



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:40 PM UTC

PDB ID : 3A13 / pdb_00003a13
Title : Crystal structure of Type III Rubisco SP4 mutant complexed with 2-CABP and activated with Ca
Authors : Nishitani, Y.; Fujihashi, M.; Doi, T.; Yoshida, S.; Atomi, H.; Imanaka, T.; Miki, K.
Deposited on : 2009-03-25
Resolution : 2.34 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

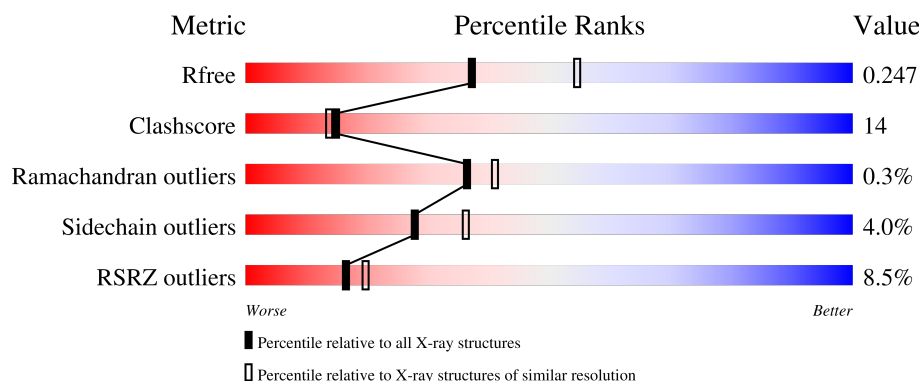
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.34 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	4% 72% 25% ..
1	B	444	9% 76% 20% ..
1	C	444	11% 76% 21% ..
1	D	444	13% 75% 21% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	444	4% 79% 17%
1	F	444	9% 75% 23%
1	G	444	9% 75% 23%
1	H	444	10% 75% 23%
1	I	444	7% 75% 21%
1	J	444	7% 75% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36193 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	436	Total	C	N	O	S	0	0	0
			3408	2186	586	626	10			
1	B	437	Total	C	N	O	S	0	0	0
			3412	2187	586	629	10			
1	C	437	Total	C	N	O	S	0	0	0
			3399	2181	584	624	10			
1	D	437	Total	C	N	O	S	0	0	0
			3392	2170	584	628	10			
1	E	432	Total	C	N	O	S	0	0	0
			3379	2163	581	625	10			
1	F	437	Total	C	N	O	S	0	0	0
			3405	2184	586	625	10			
1	G	437	Total	C	N	O	S	0	0	0
			3413	2190	585	628	10			
1	H	438	Total	C	N	O	S	0	0	0
			3412	2189	588	625	10			
1	I	437	Total	C	N	O	S	0	0	0
			3423	2195	587	631	10			
1	J	434	Total	C	N	O	S	0	0	0
			3379	2161	583	625	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

Continued on next page...

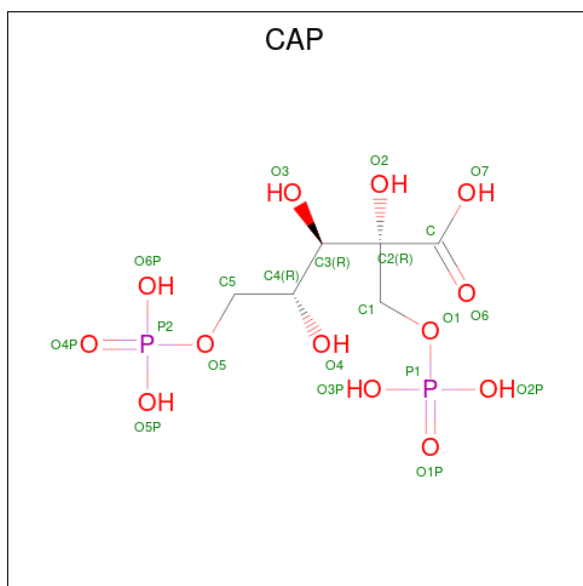
Continued from previous page...

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	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

- 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
3	B	1	Total C O P 21 6 13 2	0	0
3	C	1	Total C O P 21 6 13 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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 CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Ca	0	0
			1	1		
4	J	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	193	Total	O	0	0
			193	193		
5	B	204	Total	O	0	0
			204	204		
5	C	186	Total	O	0	0
			186	186		
5	D	210	Total	O	0	0
			210	210		
5	E	193	Total	O	0	0
			193	193		
5	F	176	Total	O	0	0
			176	176		
5	G	203	Total	O	0	0
			203	203		
5	H	180	Total	O	0	0
			180	180		

Continued on next page...

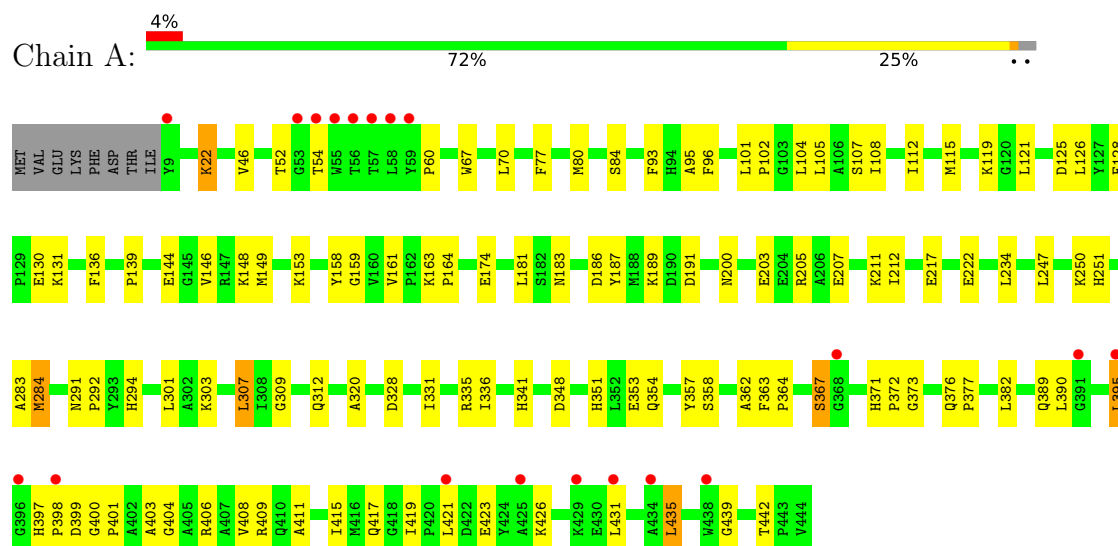
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	212	Total 212	O 212	0	0
5	J	194	Total 194	O 194	0	0

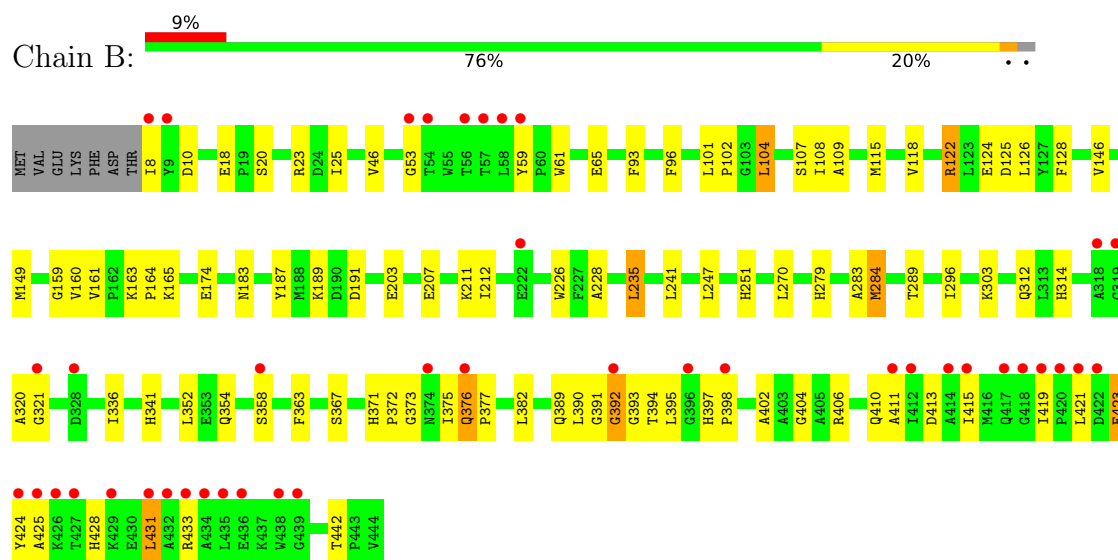
3 Residue-property plots

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

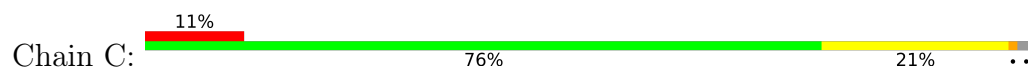
• Molecule 1: Ribulose biphosphate carboxylase

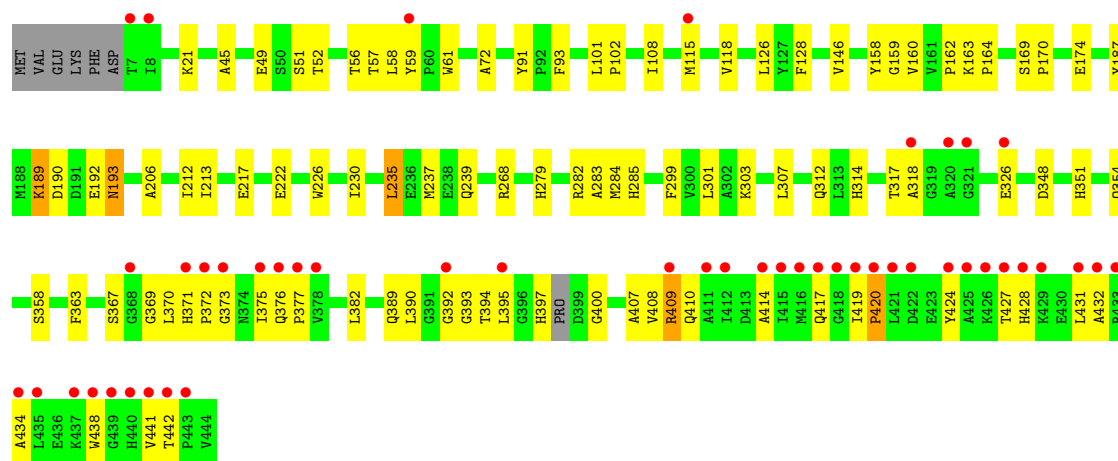


• Molecule 1: Ribulose biphosphate carboxylase

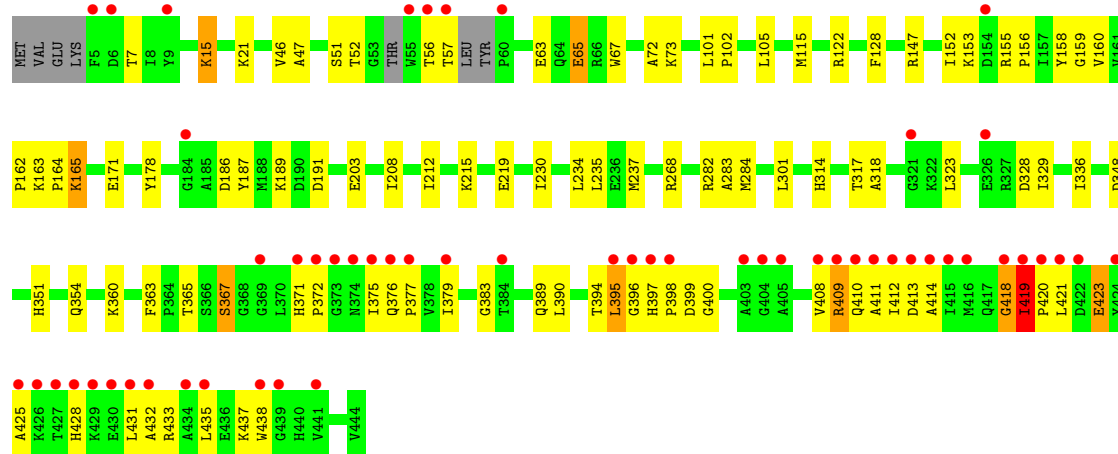
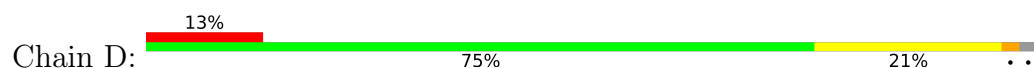


