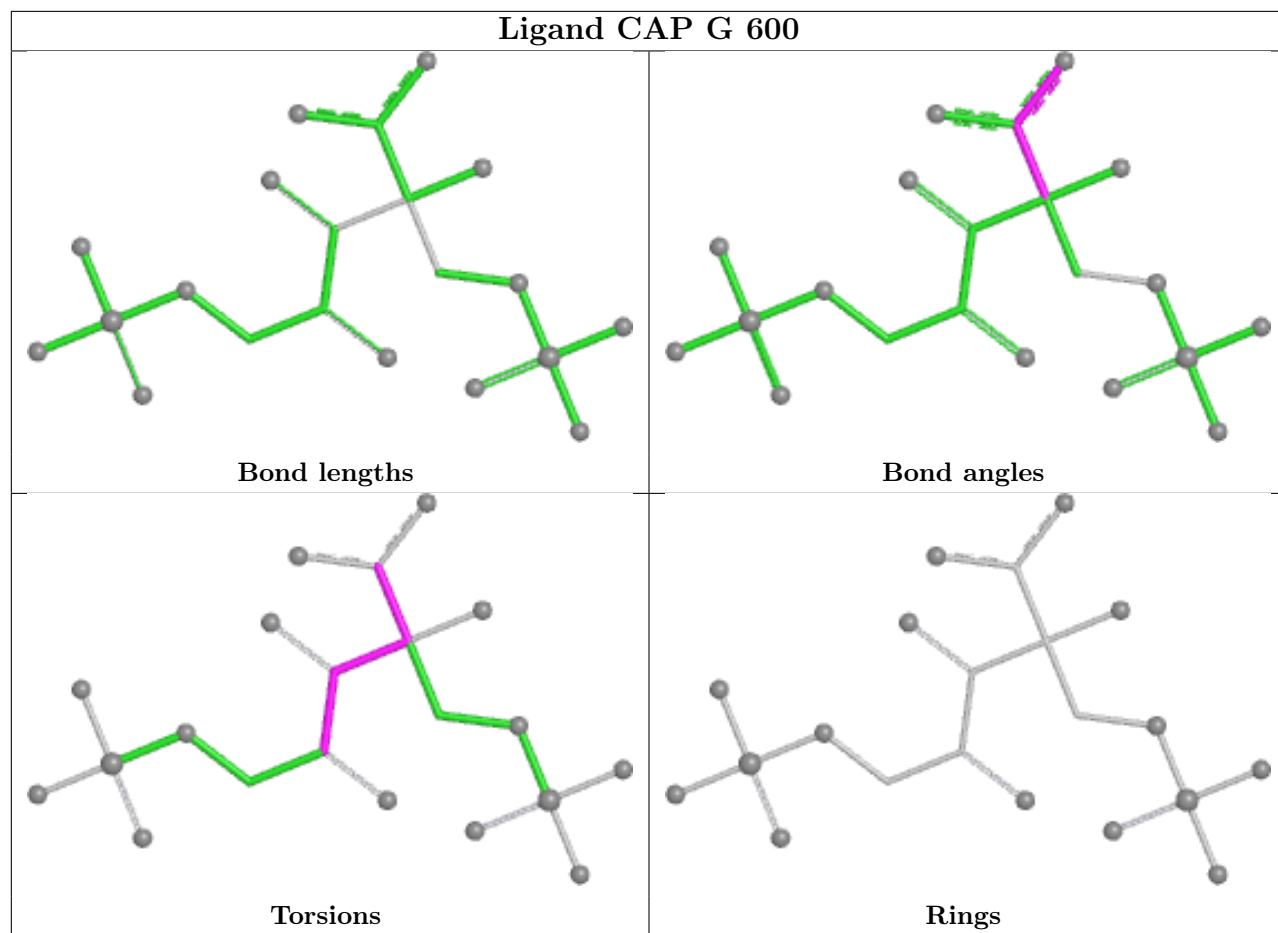


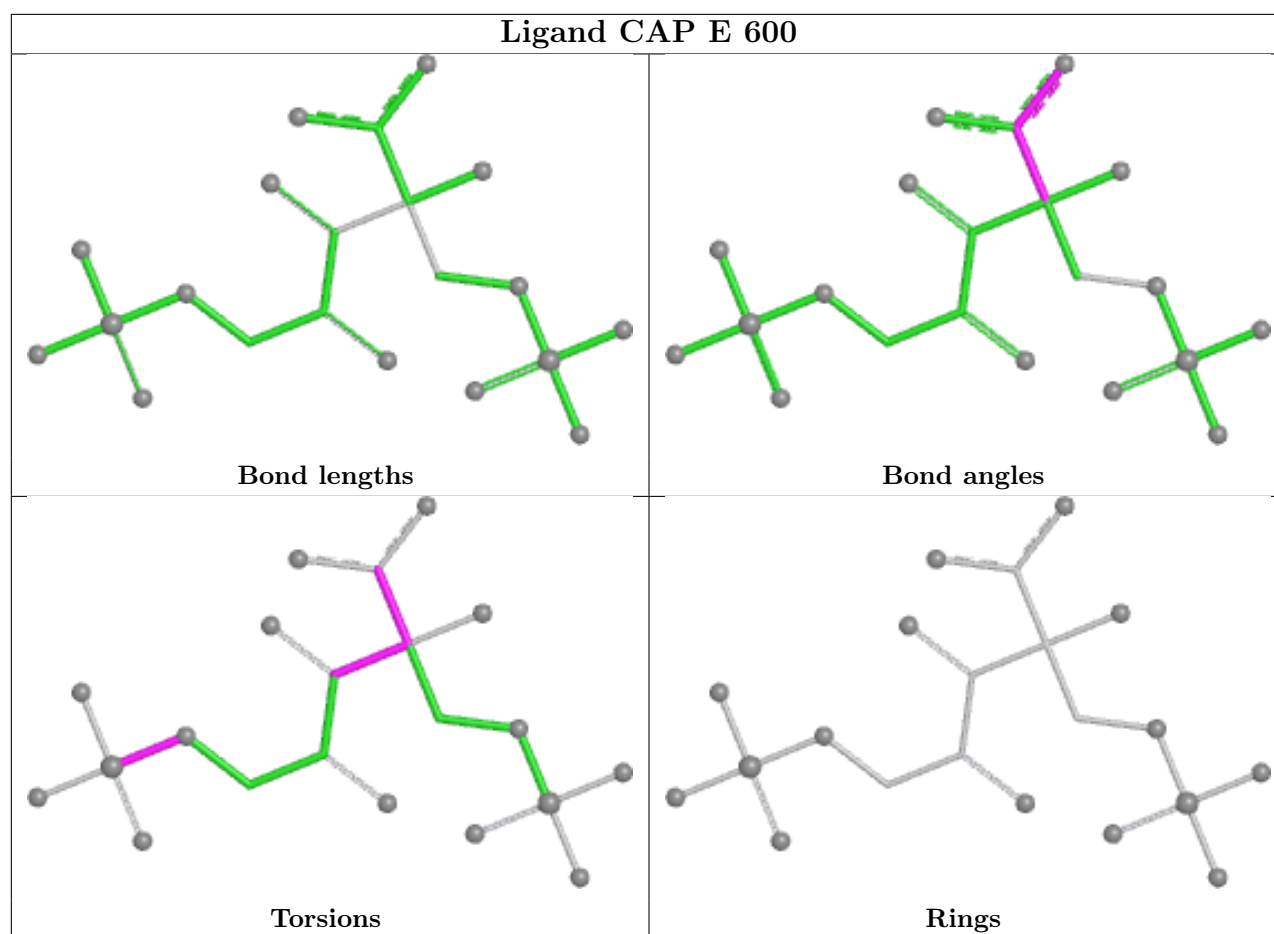












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	436/444 (98%)	1.80	187 (42%) 0 1	22, 36, 52, 58	0
1	B	436/444 (98%)	0.11	6 (1%) 73 75	13, 22, 34, 37	0
1	C	436/444 (98%)	0.19	15 (3%) 48 50	12, 21, 40, 45	0
1	D	436/444 (98%)	0.06	8 (1%) 67 70	11, 20, 32, 39	0
1	E	437/444 (98%)	0.32	29 (6%) 24 26	15, 24, 47, 51	0
1	F	436/444 (98%)	0.35	23 (5%) 32 34	12, 24, 38, 46	0
1	G	436/444 (98%)	0.18	11 (2%) 58 61	13, 24, 36, 41	0
1	H	437/444 (98%)	1.26	112 (25%) 1 2	22, 32, 57, 61	0
1	I	435/444 (97%)	0.04	8 (1%) 67 70	15, 23, 34, 40	0
1	J	436/444 (98%)	0.12	16 (3%) 45 47	11, 20, 41, 47	0
All	All	4361/4440 (98%)	0.44	415 (9%) 14 14	11, 24, 42, 61	0