• Molecule 1: Ribulose biphosphate carboxylase

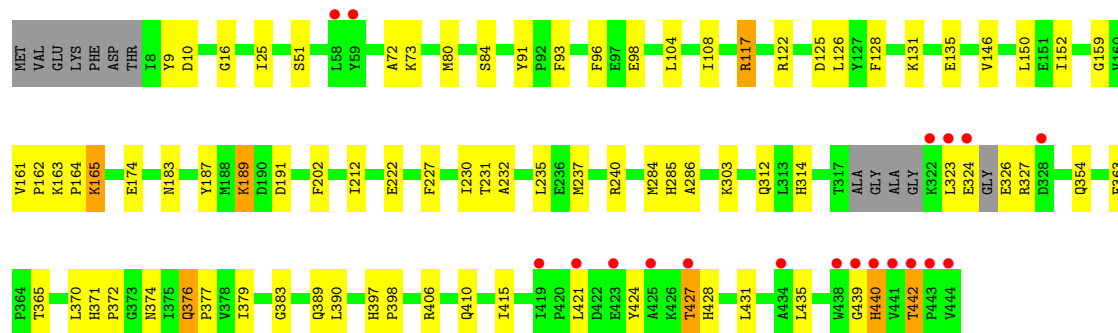
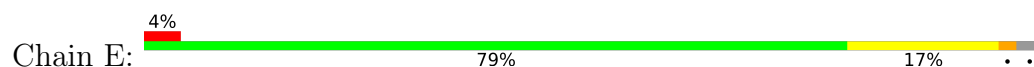




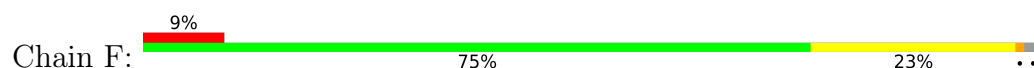
• Molecule 1: Ribulose biphosphate carboxylase

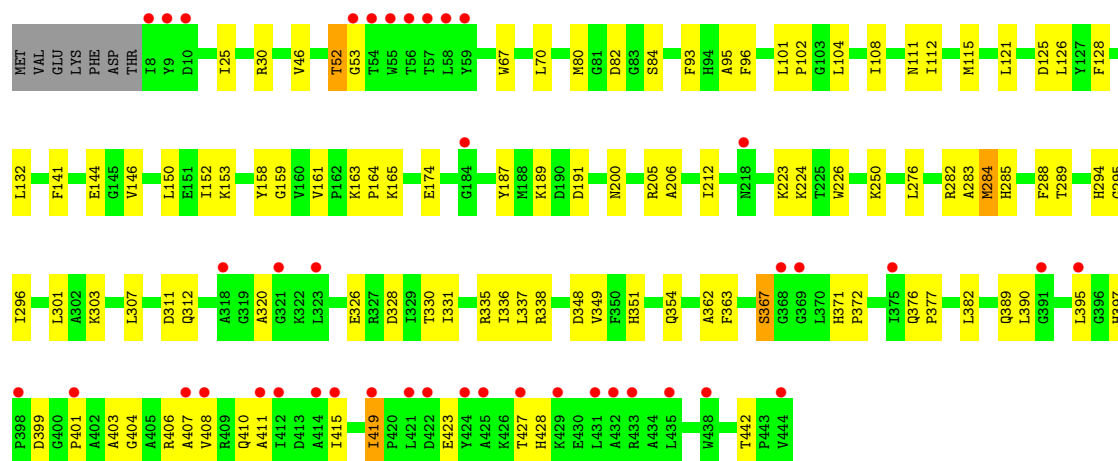


• Molecule 1: Ribulose biphosphate carboxylase

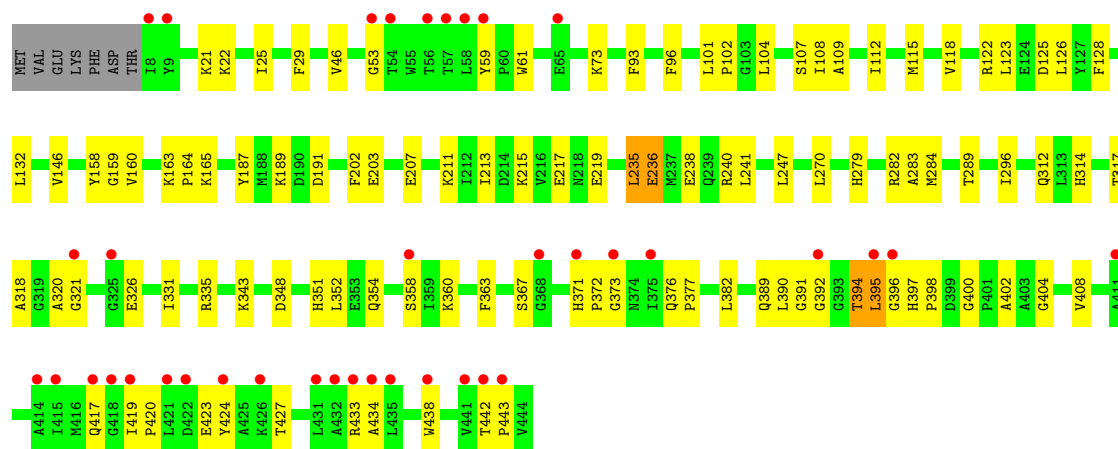
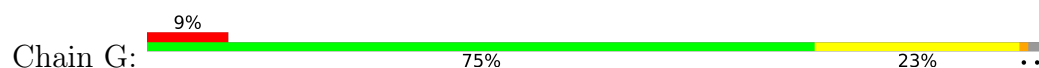


• Molecule 1: Ribulose biphosphate carboxylase

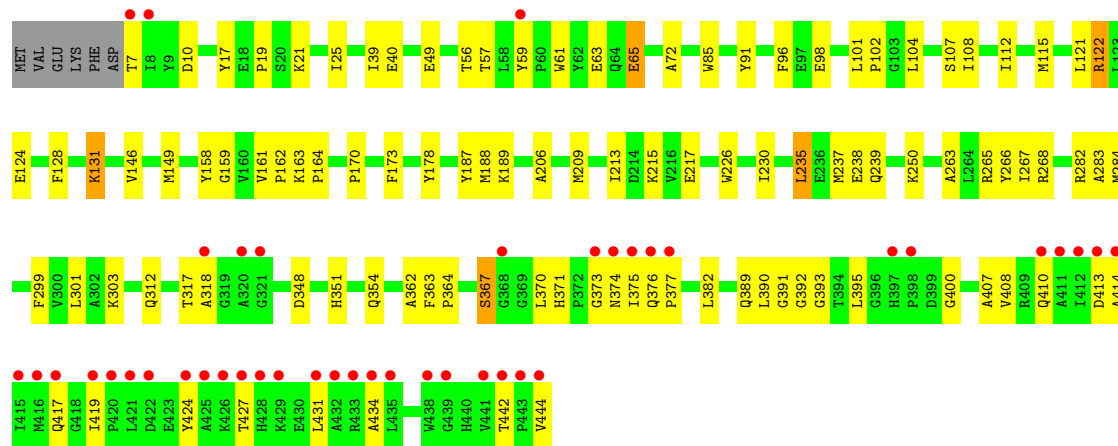
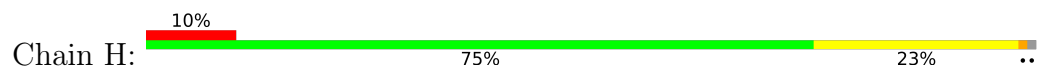




• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase



• Molecule 1: Ribulose biphosphate carboxylase

4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	173.68Å 247.09Å 144.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.22 – 2.34 42.22 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.3 (42.22-2.34) 99.6 (42.22-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.205 , 0.250 0.206 , 0.247	Depositor DCC
R_{free} test set	13142 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	28.6	Xtrriage
Anisotropy	0.039	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	36193	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.31 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5974e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CA, KCX, CAP, MG

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	0.46	0/3482	0.77	2/4722 (0.0%)
1	B	0.47	0/3486	0.77	1/4729 (0.0%)
1	C	0.46	0/3472	0.76	2/4711 (0.0%)
1	D	0.47	0/3463	0.76	4/4695 (0.1%)
1	E	0.47	0/3451	0.74	0/4680
1	F	0.46	0/3479	0.79	3/4719 (0.1%)
1	G	0.48	0/3488	0.78	4/4732 (0.1%)
1	H	0.46	0/3486	0.77	3/4729 (0.1%)
1	I	0.49	0/3495	0.76	0/4735
1	J	0.48	0/3451	0.77	4/4679 (0.1%)
All	All	0.47	0/34753	0.77	23/47131 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	53	GLY	N-CA-C	7.19	121.42	112.79
1	J	400	GLY	CA-C-N	6.28	125.77	119.24
1	J	400	GLY	C-N-CA	6.28	125.77	119.24
1	D	400	GLY	CA-C-N	6.12	127.49	119.84
1	D	400	GLY	C-N-CA	6.12	127.49	119.84
1	J	438	TRP	N-CA-C	5.99	117.89	111.36
1	H	400	GLY	CA-C-N	5.83	125.30	119.24
1	H	400	GLY	C-N-CA	5.83	125.30	119.24
1	B	53	GLY	N-CA-C	5.79	121.10	112.41
1	J	256	VAL	N-CA-C	5.79	116.56	110.72
1	F	52	THR	N-CA-C	5.74	119.59	112.59
1	G	53	GLY	N-CA-C	5.57	121.37	112.58
1	D	419	ILE	N-CA-C	5.54	113.97	107.77
1	G	400	GLY	CA-C-N	5.37	124.82	119.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	400	GLY	C-N-CA	5.37	124.82	119.24
1	H	419	ILE	N-CA-C	5.33	112.41	107.56
1	D	153	LYS	N-CA-C	5.19	117.01	111.36
1	G	396	GLY	N-CA-C	-5.08	106.77	115.61
1	A	400	GLY	CA-C-N	5.04	126.14	119.84
1	A	400	GLY	C-N-CA	5.04	126.14	119.84
1	F	153	LYS	N-CA-C	5.02	116.56	111.14
1	C	400	GLY	CA-C-N	5.01	124.45	119.24
1	C	400	GLY	C-N-CA	5.01	124.45	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	3408	0	3311	89	0
1	B	3412	0	3307	122	0
1	C	3399	0	3284	94	0
1	D	3392	0	3267	94	0
1	E	3379	0	3253	76	0
1	F	3405	0	3301	76	0
1	G	3413	0	3303	93	0
1	H	3412	0	3315	96	0
1	I	3423	0	3330	88	0
1	J	3379	0	3235	89	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	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
3	A	21	0	7	1	0
3	B	21	0	7	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	21	0	7	3	0
3	D	21	0	7	0	0
3	E	21	0	9	1	0
3	F	21	0	8	2	0
3	G	21	0	7	1	0
3	H	21	0	8	2	0
3	I	21	0	7	0	0
3	J	21	0	9	1	0
4	E	1	0	0	0	0
4	J	1	0	0	0	0
5	A	193	0	0	16	0
5	B	204	0	0	14	0
5	C	186	0	0	9	0
5	D	210	0	0	16	0
5	E	193	0	0	12	0
5	F	176	0	0	9	0
5	G	203	0	0	15	0
5	H	180	0	0	6	0
5	I	212	0	0	14	0
5	J	194	0	0	11	0
All	All	36193	0	32982	925	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 14.