All (415) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	VAL	6.9
1	H	443	PRO	6.0
1	A	421	LEU	5.6
1	F	59	TYR	5.5
1	I	59	TYR	5.4
1	H	422	ASP	5.3
1	A	59	TYR	5.3
1	E	7	THR	5.3
1	A	42	ALA	5.3
1	A	43	ALA	5.1
1	H	7	THR	4.8
1	A	39	ILE	4.7
1	A	11	TYR	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	352	LEU	4.7
1	A	415	ILE	4.6
1	A	157	ILE	4.5
1	A	29	PHE	4.5
1	H	444	VAL	4.4
1	A	31	VAL	4.4
1	F	8	ILE	4.4
1	A	443	PRO	4.3
1	E	59	TYR	4.3
1	B	59	TYR	4.2
1	A	349	VAL	4.2
1	A	408	VAL	4.2
1	A	38	THR	4.2
1	D	8	ILE	4.2
1	H	8	ILE	4.2
1	D	59	TYR	4.1
1	A	85	TRP	4.1
1	A	13	VAL	4.1
1	A	444	VAL	4.1
1	H	431	LEU	4.0
1	A	329	ILE	4.0
1	A	334	ALA	3.9
1	A	12	TYR	3.9
1	H	414	ALA	3.9
1	A	344	PRO	3.9
1	H	382	LEU	3.9
1	A	54	THR	3.9
1	H	398	PRO	3.9
1	A	8	ILE	3.8
1	H	415	ILE	3.8
1	F	421	LEU	3.8
1	G	59	TYR	3.8
1	H	435	LEU	3.8
1	A	438	TRP	3.8
1	A	9	TYR	3.8
1	A	293	TYR	3.8
1	A	412	ILE	3.7
1	A	414	ALA	3.7
1	A	425	ALA	3.7
1	H	411	ALA	3.7
1	F	81	GLY	3.7
1	A	17	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	G	8	ILE	3.6
1	H	419	ILE	3.6
1	A	411	ALA	3.6
1	H	438	TRP	3.6
1	A	345	ASP	3.6
1	A	115	MET	3.6
1	H	85	TRP	3.6
1	J	59	TYR	3.6
1	A	378	VAL	3.5
1	A	429	LYS	3.5
1	H	320	ALA	3.5
1	H	391	GLY	3.5
1	H	286	ALA	3.5
1	A	435	LEU	3.5
1	A	351	HIS	3.5
1	A	152	ILE	3.4
1	A	395	LEU	3.4
1	A	47	ALA	3.4
1	A	185	ALA	3.4
1	H	408	VAL	3.4
1	H	325	GLY	3.4
1	A	45	ALA	3.4
1	A	442	THR	3.4
1	H	293	TYR	3.4
1	A	325	GLY	3.4
1	A	404	GLY	3.4
1	H	421	LEU	3.4
1	A	121	LEU	3.3
1	H	323	LEU	3.3
1	H	395	LEU	3.3
1	A	376	GLN	3.3
1	A	86	ILE	3.3
1	H	434	ALA	3.3
1	J	419	ILE	3.3
1	A	40	GLU	3.3
1	A	46	VAL	3.3
1	A	407	ALA	3.3
1	A	44	GLY	3.2
1	A	419	ILE	3.2
1	A	14	ASP	3.2
1	A	79	ASP	3.2
1	H	115	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	378	VAL	3.2
1	H	375	ILE	3.2
1	A	77	PHE	3.2
1	A	377	PRO	3.2
1	A	380	GLU	3.2
1	H	432	ALA	3.2
1	A	75	TYR	3.2
1	A	336	ILE	3.2
1	J	58	LEU	3.2
1	H	429	LYS	3.2
1	A	74	ALA	3.1
1	A	431	LEU	3.1
1	E	419	ILE	3.1
1	D	9	TYR	3.1
1	G	347	ASN	3.1
1	A	123	LEU	3.1
1	B	347	ASN	3.1
1	H	407	ALA	3.1
1	H	59	TYR	3.1
1	C	419	ILE	3.1
1	H	412	ILE	3.1
1	A	379	ILE	3.0
1	C	8	ILE	3.0
1	A	16	GLY	3.0
1	C	422	ASP	3.0
1	A	441	VAL	3.0
1	A	331	ILE	3.0
1	A	83	GLY	3.0
1	A	350	PHE	3.0
1	A	80	MET	3.0
1	H	84	SER	3.0
1	F	347	ASN	3.0
1	H	321	GLY	3.0
1	H	420	PRO	3.0
1	A	117	ARG	2.9
1	A	90	ALA	2.9
1	H	377	PRO	2.9
1	A	434	ALA	2.9
1	H	318	ALA	2.9
1	G	58	LEU	2.9
1	A	422	ASP	2.9
1	H	416	MET	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	326	GLU	2.9
1	H	9	TYR	2.9
1	H	425	ALA	2.9
1	A	53	GLY	2.9
1	A	393	GLY	2.9
1	H	184	GLY	2.9
1	E	10	ASP	2.9
1	J	10	ASP	2.9
1	A	342	TYR	2.9
1	H	405	ALA	2.9
1	A	120	GLY	2.9
1	H	369	GLY	2.9
1	A	420	PRO	2.8
1	A	37	TYR	2.8
1	A	318	ALA	2.8
1	A	418	GLY	2.8
1	A	323	LEU	2.8
1	D	58	LEU	2.8
1	H	58	LEU	2.8
1	A	216	VAL	2.8
1	H	426	LYS	2.8
1	A	347	ASN	2.8
1	A	294	HIS	2.8
1	H	376	GLN	2.8
1	A	76	ASP	2.8
1	A	57	THR	2.8
1	H	54	THR	2.8
1	H	329	ILE	2.8
1	H	368	GLY	2.8
1	H	108	ILE	2.8
1	E	438	TRP	2.8
1	F	218	ASN	2.7
1	A	392	GLY	2.7
1	E	426	LYS	2.7
1	A	330	THR	2.7
1	H	118	VAL	2.7
1	A	51	SER	2.7
1	H	393	GLY	2.7
1	A	432	ALA	2.7
1	A	158	TYR	2.7
1	A	156	PRO	2.7
1	H	417	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	375	ILE	2.7
1	E	8	ILE	2.7
1	H	212	ILE	2.7
1	A	10	ASP	2.7
1	H	418	GLY	2.7
1	H	439	GLY	2.7
1	A	56	THR	2.7
1	E	427	THR	2.7
1	J	421	LEU	2.7
1	E	415	ILE	2.7
1	A	48	ALA	2.6
1	A	403	ALA	2.6
1	H	34	ALA	2.6
1	H	427	THR	2.6
1	A	428	HIS	2.6
1	G	20	SER	2.6
1	H	11	TYR	2.6
1	A	89	ILE	2.6
1	F	376	GLN	2.6
1	H	324	GLU	2.6
1	C	443	PRO	2.6
1	H	424	TYR	2.6
1	H	39	ILE	2.6
1	H	379	ILE	2.6
1	A	417	GLN	2.6
1	A	67	TRP	2.6
1	A	320	ALA	2.6
1	F	58	LEU	2.6
1	B	8	ILE	2.6
1	H	441	VAL	2.6
1	I	9	TYR	2.6
1	A	423	GLU	2.6
1	H	437	LYS	2.6
1	H	47	ALA	2.6
1	H	292	PRO	2.6
1	J	328	ASP	2.6
1	A	390	LEU	2.6
1	B	58	LEU	2.6
1	H	55	TRP	2.6
1	H	370	LEU	2.6
1	H	410	GLN	2.5
1	A	326	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	108	ILE	2.5
1	E	441	VAL	2.5
1	F	419	ILE	2.5
1	A	221	GLY	2.5
1	H	114	GLY	2.5
1	A	84	SER	2.5
1	A	176	LEU	2.5
1	A	337	LEU	2.5
1	A	18	GLU	2.5
1	A	288	PHE	2.5
1	A	114	GLY	2.5
1	C	412	ILE	2.5
1	H	383	GLY	2.5
1	A	291	ASN	2.5
1	H	218	ASN	2.5
1	E	425	ALA	2.5
1	G	358	SER	2.5
1	E	421	LEU	2.5
1	A	55	TRP	2.5
1	A	426	LYS	2.5
1	F	78	HIS	2.5
1	I	53	GLY	2.5
1	A	25	ILE	2.5
1	F	87	VAL	2.5
1	F	444	VAL	2.5
1	H	423	GLU	2.5
1	A	394	THR	2.5
1	H	442	THR	2.5
1	A	34	ALA	2.5
1	A	286	ALA	2.5
1	A	381	ALA	2.5
1	A	118	VAL	2.4
1	A	41	GLN	2.4
1	A	413	ASP	2.4
1	H	381	ALA	2.4
1	C	421	LEU	2.4
1	H	409	ARG	2.4
1	A	36	GLY	2.4
1	H	400	GLY	2.4
1	A	28	VAL	2.4
1	A	108	ILE	2.4
1	A	348	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	412	ILE	2.4
1	A	366	SER	2.4
1	I	54	THR	2.4
1	J	425	ALA	2.4
1	A	58	LEU	2.4
1	A	382	LEU	2.4
1	A	159	GLY	2.4
1	A	387	VAL	2.4
1	J	8	ILE	2.4
1	H	330	THR	2.4
1	J	427	THR	2.4
1	H	428	HIS	2.4
1	A	333	ASN	2.4
1	A	439	GLY	2.4
1	J	218	ASN	2.4
1	A	112	ILE	2.4
1	H	46	VAL	2.4
1	H	161	VAL	2.4
1	A	52	THR	2.4
1	A	384	THR	2.4
1	A	401	PRO	2.4
1	H	440	HIS	2.4
1	A	424	TYR	2.3
1	F	425	ALA	2.3
1	C	395	LEU	2.3
1	A	81	GLY	2.3
1	A	113	PHE	2.3
1	A	386	ILE	2.3
1	H	222	GLU	2.3
1	A	27	ALA	2.3
1	A	180	LEU	2.3
1	A	321	GLY	2.3
1	H	404	GLY	2.3
1	G	10	ASP	2.3
1	B	444	VAL	2.3
1	I	380	GLU	2.3
1	E	417	GLN	2.3
1	H	394	THR	2.3
1	A	111	ASN	2.3
1	C	347	ASN	2.3
1	H	43	ALA	2.3
1	A	319	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	424	TYR	2.3
1	J	396	GLY	2.3
1	B	65	GLU	2.3
1	G	65	GLU	2.3
1	A	427	THR	2.3
1	A	154	ASP	2.3
1	A	368	GLY	2.3
1	A	339	GLU	2.2
1	E	358	SER	2.2
1	H	296	ILE	2.2
1	J	412	ILE	2.2
1	A	398	PRO	2.2
1	H	334	ALA	2.2
1	H	396	GLY	2.2
1	C	431	LEU	2.2
1	H	388	LEU	2.2
1	A	324	GLU	2.2
1	E	380	GLU	2.2
1	A	20	SER	2.2
1	D	340	SER	2.2
1	A	213	ILE	2.2
1	A	296	ILE	2.2
1	H	331	ILE	2.2
1	F	79	ASP	2.2
1	H	328	ASP	2.2
1	A	369	GLY	2.2
1	E	18	GLU	2.2
1	J	414	ALA	2.2
1	A	297	SER	2.2
1	A	26	ILE	2.2
1	G	419	ILE	2.2
1	E	444	VAL	2.2
1	D	380	GLU	2.2
1	E	434	ALA	2.2
1	A	388	LEU	2.2
1	H	121	LEU	2.2
1	F	429	LYS	2.2
1	A	416	MET	2.2
1	J	438	TRP	2.2
1	A	220	THR	2.2
1	E	422	ASP	2.2
1	H	372	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	413	ASP	2.2
1	I	56	THR	2.2
1	A	35	GLU	2.1
1	C	444	VAL	2.1
1	F	378	VAL	2.1
1	A	110	GLY	2.1
1	H	81	GLY	2.1
1	A	440	HIS	2.1
1	A	290	ARG	2.1
1	A	119	LYS	2.1
1	A	437	LYS	2.1
1	C	59	TYR	2.1
1	A	222	GLU	2.1
1	A	212	ILE	2.1
1	F	415	ILE	2.1
1	J	415	ILE	2.1
1	H	319	GLY	2.1
1	A	155	ARG	2.1
1	A	72	ALA	2.1
1	A	322	LYS	2.1
1	A	358	SER	2.1
1	D	421	LEU	2.1
1	E	35	GLU	2.1
1	F	345	ASP	2.1
1	G	9	TYR	2.1
1	A	292	PRO	2.1
1	E	420	PRO	2.1
1	E	442	THR	2.1
1	F	420	PRO	2.1
1	H	392	GLY	2.1
1	A	161	VAL	2.1
1	C	425	ALA	2.1
1	F	434	ALA	2.1
1	A	50	SER	2.1
1	F	416	MET	2.1
1	H	183	ASN	2.1
1	H	82	ASP	2.1
1	A	33	PRO	2.1
1	A	372	PRO	2.1
1	D	54	THR	2.1
1	H	384	THR	2.1
1	E	418	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	119	LYS	2.1
1	F	85	TRP	2.1
1	E	414	ALA	2.1
1	F	432	ALA	2.1
1	H	403	ALA	2.1
1	I	222	GLU	2.0
1	H	181	LEU	2.0
1	E	347	ASN	2.0
1	A	273	ASP	2.0
1	H	10	ASP	2.0
1	A	60	PRO	2.0
1	C	398	PRO	2.0
1	A	184	GLY	2.0
1	H	295	GLY	2.0
1	J	418	GLY	2.0
1	C	415	ILE	2.0
1	G	18	GLU	2.0
1	I	326	GLU	2.0
1	C	218	ASN	2.0
1	H	406	ARG	2.0
1	H	322	LYS	2.0
1	A	32	THR	2.0
1	H	57	THR	2.0
1	E	400	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	KCX	A	189	12/13	0.92	0.11	29,30,31,31	0
1	KCX	H	189	12/13	0.92	0.10	30,30,31,31	0
1	KCX	F	189	12/13	0.95	0.08	17,18,20,20	0
1	KCX	E	189	12/13	0.95	0.07	21,22,23,23	0
1	KCX	C	189	12/13	0.96	0.07	14,16,17,17	0
1	KCX	I	189	12/13	0.96	0.06	17,18,18,18	0
1	KCX	G	189	12/13	0.97	0.05	16,17,17,17	0
1	KCX	B	189	12/13	0.97	0.06	18,19,19,20	0
1	KCX	D	189	12/13	0.97	0.06	11,14,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	KCX	J	189	12/13	0.97	0.06	18,18,19,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