All (925) 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:F:326:GLU:HG2	5:F:602:HOH:O	1.45	1.16
1:B:104:LEU:HD23	1:B:104:LEU:C	1.72	1.14
1:J:174:GLU:HG3	1:J:212:ILE:HD11	1.29	1.13
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.18	1.12
1:J:391:GLY:O	1:J:395:LEU:HD12	1.49	1.12
1:E:174:GLU:HG3	1:E:212:ILE:HD11	1.28	1.11
1:I:429:LYS:H	1:I:429:LYS:HD3	0.98	1.09
3:C:446:CAP:H4	3:C:446:CAP:O6	1.50	1.09
1:A:358:SER:HB2	5:A:678:HOH:O	1.48	1.08
1:B:149:MET:HE1	1:B:251:HIS:CE1	1.91	1.06
1:C:49:GLU:HG3	1:C:115:MET:HE3	1.38	1.05
1:H:235:LEU:HD12	5:H:602:HOH:O	1.54	1.05
1:D:203:GLU:HG3	5:D:551:HOH:O	1.58	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:446:CAP:H4	3:H:446:CAP:O6	1.59	1.02
1:I:335:ARG:HD2	1:I:339:GLU:OE2	1.59	1.02
1:B:104:LEU:HD23	1:B:104:LEU:O	1.57	1.02
1:F:367:SER:HB2	1:F:389:GLN:HB3	1.39	1.02
1:C:417:GLN:HA	5:C:601:HOH:O	1.60	1.01
1:D:165:LYS:HB3	1:D:191:ASP:OD2	1.64	0.97
1:C:371:HIS:CE1	1:C:373:GLY:HA3	2.00	0.97
1:B:371:HIS:CE1	1:B:373:GLY:HA3	1.99	0.96
1:I:429:LYS:HD3	1:I:429:LYS:N	1.76	0.96
1:D:419:ILE:N	1:D:419:ILE:HD12	1.78	0.95
1:A:367:SER:HB2	1:A:389:GLN:HB3	1.51	0.93
1:H:371:HIS:CE1	1:H:373:GLY:HA3	2.03	0.92
1:C:235:LEU:HD12	5:C:666:HOH:O	1.69	0.91
1:H:149:MET:CE	1:H:250:LYS:HD2	2.00	0.90
1:E:431:LEU:O	1:E:435:LEU:HD13	1.69	0.90
1:B:398:PRO:HG3	1:B:433:ARG:O	1.71	0.90
1:D:438:TRP:HB2	5:D:587:HOH:O	1.71	0.90
1:C:163:LYS:H	1:C:395:LEU:CD2	1.85	0.89
1:B:104:LEU:C	1:B:104:LEU:CD2	2.46	0.89
1:J:440:HIS:CE1	5:J:694:HOH:O	2.25	0.88
1:D:383:GLY:HA3	5:D:609:HOH:O	1.73	0.88
1:B:371:HIS:HE1	1:B:373:GLY:HA3	1.38	0.88
1:G:104:LEU:HD23	1:G:104:LEU:C	1.98	0.88
1:I:429:LYS:H	1:I:429:LYS:CD	1.81	0.88
1:D:367:SER:HB2	1:D:389:GLN:HB3	1.56	0.87
1:F:174:GLU:HG3	1:F:212:ILE:HD11	1.58	0.86
1:C:193:ASN:HD22	1:C:193:ASN:H	1.23	0.86
1:G:397:HIS:ND1	1:G:398:PRO:HD2	1.91	0.86
1:B:149:MET:HE1	1:B:251:HIS:HE1	1.38	0.85
1:B:425:ALA:HB2	1:B:431:LEU:HG	1.58	0.85
1:A:174:GLU:HG3	1:A:212:ILE:HD11	1.58	0.85
1:I:329:ILE:HD11	5:I:679:HOH:O	1.77	0.84
1:C:174:GLU:HG3	1:C:212:ILE:HD11	1.57	0.84
1:B:371:HIS:CE1	1:B:373:GLY:CA	2.61	0.84
1:C:371:HIS:HE1	1:C:373:GLY:HA3	1.42	0.84
1:E:128:PHE:H	1:E:354:GLN:HE22	1.25	0.84
1:G:146:VAL:HG21	1:G:312:GLN:HE21	1.43	0.83
1:H:348:ASP:OD2	1:H:351:HIS:HD2	1.61	0.83
1:I:21:LYS:HD3	5:I:689:HOH:O	1.78	0.83
1:C:49:GLU:HG3	1:C:115:MET:CE	2.08	0.82
1:H:163:LYS:H	1:H:395:LEU:CD2	1.93	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:ARG:CZ	1:D:409:ARG:NH2	2.43	0.82
1:G:417:GLN:C	5:G:564:HOH:O	2.23	0.81
1:H:149:MET:HE1	1:H:250:LYS:HB3	1.61	0.81
1:J:128:PHE:H	1:J:354:GLN:HE22	1.27	0.81
1:D:419:ILE:N	1:D:419:ILE:CD1	2.43	0.80
1:G:159:GLY:HA3	1:G:187:TYR:CZ	2.17	0.80
1:F:163:LYS:H	1:F:395:LEU:HD22	1.47	0.79
1:G:398:PRO:HG2	1:G:433:ARG:O	1.81	0.79
1:D:413:ASP:HA	5:D:594:HOH:O	1.82	0.79
1:D:395:LEU:N	1:D:395:LEU:CD1	2.45	0.79
1:H:149:MET:HE1	1:H:250:LYS:CB	2.14	0.78
1:I:410:GLN:HE22	1:I:430:GLU:CG	1.97	0.77
1:J:174:GLU:CG	1:J:212:ILE:HD11	2.14	0.77
1:A:121:LEU:H	1:A:294:HIS:HD2	1.31	0.76
1:C:367:SER:HB2	1:C:389:GLN:HB3	1.66	0.76
1:I:348:ASP:OD2	1:I:351:HIS:HD2	1.68	0.76
1:A:331:ILE:O	1:A:335:ARG:HG3	1.85	0.76
1:F:338:ARG:HD2	5:F:574:HOH:O	1.86	0.76
1:E:440:HIS:CD2	5:E:691:HOH:O	2.38	0.76
1:J:410:GLN:NE2	1:J:431:LEU:H	1.83	0.76
1:A:411:ALA:O	1:A:415:ILE:HG13	1.85	0.76
1:B:371:HIS:ND1	1:B:373:GLY:N	2.33	0.76
1:D:397:HIS:ND1	1:D:398:PRO:HD2	2.00	0.76
1:H:161:VAL:H	1:H:389:GLN:NE2	1.83	0.76
1:D:428:HIS:CE1	5:D:583:HOH:O	2.37	0.76
1:D:21:LYS:HD3	5:D:709:HOH:O	1.84	0.76
1:H:371:HIS:HE1	1:H:373:GLY:HA3	1.49	0.75
1:C:159:GLY:HA3	1:C:187:TYR:CZ	2.22	0.75
1:D:395:LEU:N	1:D:395:LEU:HD12	2.00	0.75
1:H:128:PHE:H	1:H:354:GLN:HE22	1.35	0.75
1:I:128:PHE:H	1:I:354:GLN:HE22	1.33	0.75
1:C:348:ASP:OD2	1:C:351:HIS:HD2	1.70	0.74
1:A:389:GLN:C	1:A:390:LEU:HD12	2.12	0.74
1:E:9:TYR:HD2	1:E:117:ARG:NH1	1.84	0.74
1:C:159:GLY:HA3	1:C:187:TYR:CE2	2.22	0.74
1:I:389:GLN:C	1:I:390:LEU:HD12	2.13	0.74
1:B:423:GLU:HG3	1:B:424:TYR:N	2.02	0.74
1:E:163:LYS:HD2	5:E:630:HOH:O	1.87	0.74
1:H:367:SER:HB2	1:H:389:GLN:HB3	1.69	0.73
1:J:368:GLY:O	1:J:370:LEU:HD13	1.88	0.73
1:C:128:PHE:H	1:C:354:GLN:HE22	1.36	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:CB	1:D:191:ASP:OD2	2.36	0.73
1:E:376:GLN:N	1:E:377:PRO:HD2	2.03	0.73
1:B:423:GLU:HG3	1:B:424:TYR:H	1.52	0.73
1:B:174:GLU:HG3	1:B:212:ILE:HD11	1.70	0.73
1:E:174:GLU:CG	1:E:212:ILE:HD11	2.14	0.73
1:I:438:TRP:HB2	5:I:597:HOH:O	1.88	0.73
1:B:128:PHE:H	1:B:354:GLN:HE22	1.37	0.72
1:A:121:LEU:H	1:A:294:HIS:CD2	2.07	0.72
1:C:162:PRO:HA	1:C:395:LEU:HD21	1.71	0.71
1:D:128:PHE:H	1:D:354:GLN:HE22	1.38	0.71
1:E:440:HIS:HB3	5:E:692:HOH:O	1.91	0.71
1:B:410:GLN:CG	5:B:628:HOH:O	2.38	0.71
1:D:159:GLY:HA3	1:D:187:TYR:CZ	2.26	0.71
1:G:159:GLY:HA3	1:G:187:TYR:CE1	2.25	0.71
1:H:317:THR:O	1:H:318:ALA:HB3	1.91	0.71
1:D:63:GLU:HG2	1:D:65:GLU:HG2	1.73	0.70
1:F:389:GLN:C	1:F:390:LEU:HD12	2.16	0.70
1:G:427:THR:HB	5:G:614:HOH:O	1.91	0.70
1:B:419:ILE:HG23	1:B:423:GLU:CG	2.21	0.70
1:E:93:PHE:CE1	1:E:131:LYS:HE3	2.27	0.70
1:E:442:THR:HG23	5:E:693:HOH:O	1.92	0.70
1:B:159:GLY:HA3	1:B:187:TYR:CZ	2.27	0.70
1:E:326:GLU:HG2	1:E:327:ARG:H	1.57	0.70
1:F:423:GLU:CB	5:F:633:HOH:O	2.39	0.70
1:I:370:LEU:HB2	5:I:659:HOH:O	1.92	0.70
1:G:128:PHE:H	1:G:354:GLN:HE22	1.40	0.70
1:G:320:ALA:O	1:G:442:THR:HG23	1.92	0.69
1:G:360:LYS:HE2	5:G:645:HOH:O	1.91	0.69
1:B:146:VAL:HG21	1:B:312:GLN:HE21	1.56	0.69
1:A:320:ALA:O	1:A:442:THR:HG23	1.92	0.69
1:J:163:LYS:HA	1:J:164:PRO:C	2.17	0.69
1:F:121:LEU:H	1:F:294:HIS:HD2	1.38	0.69
1:J:410:GLN:HE21	1:J:431:LEU:N	1.89	0.69
1:C:317:THR:O	1:C:318:ALA:HB3	1.92	0.69
1:F:163:LYS:HE3	3:F:446:CAP:O2P	1.92	0.69
1:F:320:ALA:O	1:F:442:THR:HG23	1.93	0.69
1:G:371:HIS:CE1	1:G:373:GLY:HA3	2.26	0.69
1:E:159:GLY:HA3	1:E:187:TYR:CZ	2.27	0.68
1:C:235:LEU:CD1	5:C:666:HOH:O	2.35	0.68
1:E:371:HIS:CE1	1:E:439:GLY:O	2.46	0.68
1:E:410:GLN:HE21	1:E:431:LEU:HB2	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:410:GLN:NE2	1:I:430:GLU:CG	2.56	0.68
1:G:104:LEU:HD23	1:G:104:LEU:O	1.92	0.68
1:J:326:GLU:HG2	1:J:327:ARG:N	2.08	0.68
1:B:397:HIS:CG	1:B:398:PRO:HD2	2.27	0.68
1:D:348:ASP:OD2	1:D:351:HIS:HD2	1.76	0.68
1:H:39:ILE:HD13	1:H:85:TRP:CD1	2.28	0.68
1:I:428:HIS:NE2	5:I:531:HOH:O	2.26	0.68
1:B:419:ILE:CG2	1:B:423:GLU:CG	2.72	0.68
1:E:16:GLY:HA3	5:E:657:HOH:O	1.93	0.68
1:G:46:VAL:HG22	1:G:115:MET:HE1	1.75	0.67
1:J:159:GLY:HA3	1:J:187:TYR:CZ	2.29	0.67
1:A:163:LYS:H	1:A:395:LEU:HD11	1.58	0.67
1:H:376:GLN:N	1:H:377:PRO:HD2	2.09	0.67
1:I:159:GLY:HA3	1:I:187:TYR:CE2	2.30	0.67
1:B:397:HIS:ND1	1:B:398:PRO:HD2	2.10	0.67
1:G:25:ILE:HD13	1:G:96:PHE:CE2	2.30	0.67
1:J:410:GLN:HE21	1:J:431:LEU:H	1.40	0.67
1:J:326:GLU:HG2	1:J:327:ARG:H	1.60	0.67
1:E:159:GLY:HA3	1:E:187:TYR:CE2	2.30	0.66
1:J:389:GLN:C	1:J:390:LEU:HD12	2.20	0.66
1:D:395:LEU:CD1	1:D:395:LEU:H	2.07	0.66