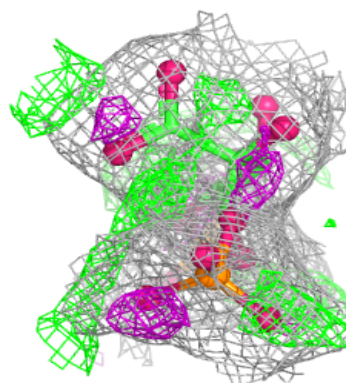
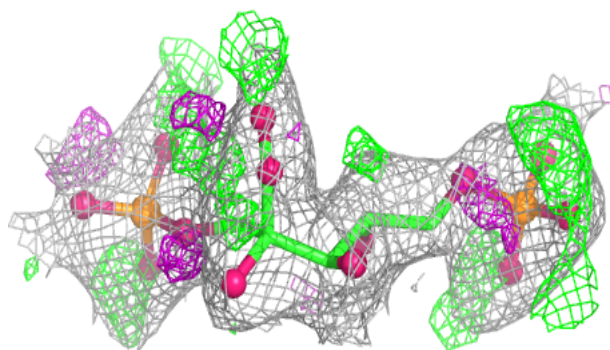
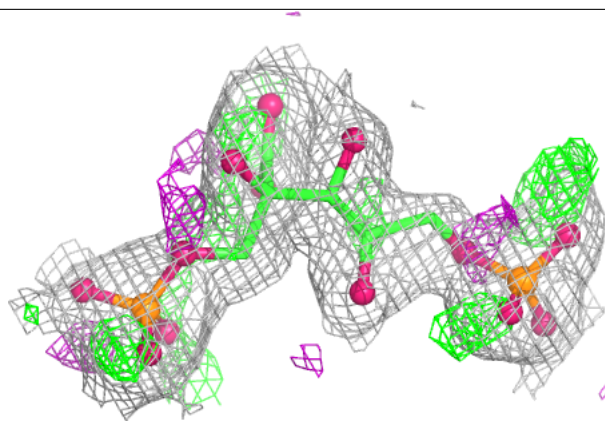
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CAP	H	600	21/21	0.87	0.13	31,34,36,37	0
3	CAP	A	600	21/21	0.88	0.13	27,33,34,35	0
2	MG	H	500	1/1	0.96	0.05	29,29,29,29	0
3	CAP	J	600	21/21	0.96	0.08	17,21,22,22	0
3	CAP	C	600	21/21	0.97	0.06	19,21,22,23	0
3	CAP	E	600	21/21	0.97	0.07	21,24,26,26	0
3	CAP	G	600	21/21	0.97	0.06	17,17,18,18	0
2	MG	A	500	1/1	0.97	0.04	29,29,29,29	0
3	CAP	B	600	21/21	0.97	0.06	17,20,21,22	0
3	CAP	F	600	21/21	0.98	0.05	15,17,17,18	0
2	MG	G	500	1/1	0.98	0.05	16,16,16,16	0
3	CAP	D	600	21/21	0.98	0.05	13,14,15,16	0
3	CAP	I	600	21/21	0.98	0.05	16,18,18,19	0
2	MG	C	500	1/1	0.98	0.02	16,16,16,16	0
2	MG	I	500	1/1	0.99	0.02	13,13,13,13	0
2	MG	J	500	1/1	0.99	0.02	16,16,16,16	0
2	MG	E	500	1/1	0.99	0.02	21,21,21,21	0
2	MG	F	500	1/1	0.99	0.02	19,19,19,19	0
2	MG	B	500	1/1	0.99	0.03	18,18,18,18	0
2	MG	D	500	1/1	0.99	0.02	11,11,11,11	0