1:I:431:LEU:HD12	1:I:431:LEU:O	1.94	0.66
1:B:241:LEU:HD12	1:B:270:LEU:HD23	1.78	0.66
1:A:341:HIS:HE1	1:A:353:GLU:OE2	1.78	0.66
1:I:159:GLY:HA3	1:I:187:TYR:CZ	2.31	0.66
1:D:155:ARG:CZ	1:D:409:ARG:HH22	2.09	0.66
1:D:159:GLY:HA3	1:D:187:TYR:CE2	2.30	0.66
1:H:63:GLU:HG2	1:H:65:GLU:HG2	1.78	0.66
1:G:348:ASP:OD2	1:G:351:HIS:HD2	1.77	0.65
1:I:410:GLN:HE22	1:I:430:GLU:HG2	1.59	0.65
1:C:193:ASN:HD22	1:C:193:ASN:N	1.88	0.65
1:D:155:ARG:NE	1:D:409:ARG:HH22	1.94	0.65
1:B:367:SER:HB2	1:B:389:GLN:HB3	1.79	0.65
1:C:163:LYS:H	1:C:395:LEU:HD23	1.60	0.65
1:A:411:ALA:HA	1:A:421:LEU:HD11	1.79	0.64
1:F:46:VAL:HG22	1:F:115:MET:HE1	1.79	0.64
1:H:348:ASP:OD2	1:H:351:HIS:CD2	2.47	0.64
1:C:371:HIS:CE1	1:C:373:GLY:CA	2.78	0.64
1:D:329:ILE:HD11	5:D:669:HOH:O	1.97	0.64
1:D:360:LYS:HE2	5:D:612:HOH:O	1.96	0.64
1:C:427:THR:O	1:C:427:THR:HG22	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:ILE:HD12	1:E:96:PHE:CE2	2.33	0.64
1:A:149:MET:HE1	1:A:251:HIS:CE1	2.32	0.64
1:H:427:THR:O	1:H:427:THR:HG22	1.96	0.64
1:C:376:GLN:N	1:C:377:PRO:CD	2.60	0.64
1:D:163:LYS:H	1:D:395:LEU:CD2	2.10	0.64
1:H:159:GLY:HA3	1:H:187:TYR:CE2	2.32	0.64
1:I:410:GLN:NE2	1:I:430:GLU:HG3	2.13	0.64
1:J:163:LYS:HD2	5:J:553:HOH:O	1.96	0.64
1:B:203:GLU:O	1:B:207:GLU:HG2	1.98	0.64
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.33	0.64
1:B:65:GLU:OE1	1:B:65:GLU:HA	1.96	0.64
1:E:162:PRO:O	1:E:163:LYS:HD3	1.98	0.64
1:H:161:VAL:H	1:H:389:GLN:HE21	1.46	0.64
1:H:371:HIS:ND1	1:H:373:GLY:N	2.46	0.63
1:E:442:THR:N	5:E:693:HOH:O	2.31	0.63
1:F:128:PHE:H	1:F:354:GLN:HE22	1.45	0.63
1:H:371:HIS:CE1	1:H:373:GLY:CA	2.81	0.63
1:I:376:GLN:N	1:I:377:PRO:CD	2.61	0.63
1:A:128:PHE:H	1:A:354:GLN:HE22	1.44	0.63
1:E:410:GLN:HE22	1:E:431:LEU:H	1.46	0.63
1:H:159:GLY:HA3	1:H:187:TYR:CZ	2.33	0.63
1:B:159:GLY:HA3	1:B:187:TYR:CE2	2.34	0.63
1:G:427:THR:CB	5:G:614:HOH:O	2.45	0.63
1:H:158:TYR:CD1	1:H:408:VAL:HG11	2.33	0.63
1:A:54:THR:CB	5:A:568:HOH:O	2.46	0.63
1:D:414:ALA:HB1	1:D:419:ILE:O	1.98	0.63
1:H:213:ILE:O	1:H:217:GLU:HG3	1.99	0.63
1:J:385:ASP:HB2	5:J:619:HOH:O	1.99	0.63
1:D:412:ILE:HG22	5:D:594:HOH:O	1.99	0.62
1:C:371:HIS:ND1	1:C:373:GLY:N	2.44	0.62
1:F:348:ASP:OD2	1:F:351:HIS:HD2	1.82	0.62
1:I:63:GLU:HG2	1:I:65:GLU:HG2	1.81	0.62
1:J:391:GLY:O	1:J:395:LEU:CD1	2.38	0.62
1:B:149:MET:CE	1:B:251:HIS:HE1	2.12	0.62
1:G:163:LYS:HA	1:G:164:PRO:C	2.23	0.62
1:D:418:GLY:C	1:D:419:ILE:HD12	2.23	0.62
1:I:119:LYS:HE2	5:I:562:HOH:O	2.00	0.62
1:A:421:LEU:HD23	5:A:641:HOH:O	2.00	0.62
1:C:163:LYS:H	1:C:395:LEU:HD22	1.65	0.62
1:G:159:GLY:HA3	1:G:187:TYR:CE2	2.35	0.62
1:I:438:TRP:HE3	5:I:597:HOH:O	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ASP:OD2	1:A:351:HIS:HD2	1.83	0.62
1:D:395:LEU:H	1:D:395:LEU:HD13	1.62	0.62
1:D:160:VAL:HG11	1:D:395:LEU:HD11	1.82	0.62
1:F:121:LEU:H	1:F:294:HIS:CD2	2.17	0.62
1:I:165:LYS:HG2	1:I:191:ASP:OD2	2.00	0.61
1:A:22:LYS:HE3	5:A:558:HOH:O	1.98	0.61
1:I:207:GLU:HG3	5:I:574:HOH:O	2.01	0.61
1:J:391:GLY:C	1:J:395:LEU:HD12	2.25	0.61
1:G:73:LYS:HG3	5:G:683:HOH:O	1.99	0.61
1:B:108:ILE:HD12	1:B:108:ILE:C	2.25	0.61
1:I:65:GLU:HG3	5:I:711:HOH:O	2.00	0.61
1:A:397:HIS:ND1	1:A:398:PRO:HD2	2.16	0.61
1:B:373:GLY:C	5:B:608:HOH:O	2.43	0.61
1:F:93:PHE:CE2	5:F:665:HOH:O	2.50	0.60
1:G:397:HIS:CE1	1:G:398:PRO:HD2	2.36	0.60
1:J:371:HIS:CE1	1:J:439:GLY:O	2.53	0.60
1:A:159:GLY:HA3	1:A:187:TYR:CZ	2.36	0.60
1:B:320:ALA:O	1:B:442:THR:HG23	2.01	0.60
1:H:407:ALA:O	1:H:410:GLN:HB2	2.01	0.60
1:A:149:MET:HE1	1:A:251:HIS:ND1	2.17	0.60
1:A:149:MET:HE3	1:A:250:LYS:HE3	1.82	0.60
1:F:125:ASP:OD1	1:F:126:LEU:N	2.33	0.60
1:F:404:GLY:O	1:F:408:VAL:HG23	2.02	0.60
1:A:54:THR:HA	5:A:568:HOH:O	2.00	0.60
1:B:391:GLY:O	1:B:394:THR:N	2.22	0.60
1:D:155:ARG:HB2	1:D:156:PRO:HD2	1.84	0.60
1:F:163:LYS:H	1:F:395:LEU:CD2	2.12	0.60
3:B:446:CAP:O6	3:B:446:CAP:H4	2.02	0.59
1:C:235:LEU:CG	5:C:666:HOH:O	2.50	0.59
1:D:155:ARG:NE	1:D:409:ARG:NH2	2.49	0.59
1:G:93:PHE:CD1	1:G:93:PHE:C	2.80	0.59
1:A:376:GLN:N	1:A:377:PRO:CD	2.64	0.59
1:E:323:LEU:O	1:E:324:GLU:C	2.45	0.59
1:F:399:ASP:HB2	1:F:403:ALA:CB	2.32	0.59
1:H:158:TYR:CE1	1:H:408:VAL:HG11	2.38	0.59
1:A:423:GLU:OE2	1:A:426:LYS:NZ	2.30	0.59
1:B:423:GLU:CG	1:B:424:TYR:N	2.64	0.59
1:D:163:LYS:HA	1:D:164:PRO:C	2.26	0.59
1:A:104:LEU:HD13	1:A:104:LEU:C	2.28	0.59
1:C:410:GLN:NE2	1:C:431:LEU:H	2.01	0.59
1:C:371:HIS:O	1:C:375:ILE:HG23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:349:VAL:HG22	5:F:537:HOH:O	2.03	0.59
1:H:39:ILE:HD13	1:H:85:TRP:CG	2.37	0.59
1:D:371:HIS:HA	1:D:390:LEU:HD23	1.85	0.58
1:G:165:LYS:HZ1	1:G:191:ASP:CG	2.09	0.58
1:B:163:LYS:HA	1:B:164:PRO:C	2.29	0.58
1:G:108:ILE:C	1:G:108:ILE:HD12	2.27	0.58
1:G:389:GLN:C	1:G:390:LEU:HD12	2.29	0.58
1:A:119:LYS:HG3	5:A:691:HOH:O	2.02	0.58
1:E:326:GLU:HG2	1:E:327:ARG:N	2.18	0.58
1:B:411:ALA:O	1:B:415:ILE:HG13	2.04	0.58
1:B:341:HIS:ND1	5:B:604:HOH:O	2.32	0.58
1:B:372:PRO:O	1:B:421:LEU:HD21	2.02	0.58
1:B:391:GLY:O	1:B:392:GLY:C	2.44	0.58
1:I:46:VAL:HG22	1:I:115:MET:HE1	1.86	0.58
1:C:348:ASP:OD2	1:C:351:HIS:CD2	2.55	0.58
1:D:147:ARG:NH1	1:D:155:ARG:O	2.27	0.58
1:E:98:GLU:HG3	1:E:135:GLU:OE2	2.03	0.57
1:E:397:HIS:CG	1:E:398:PRO:HD2	2.39	0.57
1:G:279:HIS:HE1	1:G:314:HIS:NE2	2.01	0.57
1:J:159:GLY:HA3	1:J:187:TYR:CE2	2.39	0.57
1:G:59:TYR:O	1:G:61:TRP:HD1	1.87	0.57
1:I:335:ARG:CD	1:I:339:GLU:OE2	2.46	0.57
1:G:397:HIS:ND1	1:G:398:PRO:CD	2.66	0.57
1:H:149:MET:CE	1:H:250:LYS:HB3	2.33	0.57
1:J:159:GLY:HA3	1:J:187:TYR:CE1	2.39	0.57
1:F:158:TYR:CE1	1:F:408:VAL:HG11	2.39	0.57
1:F:159:GLY:HA3	1:F:187:TYR:CZ	2.39	0.57
1:D:371:HIS:HB2	1:D:372:PRO:CD	2.35	0.57
1:F:25:ILE:HD11	1:F:132:LEU:CD2	2.34	0.57
1:F:376:GLN:HB3	1:F:377:PRO:HD3	1.86	0.57
1:A:46:VAL:HG22	1:A:115:MET:HE1	1.85	0.57
1:A:146:VAL:HG21	1:A:312:GLN:HE21	1.69	0.57
1:B:183:ASN:OD1	1:B:406:ARG:NH1	2.37	0.57
1:I:163:LYS:HA	1:I:164:PRO:C	2.30	0.57
1:D:158:TYR:CE1	1:D:408:VAL:HG11	2.40	0.56
1:E:374:ASN:O	1:E:377:PRO:HG2	2.05	0.56
1:J:163:LYS:CD	5:J:553:HOH:O	2.52	0.56
1:F:25:ILE:HD11	1:F:132:LEU:HD21	1.86	0.56
1:F:223:LYS:O	1:F:224:LYS:HD3	2.05	0.56
1:A:54:THR:N	5:A:547:HOH:O	2.38	0.56
1:B:419:ILE:CG2	1:B:423:GLU:CD	2.78	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASN:H	1:C:193:ASN:ND2	2.00	0.56
1:D:394:THR:HB	1:D:395:LEU:CD1	2.35	0.56
1:F:112:ILE:O	1:F:115:MET:HE2	2.06	0.56
1:H:389:GLN:C	1:H:390:LEU:HD12	2.30	0.56
1:A:419:ILE:HD12	1:A:419:ILE:H	1.69	0.56
1:J:9:TYR:HD2	1:J:117:ARG:NH1	2.03	0.56
1:B:10:ASP:CB	5:B:654:HOH:O	2.53	0.56
1:B:397:HIS:ND1	1:B:398:PRO:CD	2.69	0.56
1:F:376:GLN:N	1:F:377:PRO:CD	2.69	0.56
1:G:417:GLN:HA	5:G:564:HOH:O	2.04	0.56
1:H:230:ILE:O	1:H:237:MET:HG2	2.06	0.56
1:H:238:GLU:OE2	1:H:266:TYR:OH	2.21	0.56
1:J:326:GLU:N	5:J:664:HOH:O	2.37	0.56
1:B:46:VAL:HG22	1:B:115:MET:HE1	1.86	0.56
1:B:59:TYR:O	1:B:61:TRP:HD1	1.88	0.56
1:D:438:TRP:HE3	5:D:587:HOH:O	1.88	0.56