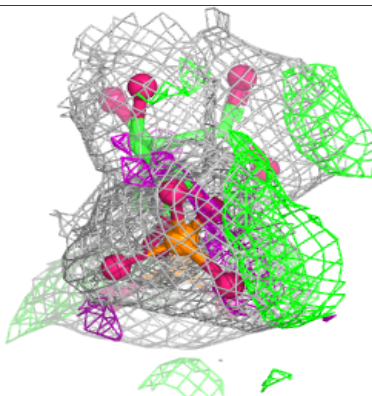
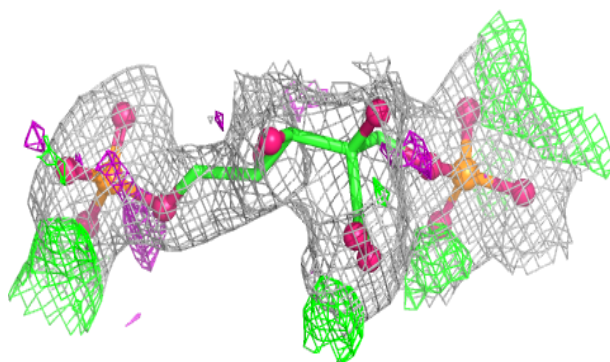
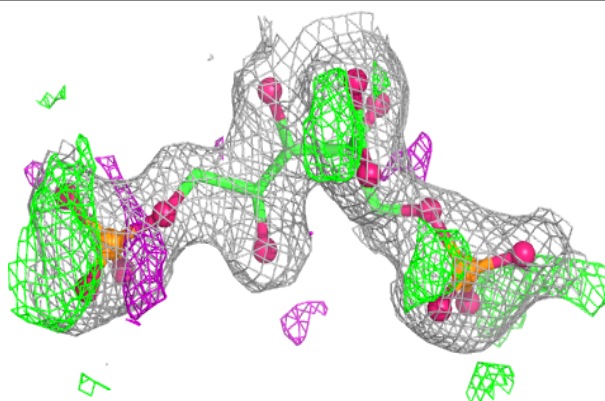
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP H 600:

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

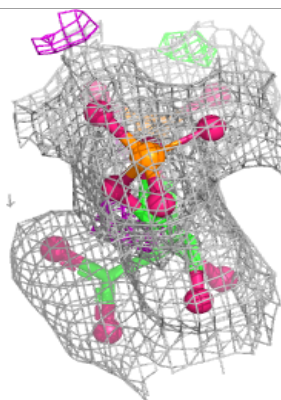
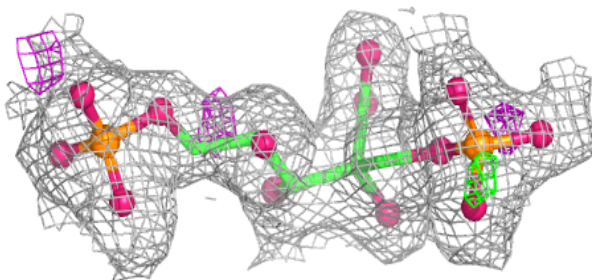
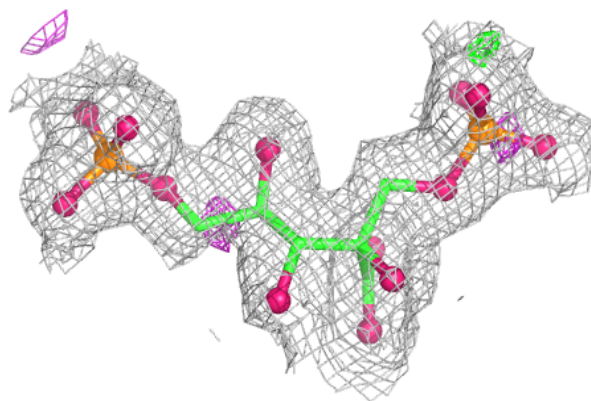
**Electron density around CAP A 600:**

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

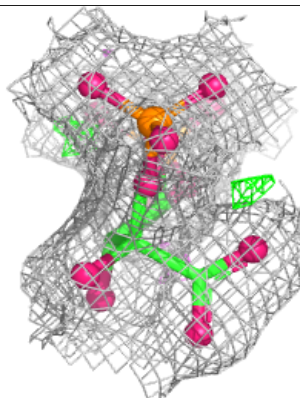
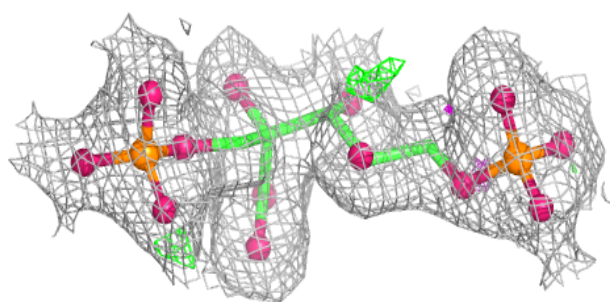
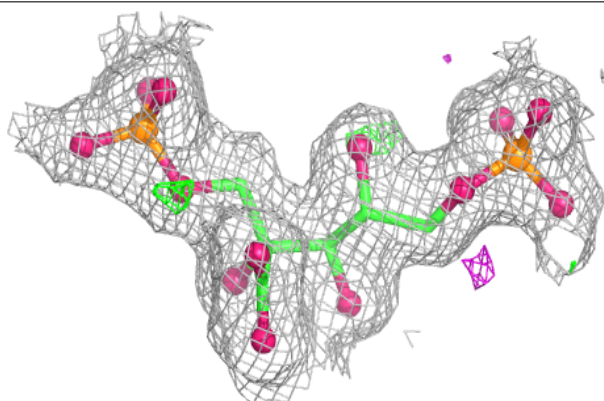


Electron density around CAP J 600:

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

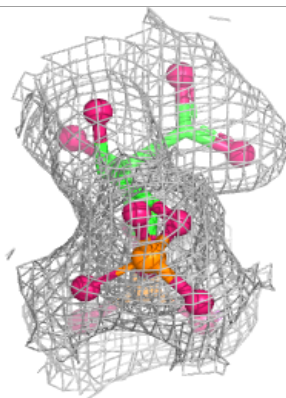
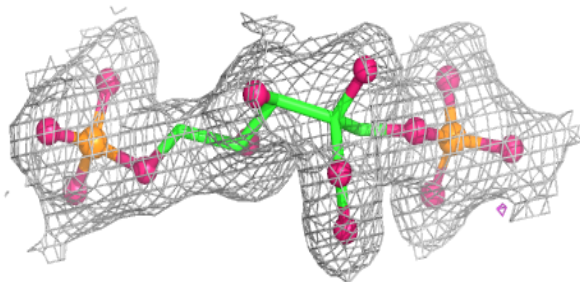
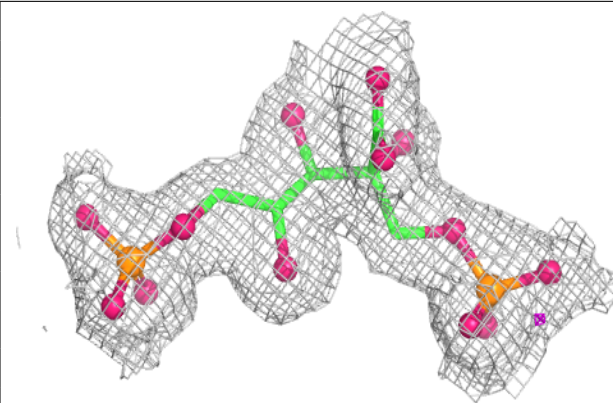
**Electron density around CAP C 600:**

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

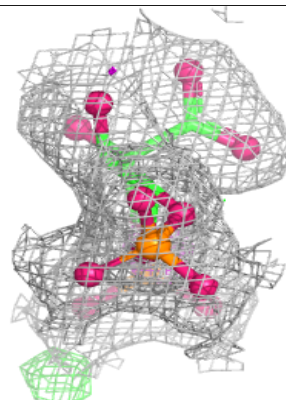
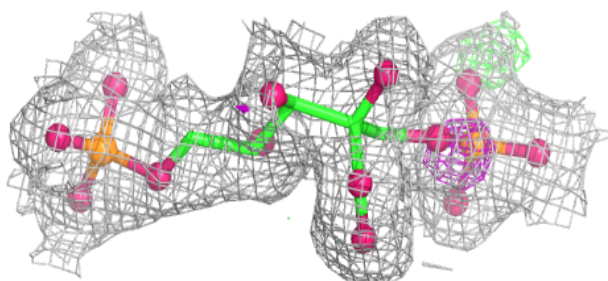
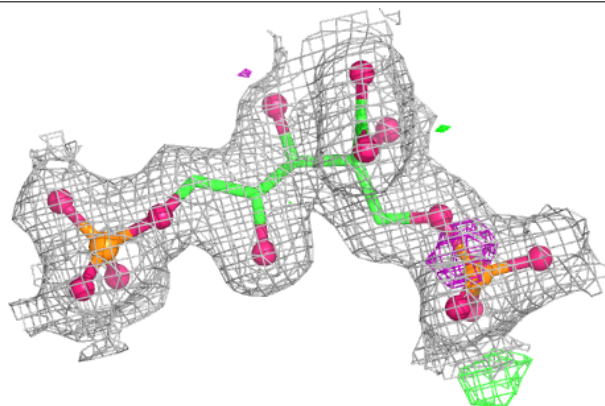


Electron density around CAP E 600:

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

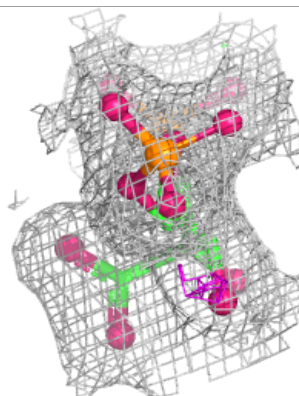
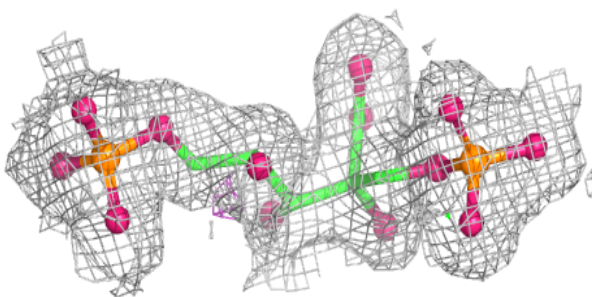
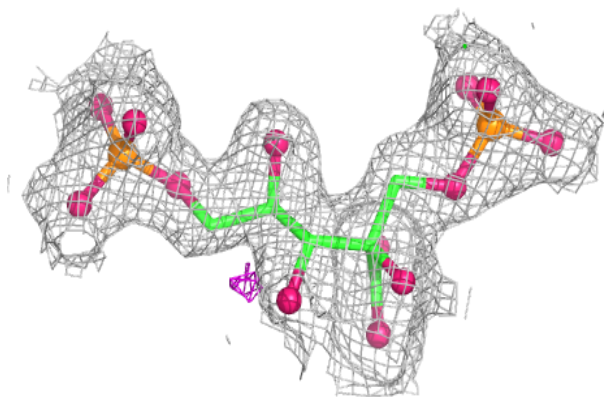
**Electron density around CAP G 600:**