1:J:326:GLU:HB3	1:J:329:ILE:HD13	1.88	0.56
1:A:163:LYS:HA	1:A:164:PRO:C	2.30	0.56
1:B:419:ILE:HG22	1:B:423:GLU:HG3	1.88	0.56
1:H:56:THR:OG1	1:H:57:THR:N	2.31	0.56
1:H:188:MET:HB3	5:H:597:HOH:O	2.06	0.56
1:J:375:ILE:O	1:J:379:ILE:HG13	2.05	0.56
1:B:104:LEU:HD21	1:B:108:ILE:CG1	2.35	0.56
1:E:163:LYS:HA	1:E:164:PRO:C	2.30	0.56
1:H:163:LYS:H	1:H:395:LEU:HD22	1.67	0.56
1:J:174:GLU:HG3	1:J:212:ILE:CD1	2.20	0.56
1:H:235:LEU:HD23	1:H:239:GLN:NE2	2.21	0.55
1:I:438:TRP:O	1:I:441:VAL:HG12	2.06	0.55
1:A:371:HIS:HB2	1:A:372:PRO:CD	2.36	0.55
1:E:376:GLN:CG	1:E:415:ILE:HG12	2.37	0.55
1:A:161:VAL:HG23	1:A:389:GLN:CD	2.30	0.55
1:H:65:GLU:CD	1:H:65:GLU:H	2.11	0.55
1:E:371:HIS:HB2	1:E:372:PRO:HD2	1.89	0.55
1:F:163:LYS:HA	1:F:164:PRO:C	2.30	0.55
1:E:427:THR:HB	1:E:428:HIS:CE1	2.41	0.55
1:G:417:GLN:O	1:G:419:ILE:HD12	2.06	0.55
3:J:446:CAP:O4	3:J:446:CAP:C	2.55	0.55
1:C:213:ILE:O	1:C:217:GLU:HG3	2.07	0.55
1:G:343:LYS:HE3	5:G:588:HOH:O	2.06	0.55
1:I:431:LEU:HD12	1:I:431:LEU:C	2.31	0.55
1:B:402:ALA:CB	5:B:550:HOH:O	2.54	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:THR:OG1	1:C:57:THR:N	2.40	0.55
1:B:93:PHE:CD1	1:B:93:PHE:C	2.84	0.55
1:E:376:GLN:HG2	1:E:415:ILE:HG12	1.88	0.55
1:F:150:LEU:O	1:F:152:ILE:HG13	2.07	0.55
1:G:395:LEU:C	1:G:395:LEU:HD12	2.32	0.55
1:B:419:ILE:HG23	1:B:423:GLU:HG2	1.88	0.54
1:G:376:GLN:N	1:G:377:PRO:HD2	2.23	0.54
1:A:283:ALA:O	1:A:284:MET:CB	2.55	0.54
1:B:371:HIS:ND1	1:B:373:GLY:CA	2.70	0.54
1:F:428:HIS:NE2	5:F:553:HOH:O	2.34	0.54
1:J:371:HIS:HB2	1:J:372:PRO:CD	2.36	0.54
1:J:376:GLN:N	1:J:377:PRO:HD2	2.23	0.54
1:A:149:MET:CE	1:A:251:HIS:CE1	2.90	0.54
1:B:372:PRO:O	1:B:421:LEU:CD2	2.56	0.54
1:B:389:GLN:C	1:B:390:LEU:HD12	2.33	0.54
1:C:21:LYS:HE2	5:C:682:HOH:O	2.07	0.54
1:F:371:HIS:HB2	1:F:372:PRO:CD	2.38	0.54
1:J:65:GLU:CD	1:J:65:GLU:H	2.14	0.54
1:A:200:ASN:OD1	1:A:205:ARG:HD3	2.07	0.54
1:D:46:VAL:CG2	1:D:115:MET:HE1	2.37	0.54
1:G:104:LEU:C	1:G:104:LEU:CD2	2.73	0.54
1:A:341:HIS:CE1	1:A:353:GLU:OE2	2.61	0.54
1:B:398:PRO:CG	1:B:433:ARG:O	2.51	0.54
1:B:419:ILE:HG23	1:B:423:GLU:CD	2.33	0.54
1:J:424:TYR:CZ	1:J:428:HIS:CE1	2.96	0.54
1:B:241:LEU:CD1	1:B:270:LEU:HD23	2.38	0.54
1:H:303:LYS:NZ	1:H:354:GLN:HE21	2.06	0.54
1:A:371:HIS:HB2	1:A:372:PRO:HD2	1.90	0.54
1:B:25:ILE:HD12	1:B:96:PHE:CE2	2.43	0.54
1:B:371:HIS:HB2	1:B:372:PRO:CD	2.38	0.54
1:D:419:ILE:CD1	1:D:419:ILE:H	2.17	0.54
1:A:159:GLY:HA3	1:A:187:TYR:CE2	2.42	0.54
1:C:59:TYR:O	1:C:61:TRP:HD1	1.91	0.54
1:C:159:GLY:HA3	1:C:187:TYR:CD2	2.43	0.54
1:E:25:ILE:HD12	1:E:96:PHE:HE2	1.73	0.54
1:H:178:TYR:CE1	1:H:215:LYS:HD3	2.42	0.54
1:A:191:ASP:HB2	5:A:567:HOH:O	2.08	0.53
1:C:230:ILE:O	1:C:237:MET:HG2	2.08	0.53
1:E:376:GLN:N	1:E:377:PRO:CD	2.72	0.53
1:E:427:THR:HB	1:E:428:HIS:ND1	2.23	0.53
1:F:331:ILE:O	1:F:335:ARG:HG3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:ILE:CD1	1:H:85:TRP:HB2	2.38	0.53
1:H:263:ALA:O	1:H:267:ILE:HG12	2.08	0.53
1:I:320:ALA:O	1:I:442:THR:HG23	2.09	0.53
1:A:389:GLN:O	1:A:390:LEU:HD12	2.08	0.53
1:C:159:GLY:HA3	1:C:187:TYR:CE1	2.44	0.53
1:E:410:GLN:HE21	1:E:431:LEU:CB	2.21	0.53
1:E:439:GLY:C	1:E:440:HIS:CD2	2.86	0.53
1:J:93:PHE:CD1	1:J:93:PHE:C	2.86	0.53
1:A:121:LEU:N	1:A:294:HIS:HD2	2.05	0.53
1:G:371:HIS:HB2	1:G:372:PRO:CD	2.39	0.53
1:I:202:PHE:CD2	1:I:240:ARG:HG2	2.43	0.53
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.43	0.53
1:G:419:ILE:O	1:G:420:PRO:C	2.51	0.53
1:I:65:GLU:H	1:I:65:GLU:CD	2.16	0.53
1:I:158:TYR:CE1	1:I:408:VAL:HG11	2.43	0.53
1:J:183:ASN:OD1	1:J:406:ARG:NH1	2.41	0.53
1:B:419:ILE:CG2	1:B:423:GLU:HG3	2.38	0.53
1:F:250:LYS:NZ	5:F:651:HOH:O	2.41	0.53
1:G:25:ILE:HD13	1:G:96:PHE:HE2	1.73	0.53
1:C:432:ALA:C	1:C:434:ALA:H	2.15	0.53
1:G:22:LYS:HG2	5:G:521:HOH:O	2.08	0.53
1:B:421:LEU:HD22	5:B:692:HOH:O	2.08	0.53
1:C:158:TYR:CE1	1:C:408:VAL:HG11	2.44	0.53
1:C:389:GLN:C	1:C:390:LEU:HD12	2.33	0.53
1:H:161:VAL:N	1:H:389:GLN:HE21	2.05	0.53
1:B:283:ALA:O	1:B:284:MET:HB3	2.08	0.52
1:F:108:ILE:C	1:F:108:ILE:HD12	2.34	0.52
1:H:122:ARG:HD2	1:H:124:GLU:OE2	2.08	0.52
1:H:159:GLY:HA3	1:H:187:TYR:CD2	2.44	0.52
1:H:162:PRO:O	1:H:163:LYS:HD3	2.09	0.52
1:I:47:ALA:O	1:I:51:SER:HB2	2.10	0.52
1:I:371:HIS:HB2	1:I:372:PRO:CD	2.39	0.52
1:B:149:MET:HE1	1:B:251:HIS:ND1	2.21	0.52
1:B:423:GLU:OE1	1:B:424:TYR:HA	2.10	0.52
1:E:371:HIS:HB2	1:E:372:PRO:CD	2.40	0.52
1:F:348:ASP:OD2	1:F:351:HIS:CD2	2.62	0.52
1:G:236:GLU:HG3	5:G:523:HOH:O	2.09	0.52
1:G:279:HIS:CE1	1:G:314:HIS:NE2	2.76	0.52
1:J:376:GLN:N	1:J:377:PRO:CD	2.73	0.52
1:B:163:LYS:H	1:B:395:LEU:HD22	1.73	0.52
1:D:65:GLU:H	1:D:65:GLU:CD	2.16	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LEU:HD12	1:G:238:GLU:OE1	2.10	0.52
1:I:250:LYS:HD3	5:I:667:HOH:O	2.08	0.52
1:B:104:LEU:HD21	1:B:108:ILE:HG12	1.92	0.52
1:C:397:HIS:HA	1:C:438:TRP:CH2	2.45	0.52
1:A:93:PHE:C	1:A:93:PHE:CD1	2.88	0.52
1:A:158:TYR:O	1:A:186:ASP:HB2	2.09	0.52
1:D:72:ALA:O	1:D:73:LYS:HD3	2.09	0.52
1:E:146:VAL:HG21	1:E:312:GLN:HE21	1.75	0.52
1:E:440:HIS:CD2	1:E:440:HIS:N	2.78	0.52
1:B:8:ILE:N	5:B:654:HOH:O	2.43	0.52
1:H:371:HIS:O	1:H:375:ILE:HG23	2.09	0.52
1:J:323:LEU:O	1:J:324:GLU:C	2.52	0.52
1:B:279:HIS:HE1	1:B:314:HIS:NE2	2.08	0.52
1:B:376:GLN:N	1:B:377:PRO:HD2	2.25	0.52
1:D:163:LYS:H	1:D:395:LEU:HD23	1.74	0.52
1:D:282:ARG:O	1:D:283:ALA:C	2.53	0.51
1:G:125:ASP:OD1	1:G:126:LEU:N	2.42	0.51
1:H:104:LEU:C	1:H:104:LEU:HD23	2.35	0.51
1:A:54:THR:CA	5:A:568:HOH:O	2.56	0.51
1:A:283:ALA:O	1:A:284:MET:HB3	2.10	0.51
1:E:72:ALA:O	1:E:73:LYS:HD3	2.10	0.51
1:E:439:GLY:C	5:E:691:HOH:O	2.53	0.51
1:F:146:VAL:HG21	1:F:312:GLN:HE21	1.76	0.51
1:H:376:GLN:N	1:H:377:PRO:CD	2.73	0.51
1:I:117:ARG:HH11	1:I:117:ARG:HG3	1.74	0.51
1:I:348:ASP:OD2	1:I:351:HIS:CD2	2.56	0.51
1:D:371:HIS:HB2	1:D:372:PRO:HD2	1.93	0.51
1:F:303:LYS:NZ	1:F:354:GLN:HE21	2.08	0.51
1:J:282:ARG:HG3	1:J:285:HIS:CD2	2.46	0.51
1:D:397:HIS:HE1	1:D:399:ASP:OD2	1.94	0.51
1:D:412:ILE:C	5:D:594:HOH:O	2.53	0.51
1:I:93:PHE:CD1	1:I:93:PHE:C	2.89	0.51
1:I:206:ALA:HA	1:I:226:TRP:CZ3	2.46	0.51
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.45	0.51
1:F:283:ALA:O	1:F:284:MET:CB	2.58	0.51
1:B:375:ILE:HG13	1:B:415:ILE:CD1	2.41	0.50
1:C:160:VAL:HG11	1:C:395:LEU:HD11	1.93	0.50
1:H:146:VAL:HG21	1:H:312:GLN:HE21	1.76	0.50
1:B:371:HIS:HA	1:B:390:LEU:HD23	1.93	0.50
1:G:397:HIS:CD2	1:G:404:GLY:HA2	2.47	0.50
1:C:235:LEU:HD23	1:C:239:GLN:NE2	2.26	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:ILE:HG22	1:D:423:GLU:CB	2.41	0.50
1:F:80:MET:HB2	1:F:84:SER:O	2.11	0.50
1:F:330:THR:HG22	1:F:382:LEU:HD21	1.92	0.50
1:A:303:LYS:NZ	1:A:354:GLN:HE21	2.10	0.50
1:B:104:LEU:HD23	1:B:108:ILE:HG13	1.93	0.50
1:C:419:ILE:O	1:C:420:PRO:C	2.54	0.50
1:C:158:TYR:CD1	1:C:408:VAL:HG11	2.47	0.50
1:C:317:THR:O	1:C:318:ALA:CB	2.59	0.50
1:D:162:PRO:HA	1:D:395:LEU:HD21	1.93	0.50
1:F:337:LEU:HD22	1:F:362:ALA:HB3	1.92	0.50
1:G:371:HIS:CE1	1:G:373:GLY:CA	2.94	0.50
1:G:402:ALA:CB	5:G:599:HOH:O	2.59	0.50
1:I:65:GLU:CG	5:I:711:HOH:O	2.59	0.50
1:A:431:LEU:HD12	1:A:435:LEU:HD13	1.94	0.50
1:G:371:HIS:HE1	1:G:373:GLY:HA3	1.71	0.50
1:H:282:ARG:O	1:H:283:ALA:C	2.53	0.50
3:E:446:CAP:O4	3:E:446:CAP:C	2.59	0.50
1:F:283:ALA:O	1:F:284:MET:HB3	2.12	0.50
1:H:209:MET:HE2	1:H:226:TRP:HB2	1.93	0.50
1:I:72:ALA:O	1:I:73:LYS:HD3	2.11	0.50
1:J:303:LYS:NZ	1:J:354:GLN:HE21	2.10	0.50
1:A:52:THR:HB	1:A:67:TRP:NE1	2.27	0.49
1:A:125:ASP:OD1	1:A:126:LEU:N	2.44	0.49
1:C:159:GLY:CA	1:C:187:TYR:CE2	2.94	0.49
1:G:417:GLN:HB3	1:G:419:ILE:HD13	1.93	0.49
1:H:159:GLY:HA3	1:H:187:TYR:CE1	2.47	0.49
1:H:371:HIS:ND1	1:H:373:GLY:CA	2.75	0.49
1:J:391:GLY:C	1:J:395:LEU:CD1	2.84	0.49
1:A:70:LEU:HD22	1:A:95:ALA:HA	1.93	0.49
1:F:411:ALA:O	1:F:415:ILE:HG13	2.12	0.49
1:F:419:ILE:HD13	1:F:419:ILE:N	2.27	0.49
1:B:25:ILE:HD12	1:B:96:PHE:HE2	1.77	0.49
1:D:152:ILE:HD13	1:D:155:ARG:NH2	2.27	0.49
1:B:283:ALA:O	1:B:284:MET:CB	2.60	0.49
1:B:20:SER:OG	1:B:23:ARG:HG3	2.12	0.49
1:B:25:ILE:CD1	1:B:96:PHE:CE2	2.95	0.49
1:B:104:LEU:CD2	1:B:108:ILE:HG13	2.42	0.49
1:J:161:VAL:HG12	1:J:163:LYS:HE2	1.95	0.49
1:E:159:GLY:HA3	1:E:187:TYR:CE1	2.47	0.49
1:I:335:ARG:NH2	5:I:549:HOH:O	2.40	0.49
1:J:329:ILE:HD12	1:J:329:ILE:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:TYR:CD2	1:E:117:ARG:NH1	2.74	0.49
1:E:410:GLN:NE2	1:E:431:LEU:H	2.09	0.49
1:F:141:PHE:HB2	1:F:311:ASP:OD1	2.12	0.49
1:H:268:ARG:HD3	1:H:268:ARG:C	2.38	0.49
1:H:442:THR:O	1:H:444:VAL:HG23	2.11	0.49
1:I:46:VAL:CG2	1:I:115:MET:HE1	2.43	0.49
1:F:289:THR:HG22	1:F:296:ILE:O	2.12	0.49
1:B:160:VAL:HG21	1:B:394:THR:HG21	1.95	0.48
1:B:289:THR:HG22	1:B:296:ILE:O	2.13	0.48
1:D:46:VAL:HG22	1:D:115:MET:HE1	1.94	0.48
1:D:397:HIS:ND1	1:D:398:PRO:CD	2.74	0.48
1:D:65:GLU:HG3	5:D:648:HOH:O	2.13	0.48
1:J:440:HIS:ND1	5:J:694:HOH:O	2.33	0.48
1:C:163:LYS:HA	1:C:164:PRO:C	2.37	0.48
1:D:159:GLY:HA3	1:D:187:TYR:CE1	2.49	0.48
1:B:165:LYS:NZ	1:B:191:ASP:OD2	2.33	0.48
1:J:93:PHE:CE1	1:J:131:LYS:HE3	2.48	0.48
1:J:101:LEU:HB3	1:J:102:PRO:HD3	1.96	0.48
1:C:414:ALA:HB2	1:C:424:TYR:CD2	2.48	0.48
1:A:397:HIS:ND1	1:A:398:PRO:CD	2.77	0.48
1:C:424:TYR:HA	5:C:577:HOH:O	2.14	0.48
1:C:441:VAL:CG1	1:C:442:THR:N	2.76	0.48
1:G:367:SER:HB2	1:G:389:GLN:HB3	1.95	0.48
1:I:424:TYR:CE2	1:I:428:HIS:CE1	3.01	0.48
1:D:348:ASP:OD2	1:D:351:HIS:CD2	2.63	0.48
1:F:159:GLY:HA3	1:F:187:TYR:CE1	2.49	0.48
1:G:165:LYS:NZ	1:G:191:ASP:OD2	2.26	0.48
1:I:371:HIS:HB2	1:I:372:PRO:HD2	1.94	0.48
1:J:131:LYS:NZ	5:J:653:HOH:O	2.29	0.48
1:A:207:GLU:O	5:A:675:HOH:O	2.20	0.48
1:A:411:ALA:HA	1:A:421:LEU:CD1	2.43	0.48
1:B:161:VAL:HG12	1:B:163:LYS:HE2	1.95	0.48
1:B:371:HIS:HB2	1:B:372:PRO:HD2	1.95	0.48
1:B:279:HIS:CE1	1:B:314:HIS:NE2	2.82	0.48
1:D:397:HIS:CG	1:D:398:PRO:HD2	2.49	0.48
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.62	0.48
1:G:390:LEU:O	1:G:394:THR:HB	2.14	0.48
1:G:397:HIS:CD2	1:G:434:ALA:HB2	2.49	0.48
1:H:21:LYS:HG3	5:H:578:HOH:O	2.12	0.48
1:G:159:GLY:HA3	1:G:187:TYR:CD1	2.49	0.47
1:H:265:ARG:CD	5:H:564:HOH:O	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:118:VAL:HG23	1:I:118:VAL:O	2.14	0.47
1:B:174:GLU:HG3	1:B:212:ILE:CD1	2.43	0.47
1:C:222:GLU:OE2	1:C:409:ARG:NH1	2.47	0.47
1:E:303:LYS:NZ	1:E:354:GLN:HE21	2.12	0.47
1:H:131:LYS:HG2	1:I:198:TRP:CD2	2.49	0.47
1:I:211:LYS:HG3	1:I:212:ILE:N	2.29	0.47
1:J:25:ILE:HD12	1:J:96:PHE:CE2	2.49	0.47
1:B:108:ILE:HD12	1:B:109:ALA:N	2.30	0.47
1:D:47:ALA:O	1:D:51:SER:CB	2.62	0.47
1:H:389:GLN:O	1:H:390:LEU:HD12	2.14	0.47
1:I:101:LEU:N	1:I:102:PRO:CD	2.76	0.47
1:B:174:GLU:CG	1:B:212:ILE:HD11	2.41	0.47
1:I:390:LEU:HD12	1:I:390:LEU:N	2.29	0.47
1:A:399:ASP:HB2	1:A:403:ALA:CB	2.44	0.47
1:B:46:VAL:CG2	1:B:115:MET:HE1	2.44	0.47
1:B:376:GLN:HG3	1:B:377:PRO:N	2.30	0.47
1:B:410:GLN:HG2	5:B:628:HOH:O	2.09	0.47
1:B:410:GLN:NE2	5:B:628:HOH:O	2.47	0.47
1:C:268:ARG:HD3	1:C:268:ARG:C	2.39	0.47
1:G:351:HIS:HE1	5:G:526:HOH:O	1.97	0.47
1:H:163:LYS:HA	1:H:164:PRO:C	2.39	0.47
1:J:17:TYR:OH	1:J:24:ASP:OD2	2.27	0.47
1:G:371:HIS:ND1	1:G:373:GLY:N	2.59	0.47
1:J:395:LEU:HD12	1:J:395:LEU:H	1.80	0.47
1:B:371:HIS:CE1	1:B:373:GLY:C	2.92	0.47
1:B:371:HIS:HE1	1:B:373:GLY:CA	2.09	0.47
1:C:282:ARG:HD2	1:C:285:HIS:CD2	2.49	0.47
1:D:47:ALA:O	1:D:51:SER:HB2	2.13	0.47
1:D:376:GLN:N	1:D:377:PRO:CD	2.77	0.47
1:D:399:ASP:OD2	1:D:433:ARG:HG3	2.14	0.47
1:E:285:HIS:CG	1:E:286:ALA:N	2.83	0.47
1:J:410:GLN:NE2	1:J:431:LEU:N	2.51	0.47
1:D:215:LYS:O	1:D:219:GLU:HG3	2.15	0.47
1:E:389:GLN:C	1:E:390:LEU:HD12	2.40	0.47
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.97	0.47
1:I:47:ALA:O	1:I:51:SER:CB	2.63	0.47
1:J:371:HIS:O	1:J:375:ILE:HG23	2.15	0.47
1:J:17:TYR:CE2	1:J:19:PRO:HA	2.50	0.47
1:J:439:GLY:C	1:J:440:HIS:ND1	2.73	0.47
1:B:410:GLN:O	1:B:413:ASP:HB2	2.15	0.47
1:G:93:PHE:HB2	1:G:132:LEU:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:331:ILE:O	1:G:335:ARG:HG3	2.15	0.47
1:I:117:ARG:HG3	1:I:117:ARG:NH1	2.30	0.47
1:J:46:VAL:HG22	1:J:115:MET:HE1	1.97	0.47
1:E:150:LEU:O	1:E:152:ILE:HG13	2.15	0.46
1:F:371:HIS:HB2	1:F:372:PRO:HD2	1.97	0.46
1:C:371:HIS:ND1	1:C:373:GLY:CA	2.77	0.46
1:D:420:PRO:O	1:D:423:GLU:CB	2.63	0.46
1:E:431:LEU:O	1:E:435:LEU:CD1	2.54	0.46
1:H:59:TYR:O	1:H:61:TRP:HD1	1.98	0.46
1:H:413:ASP:O	1:H:417:GLN:HG3	2.16	0.46
1:I:146:VAL:HG21	1:I:312:GLN:HE21	1.79	0.46
1:J:16:GLY:HA3	5:J:645:HOH:O	2.14	0.46
1:B:108:ILE:C	1:B:108:ILE:CD1	2.88	0.46
1:E:370:LEU:HB2	1:E:390:LEU:HG	1.97	0.46
1:E:431:LEU:HD11	1:E:435:LEU:HD11	1.98	0.46
1:F:165:LYS:HZ1	1:F:191:ASP:CG	2.24	0.46
1:C:369:GLY:N	3:C:446:CAP:O3P	2.41	0.46
1:F:159:GLY:HA3	1:F:187:TYR:CE2	2.50	0.46
1:A:203:GLU:CB	5:A:633:HOH:O	2.62	0.46
1:C:358:SER:HB3	1:D:171:GLU:OE2	2.16	0.46
1:D:396:GLY:O	1:D:437:LYS:NZ	2.38	0.46
1:E:230:ILE:O	1:E:231:THR:C	2.59	0.46
1:H:303:LYS:HZ3	1:H:354:GLN:HE21	1.63	0.46
1:J:433:ARG:O	1:J:436:GLU:HG2	2.15	0.46
1:G:417:GLN:HB3	1:G:419:ILE:CD1	2.46	0.46
1:A:96:PHE:HE1	1:A:107:SER:OG	1.97	0.46
1:J:355:LYS:HE3	5:J:558:HOH:O	2.15	0.46
1:A:158:TYR:CE1	1:A:408:VAL:HG11	2.50	0.46
1:C:235:LEU:HG	5:C:666:HOH:O	2.12	0.46
1:J:320:ALA:O	1:J:442:THR:CB	2.64	0.46
1:A:348:ASP:OD2	1:A:351:HIS:CD2	2.67	0.46
1:D:314:HIS:HA	1:D:365:THR:O	2.15	0.46
1:D:282:ARG:HG2	5:D:532:HOH:O	2.15	0.46
1:E:314:HIS:HA	1:E:365:THR:O	2.15	0.46
1:H:414:ALA:HB2	1:H:424:TYR:CD2	2.51	0.46
1:J:157:ILE:HD13	1:J:363:PHE:CZ	2.51	0.46
1:J:440:HIS:ND1	1:J:440:HIS:N	2.64	0.46
1:C:371:HIS:HB2	1:C:372:PRO:CD	2.46	0.45
1:D:420:PRO:O	1:D:423:GLU:N	2.48	0.45
1:G:326:GLU:HB3	5:G:674:HOH:O	2.16	0.45
1:I:155:ARG:NH2	1:I:409:ARG:NH1	2.63	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:GLY:HA3	1:A:187:TYR:CE1	2.51	0.45
1:C:303:LYS:NZ	1:C:354:GLN:HE21	2.14	0.45
1:F:93:PHE:CD1	1:F:93:PHE:C	2.94	0.45
1:I:159:GLY:HA3	1:I:187:TYR:CD2	2.50	0.45
1:I:410:GLN:NE2	1:I:430:GLU:HG2	2.27	0.45