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

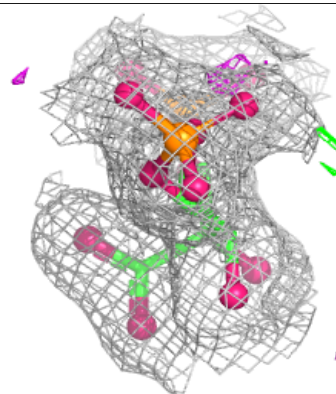
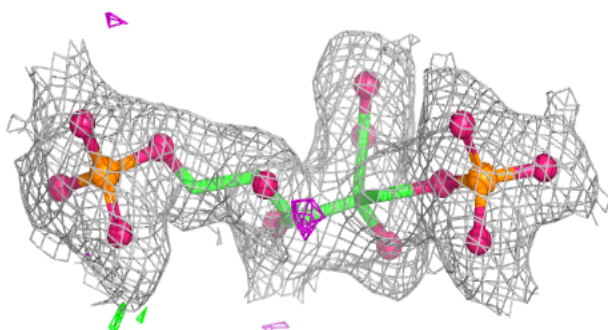
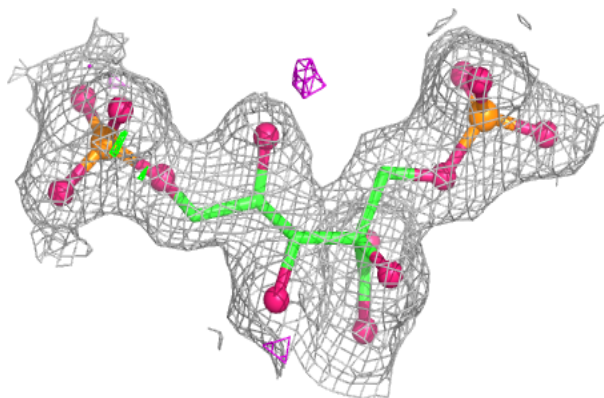


Electron density around CAP B 600:

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

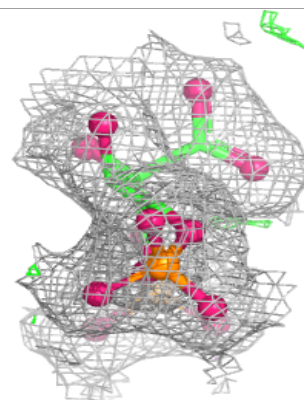
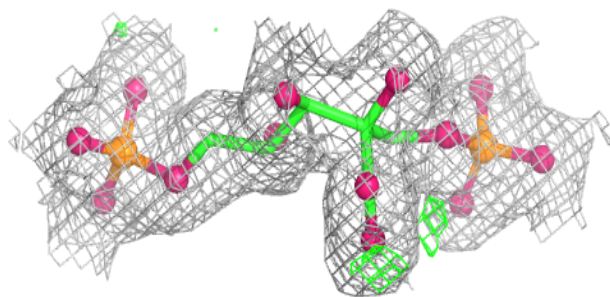
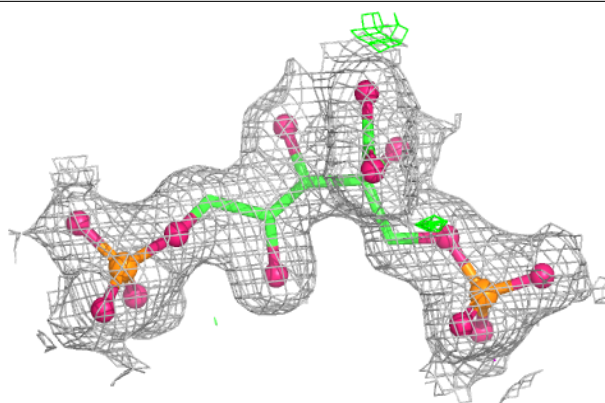
**Electron density around CAP F 600:**

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

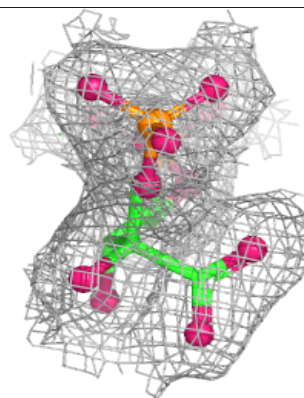
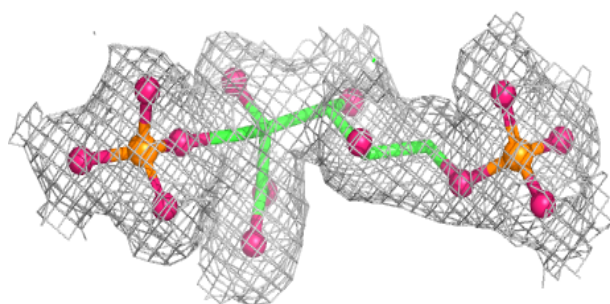
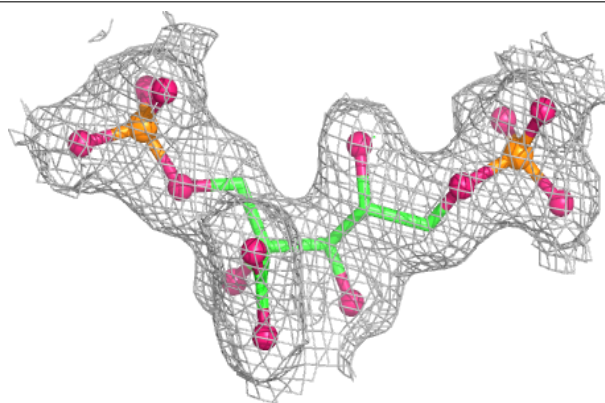


Electron density around CAP D 600:

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

**Electron density around CAP I 600:**

$2mF_o-DF_c$ (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.