1:B:371:HIS:O	1:B:375:ILE:HG23	2.16	0.45
1:C:432:ALA:C	1:C:434:ALA:N	2.74	0.45
1:F:206:ALA:HA	1:F:226:TRP:CZ3	2.51	0.45
1:G:419:ILE:CG2	1:G:423:GLU:HG2	2.46	0.45
1:H:161:VAL:N	1:H:389:GLN:NE2	2.57	0.45
1:J:371:HIS:HB2	1:J:372:PRO:HD2	1.96	0.45
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.81	0.45
3:F:446:CAP:O4	3:F:446:CAP:H11	2.16	0.45
1:A:362:ALA:O	1:A:364:PRO:HD3	2.15	0.45
1:B:101:LEU:HB3	1:B:102:PRO:HD3	1.97	0.45
1:B:425:ALA:CB	1:B:431:LEU:HG	2.38	0.45
1:C:162:PRO:HA	1:C:395:LEU:CD2	2.43	0.45
1:D:208:ILE:O	1:D:212:ILE:HG12	2.16	0.45
1:E:222:GLU:CD	5:E:586:HOH:O	2.59	0.45
1:G:108:ILE:C	1:G:108:ILE:CD1	2.89	0.45
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.51	0.45
1:H:149:MET:CE	1:H:250:LYS:CB	2.91	0.45
1:A:130:GLU:HG3	1:A:357:TYR:CE2	2.51	0.45
1:C:427:THR:O	1:C:428:HIS:CG	2.70	0.45
1:B:428:HIS:CE1	5:B:596:HOH:O	2.70	0.45
1:E:80:MET:HB2	1:E:84:SER:O	2.17	0.45
1:E:202:PHE:CD2	1:E:240:ARG:HG2	2.52	0.45
1:F:250:LYS:HA	1:F:276:LEU:HD23	1.99	0.45
1:F:205:ARG:HG3	1:F:205:ARG:HH11	1.81	0.45
1:J:326:GLU:OE1	1:J:329:ILE:CD1	2.64	0.45
1:C:159:GLY:CA	1:C:187:TYR:CZ	2.98	0.45
1:E:131:LYS:NZ	5:E:642:HOH:O	2.37	0.45
1:G:101:LEU:N	1:G:102:PRO:CD	2.80	0.45
1:G:423:GLU:HG2	1:G:424:TYR:N	2.32	0.45
1:H:131:LYS:HD3	5:H:522:HOH:O	2.15	0.45
1:H:149:MET:HE1	1:H:250:LYS:HB2	1.94	0.45
1:C:371:HIS:HB2	1:C:372:PRO:HD2	1.99	0.45
1:I:5:PHE:O	1:I:6:ASP:C	2.60	0.45
1:I:322:LYS:HG3	1:I:323:LEU:HD13	1.99	0.45
1:C:101:LEU:HB3	1:C:102:PRO:HD3	1.99	0.44
1:C:283:ALA:O	1:C:284:MET:HB3	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:370:LEU:N	1:J:370:LEU:CD1	2.79	0.44
1:B:104:LEU:CD2	1:B:108:ILE:CG1	2.94	0.44
1:C:283:ALA:O	1:C:284:MET:CB	2.65	0.44
1:C:410:GLN:NE2	1:C:428:HIS:HB3	2.32	0.44
1:E:159:GLY:HA3	1:E:187:TYR:CD2	2.52	0.44
1:F:82:ASP:OD1	1:F:82:ASP:C	2.60	0.44
1:I:155:ARG:HH21	1:I:409:ARG:NH1	2.15	0.44
3:A:446:CAP:O4	3:A:446:CAP:H11	2.17	0.44
1:B:118:VAL:O	1:B:118:VAL:HG23	2.17	0.44
1:F:191:ASP:HB2	5:F:536:HOH:O	2.17	0.44
1:H:370:LEU:O	1:H:393:GLY:HA3	2.17	0.44
1:A:136:PHE:HB3	1:A:307:LEU:O	2.17	0.44
1:B:410:GLN:HG3	5:B:628:HOH:O	2.12	0.44
1:C:410:GLN:HE21	1:C:431:LEU:H	1.63	0.44
3:C:446:CAP:O6	3:C:446:CAP:C4	2.40	0.44
1:F:303:LYS:HZ1	1:F:354:GLN:HE21	1.64	0.44
1:G:158:TYR:CE1	1:G:408:VAL:HG11	2.52	0.44
1:G:202:PHE:CD2	1:G:240:ARG:HG2	2.52	0.44
1:H:39:ILE:HD13	1:H:85:TRP:HB2	2.00	0.44
1:H:39:ILE:HG23	1:H:40:GLU:N	2.32	0.44
1:A:419:ILE:HD12	1:A:419:ILE:N	2.32	0.44
1:B:397:HIS:CE1	1:B:398:PRO:HG2	2.53	0.44
1:C:108:ILE:HG22	1:C:108:ILE:O	2.16	0.44
1:G:215:LYS:HE2	1:G:219:GLU:OE2	2.16	0.44
1:J:98:GLU:HG3	1:J:135:GLU:OE2	2.17	0.44
1:A:351:HIS:HE1	5:A:526:HOH:O	2.00	0.44
1:B:431:LEU:O	1:B:431:LEU:HD12	2.17	0.44
1:D:394:THR:HB	1:D:395:LEU:HD13	1.99	0.44
1:G:159:GLY:CA	1:G:187:TYR:CZ	2.96	0.44
1:H:101:LEU:HB3	1:H:102:PRO:HD3	1.99	0.44
1:H:362:ALA:O	1:H:364:PRO:HD3	2.18	0.44
1:I:52:THR:HB	1:I:67:TRP:NE1	2.33	0.44
1:I:101:LEU:HG	1:I:105:LEU:HD22	1.99	0.44
1:J:125:ASP:OD1	1:J:126:LEU:N	2.50	0.44
1:C:351:HIS:HE1	5:C:570:HOH:O	2.01	0.44
1:E:183:ASN:OD1	1:E:406:ARG:HD3	2.18	0.44
1:I:70:LEU:HD22	1:I:95:ALA:HA	1.99	0.44
1:J:63:GLU:HG2	1:J:65:GLU:HG2	1.98	0.44
1:C:279:HIS:NE2	1:C:314:HIS:NE2	2.59	0.44
1:F:96:PHE:CE1	1:F:104:LEU:HD12	2.53	0.44
1:H:17:TYR:CE2	1:H:19:PRO:HA	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:399:ASP:OD1	1:J:433:ARG:NH2	2.45	0.44
1:A:119:LYS:NZ	5:A:634:HOH:O	2.49	0.43
1:C:160:VAL:HG11	1:C:395:LEU:CD1	2.48	0.43
1:F:126:LEU:HA	1:F:126:LEU:HD12	1.82	0.43
1:F:200:ASN:OD1	1:F:205:ARG:HG3	2.18	0.43
1:F:390:LEU:HD12	1:F:390:LEU:N	2.33	0.43
1:I:108:ILE:HD12	1:I:108:ILE:C	2.42	0.43
1:I:283:ALA:O	1:I:284:MET:HB3	2.18	0.43
1:J:70:LEU:HD22	1:J:95:ALA:HA	1.99	0.43
1:B:125:ASP:OD1	1:B:126:LEU:N	2.50	0.43
1:B:402:ALA:HB3	5:B:550:HOH:O	2.16	0.43
1:B:410:GLN:O	1:B:413:ASP:N	2.51	0.43
1:E:165:LYS:HB2	1:E:191:ASP:CG	2.43	0.43
1:G:46:VAL:HG22	1:G:115:MET:CE	2.46	0.43
1:H:112:ILE:HD12	1:H:121:LEU:HD21	2.00	0.43
1:C:174:GLU:O	1:C:212:ILE:CD1	2.66	0.43
1:D:317:THR:O	1:D:318:ALA:C	2.61	0.43
1:E:161:VAL:HG22	1:E:189:KCX:HB2	1.99	0.43
1:F:101:LEU:HB3	1:F:102:PRO:HD3	2.00	0.43
1:I:264:LEU:HD23	1:I:264:LEU:HA	1.89	0.43
1:J:251:HIS:NE2	1:J:312:GLN:NE2	2.66	0.43
5:A:655:HOH:O	1:H:427:THR:HG21	2.18	0.43
1:C:299:PHE:HB2	5:C:574:HOH:O	2.19	0.43
1:C:424:TYR:CZ	1:C:428:HIS:CE1	3.07	0.43
1:H:108:ILE:O	1:H:108:ILE:CG2	2.66	0.43
1:I:30:ARG:NH2	1:I:82:ASP:OD2	2.51	0.43
1:J:326:GLU:OE1	1:J:329:ILE:HD13	2.19	0.43
1:A:108:ILE:C	1:A:108:ILE:HD12	2.44	0.43
1:A:183:ASN:OD1	1:A:406:ARG:NH1	2.50	0.43
1:A:417:GLN:O	1:A:419:ILE:HD12	2.19	0.43
1:C:51:SER:OG	1:C:52:THR:N	2.52	0.43
1:D:178:TYR:CE1	1:D:215:LYS:HE3	2.53	0.43
1:B:149:MET:CE	1:B:251:HIS:CE1	2.81	0.43
1:D:56:THR:OG1	1:D:57:THR:N	2.50	0.43
1:H:371:HIS:ND1	1:H:373:GLY:HA3	2.29	0.43
1:I:282:ARG:O	1:I:283:ALA:C	2.60	0.43
1:A:77:PHE:N	1:A:77:PHE:CD2	2.87	0.43
1:A:336:ILE:HD12	1:A:336:ILE:HA	1.80	0.43
1:B:336:ILE:HD12	1:B:336:ILE:HA	1.89	0.43
1:E:91:TYR:CZ	1:E:108:ILE:HG22	2.54	0.43
1:G:160:VAL:HG21	1:G:394:THR:HG21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:150:LEU:HD23	1:I:157:ILE:HD13	1.99	0.43
1:D:268:ARG:C	1:D:268:ARG:HD3	2.43	0.43
1:D:425:ALA:O	1:D:432:ALA:HB2	2.18	0.43
1:J:157:ILE:CD1	1:J:363:PHE:CZ	3.02	0.43
1:A:161:VAL:HG23	1:A:389:GLN:OE1	2.19	0.43
1:A:217:GLU:HG2	1:A:222:GLU:O	2.19	0.43
1:B:251:HIS:NE2	1:B:312:GLN:NE2	2.66	0.43
1:C:72:ALA:HB2	1:C:91:TYR:CD1	2.54	0.43
1:G:397:HIS:CG	1:G:398:PRO:HD2	2.53	0.43
1:H:410:GLN:HE22	1:H:431:LEU:H	1.66	0.43
1:A:376:GLN:HA	1:A:415:ILE:HD13	2.01	0.43
1:B:122:ARG:NH1	5:B:679:HOH:O	2.51	0.43
1:B:423:GLU:OE1	1:B:424:TYR:N	2.52	0.43
1:C:376:GLN:HB3	1:C:377:PRO:HD3	2.01	0.43
1:C:392:GLY:C	1:C:394:THR:H	2.27	0.43
1:E:379:ILE:O	1:E:383:GLY:CA	2.66	0.43
1:E:431:LEU:CD1	1:E:435:LEU:HD11	2.49	0.43
1:G:434:ALA:HB1	1:G:438:TRP:CZ3	2.54	0.43
1:H:431:LEU:O	1:H:434:ALA:HB3	2.19	0.43
1:I:336:ILE:HD12	1:I:336:ILE:HA	1.87	0.43
1:J:376:GLN:CG	1:J:415:ILE:HD13	2.48	0.43
1:A:80:MET:HB2	1:A:84:SER:O	2.19	0.42
1:C:189:KCX:HG3	1:C:190:ASP:O	2.19	0.42
1:E:227:PHE:CD1	1:E:227:PHE:N	2.87	0.42
1:G:46:VAL:CG2	1:G:115:MET:HE1	2.45	0.42
1:J:299:PHE:CE1	1:J:336:ILE:HB	2.54	0.42
1:J:362:ALA:O	1:J:364:PRO:HD3	2.19	0.42
1:A:101:LEU:HB3	1:A:102:PRO:HD3	2.00	0.42
1:D:351:HIS:HE1	5:D:548:HOH:O	2.02	0.42
1:J:333:ASN:OD1	5:J:543:HOH:O	2.21	0.42
1:A:112:ILE:O	1:A:115:MET:HE2	2.20	0.42
1:B:391:GLY:O	1:B:393:GLY:N	2.52	0.42
1:F:161:VAL:HG23	1:F:389:GLN:CD	2.43	0.42
1:H:283:ALA:O	1:H:284:MET:HB3	2.18	0.42
1:A:149:MET:HE1	1:A:251:HIS:HD1	1.84	0.42
1:C:282:ARG:O	1:C:283:ALA:C	2.60	0.42
1:D:375:ILE:O	1:D:379:ILE:HG13	2.19	0.42
1:D:397:HIS:CE1	1:D:398:PRO:HD2	2.55	0.42
1:E:125:ASP:OD1	1:E:126:LEU:N	2.52	0.42
1:G:73:LYS:NZ	5:G:683:HOH:O	2.51	0.42
1:J:336:ILE:HD12	1:J:336:ILE:HA	1.91	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:392:GLY:C	1:J:394:THR:N	2.78	0.42
1:D:419:ILE:CG2	1:D:423:GLU:CB	2.97	0.42
1:F:282:ARG:HD2	1:F:285:HIS:CD2	2.55	0.42
1:G:283:ALA:O	1:G:284:MET:HB3	2.20	0.42
1:H:25:ILE:HD12	1:H:96:PHE:CE2	2.55	0.42
1:J:157:ILE:HD12	1:J:157:ILE:N	2.34	0.42
1:J:165:LYS:HB2	1:J:191:ASP:CG	2.44	0.42
1:C:93:PHE:CD1	1:C:93:PHE:C	2.98	0.42
1:F:52:THR:HB	1:F:67:TRP:NE1	2.35	0.42
1:G:282:ARG:O	1:G:283:ALA:C	2.62	0.42
1:J:285:HIS:CG	1:J:286:ALA:N	2.87	0.42
1:C:370:LEU:O	1:C:393:GLY:HA3	2.19	0.42
1:D:421:LEU:O	1:D:425:ALA:HB2	2.19	0.42
1:F:30:ARG:NH2	1:F:82:ASP:OD2	2.51	0.42
1:G:118:VAL:O	1:G:118:VAL:HG23	2.19	0.42
1:G:203:GLU:O	1:G:207:GLU:HG2	2.20	0.42
1:G:289:THR:HG22	1:G:296:ILE:O	2.20	0.42
1:G:395:LEU:C	1:G:395:LEU:CD1	2.93	0.42
1:H:63:GLU:CG	1:H:65:GLU:HG2	2.47	0.42
1:H:371:HIS:CE1	1:H:374:ASN:H	2.37	0.42
1:H:391:GLY:O	1:H:392:GLY:C	2.63	0.42
1:I:285:HIS:CG	1:I:286:ALA:N	2.88	0.42
1:J:374:ASN:OD1	1:J:374:ASN:C	2.62	0.42
1:B:321:GLY:HA3	5:B:660:HOH:O	2.19	0.42
1:D:383:GLY:CA	5:D:609:HOH:O	2.48	0.42
1:D:410:GLN:O	1:D:413:ASP:N	2.52	0.42
1:E:25:ILE:CD1	1:E:96:PHE:CE2	3.01	0.42
1:G:442:THR:HA	1:G:443:PRO:HD3	1.85	0.42
1:I:159:GLY:HA3	1:I:187:TYR:CE1	2.54	0.42
1:D:63:GLU:CG	1:D:65:GLU:HG2	2.44	0.42
1:F:288:PHE:O	1:F:295:GLY:HA3	2.20	0.42
1:G:241:LEU:HD12	1:G:270:LEU:HD23	2.01	0.42
1:H:39:ILE:HD11	1:H:85:TRP:HB2	2.02	0.42
1:I:101:LEU:HB3	1:I:102:PRO:HD3	2.01	0.42
1:J:51:SER:HA	5:J:597:HOH:O	2.19	0.42
1:B:391:GLY:C	1:B:393:GLY:N	2.78	0.42
1:B:431:LEU:HD12	1:B:431:LEU:C	2.45	0.42
1:E:51:SER:HA	5:E:519:HOH:O	2.18	0.42
1:H:49:GLU:HG3	1:H:115:MET:SD	2.60	0.42
1:J:368:GLY:O	1:J:370:LEU:CD1	2.64	0.42
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:LYS:HE3	5:A:543:HOH:O	2.19	0.41
1:F:336:ILE:HD12	1:F:336:ILE:HA	1.78	0.41
1:G:112:ILE:HG23	5:G:635:HOH:O	2.20	0.41
1:J:118:VAL:O	1:J:118:VAL:HG23	2.20	0.41
1:J:159:GLY:CA	1:J:187:TYR:CZ	3.02	0.41
1:C:45:ALA:HB1	1:C:115:MET:HE1	2.02	0.41
1:C:192:GLU:HG3	1:C:283:ALA:HB2	2.01	0.41
1:E:376:GLN:HG3	1:E:415:ILE:HG12	2.03	0.41
1:G:283:ALA:O	1:G:284:MET:CB	2.68	0.41
1:H:317:THR:O	1:H:318:ALA:CB	2.58	0.41
1:I:441:VAL:HG22	1:I:442:THR:N	2.36	0.41
1:C:303:LYS:HZ3	1:C:354:GLN:HE21	1.67	0.41
1:H:7:THR:N	1:H:10:ASP:CB	2.83	0.41
1:I:176:LEU:HD21	1:I:395:LEU:HD11	2.01	0.41
1:J:227:PHE:N	1:J:227:PHE:CD1	2.87	0.41
1:A:284:MET:O	1:A:284:MET:HG2	2.20	0.41
1:D:152:ILE:HD11	1:D:186:ASP:OD1	2.19	0.41
1:F:397:HIS:CD2	1:F:404:GLY:HA2	2.55	0.41
1:H:178:TYR:HE1	1:H:215:LYS:HD3	1.86	0.41
3:H:446:CAP:O6	3:H:446:CAP:C4	2.46	0.41
1:J:115:MET:HE3	1:J:115:MET:HB2	1.96	0.41
1:J:389:GLN:O	1:J:390:LEU:HD12	2.20	0.41
1:A:291:ASN:HA	1:A:292:PRO:HD3	1.95	0.41
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.94	0.41
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.21	0.41
1:C:410:GLN:HE21	1:C:431:LEU:N	2.19	0.41
1:D:230:ILE:O	1:D:237:MET:HG2	2.21	0.41
1:E:73:LYS:HD3	1:E:73:LYS:HA	1.70	0.41
1:E:421:LEU:N	5:E:551:HOH:O	2.53	0.41
1:H:427:THR:O	1:H:427:THR:CG2	2.67	0.41
1:I:119:LYS:CE	5:I:562:HOH:O	2.65	0.41
1:C:206:ALA:HA	1:C:226:TRP:CZ3	2.55	0.41
1:D:52:THR:HB	1:D:67:TRP:NE1	2.36	0.41
1:D:147:ARG:HD3	1:D:152:ILE:O	2.20	0.41
1:F:406:ARG:O	1:F:410:GLN:HG3	2.21	0.41
1:G:29:PHE:CE1	1:G:123:LEU:HD13	2.56	0.41
3:G:446:CAP:O6	3:G:446:CAP:H4	2.21	0.41
1:I:230:ILE:O	1:I:237:MET:HG2	2.21	0.41
1:A:373:GLY:HA3	1:A:439:GLY:O	2.21	0.41
1:A:397:HIS:CD2	1:A:404:GLY:HA2	2.55	0.41
1:B:159:GLY:HA3	1:B:187:TYR:CD2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:410:GLN:OE1	1:D:431:LEU:N	2.54	0.41
1:F:200:ASN:OD1	1:F:205:ARG:CG	2.69	0.41
1:I:283:ALA:O	1:I:284:MET:CB	2.68	0.41
1:I:335:ARG:HH21	1:I:339:GLU:CD	2.29	0.41
1:C:169:SER:HB2	1:C:170:PRO:HD2	2.02	0.41
1:E:232:ALA:O	1:E:237:MET:HE2	2.21	0.41
1:F:111:ASN:HA	5:F:621:HOH:O	2.21	0.41
1:F:115:MET:HE3	1:F:115:MET:HB2	1.83	0.41
1:G:213:ILE:O	1:G:217:GLU:HG3	2.21	0.41
1:J:101:LEU:O	1:J:102:PRO:C	2.63	0.41
1:A:153:LYS:HA	5:A:614:HOH:O	2.20	0.40
1:A:411:ALA:CA	1:A:421:LEU:HD11	2.49	0.40
1:B:226:TRP:CE3	1:B:228:ALA:HB2	2.56	0.40
1:E:439:GLY:CA	5:E:691:HOH:O	2.69	0.40
1:F:407:ALA:HA	1:F:410:GLN:HB2	2.02	0.40
1:G:397:HIS:HA	1:G:398:PRO:HD3	1.88	0.40
1:I:148:LYS:HG3	5:I:601:HOH:O	2.20	0.40
1:I:153:LYS:NZ	1:I:154:ASP:OD2	2.55	0.40
1:J:283:ALA:O	1:J:284:MET:HB3	2.21	0.40
1:E:163:LYS:HD3	1:E:163:LYS:HA	1.81	0.40
1:F:70:LEU:HD22	1:F:95:ALA:HA	2.04	0.40
1:I:25:ILE:HD11	1:I:132:LEU:HD21	2.03	0.40
1:A:46:VAL:CG2	1:A:115:MET:HE1	2.49	0.40
1:B:122:ARG:HG3	1:B:124:GLU:OE2	2.20	0.40
1:B:424:TYR:CE2	1:B:428:HIS:CE1	3.10	0.40
1:C:407:ALA:O	1:C:410:GLN:HG2	2.20	0.40
1:G:317:THR:O	1:G:318:ALA:C	2.64	0.40
1:G:321:GLY:HA3	5:G:642:HOH:O	2.21	0.40
1:G:391:GLY:O	1:G:392:GLY:C	2.64	0.40
1:H:162:PRO:HA	1:H:395:LEU:HD21	2.04	0.40
1:B:303:LYS:NZ	1:B:354:GLN:HE21	2.19	0.40
1:C:126:LEU:HD12	1:C:126:LEU:HA	1.90	0.40
1:D:336:ILE:HD12	1:D:336:ILE:HA	1.86	0.40
1:G:108:ILE:HD12	1:G:109:ALA:N	2.35	0.40
1:G:348:ASP:OD2	1:G:351:HIS:CD2	2.66	0.40
1:G:371:HIS:HB2	1:G:372:PRO:HD2	2.03	0.40
1:H:206:ALA:HA	1:H:226:TRP:CZ3	2.57	0.40
1:H:299:PHE:HB2	5:H:659:HOH:O	2.21	0.40
1:I:367:SER:HB2	1:I:389:GLN:HB3	2.04	0.40
1:I:390:LEU:N	1:I:390:LEU:CD1	2.85	0.40
1:J:213:ILE:O	1:J:217:GLU:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:PRO:N	1:A:309:GLY:HA2	2.37	0.40
1:B:161:VAL:CG1	1:B:163:LYS:HE2	2.52	0.40
1:B:397:HIS:CD2	1:B:404:GLY:HA2	2.56	0.40
1:C:371:HIS:C	1:C:373:GLY:N	2.79	0.40
1:D:15:LYS:HG3	5:D:574:HOH:O	2.22	0.40
1:D:372:PRO:HB3	1:D:411:ALA:HB2	2.03	0.40
1:D:389:GLN:C	1:D:390:LEU:HD12	2.46	0.40
1:E:424:TYR:CZ	1:E:428:HIS:CE1	3.09	0.40
1:G:59:TYR:O	1:G:61:TRP:CD1	2.72	0.40
1:H:170:PRO:O	1:H:173:PHE:HB3	2.22	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	433/444 (98%)	417 (96%)	13 (3%)	3 (1%)	18	18
1	B	434/444 (98%)	413 (95%)	19 (4%)	2 (0%)	24	26
1	C	432/444 (97%)	408 (94%)	23 (5%)	1 (0%)	43	50
1	D	430/444 (97%)	401 (93%)	26 (6%)	3 (1%)	18	18
1	E	425/444 (96%)	410 (96%)	14 (3%)	1 (0%)	43	50
1	F	434/444 (98%)	409 (94%)	23 (5%)	2 (0%)	24	26
1	G	434/444 (98%)	411 (95%)	23 (5%)	0	100	100
1	H	435/444 (98%)	415 (95%)	20 (5%)	0	100	100
1	I	430/444 (97%)	411 (96%)	18 (4%)	1 (0%)	43	50
1	J	427/444 (96%)	407 (95%)	19 (4%)	1 (0%)	43	50
All	All	4314/4440 (97%)	4102 (95%)	198 (5%)	14 (0%)	36	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	MET
1	E	284	MET
1	F	284	MET
1	F	401	PRO
1	I	284	MET
1	A	60	PRO
1	C	420	PRO
1	D	284	MET
1	D	423	GLU
1	B	284	MET
1	B	392	GLY
1	J	284	MET
1	D	418	GLY
1	A	401	PRO

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	336/356 (94%)	319 (95%)	17 (5%)	21	26
1	B	336/356 (94%)	322 (96%)	14 (4%)	26	34
1	C	332/356 (93%)	322 (97%)	10 (3%)	36	47
1	D	332/356 (93%)	315 (95%)	17 (5%)	21	26
1	E	333/356 (94%)	322 (97%)	11 (3%)	33	43
1	F	334/356 (94%)	326 (98%)	8 (2%)	43	55
1	G	335/356 (94%)	322 (96%)	13 (4%)	28	37
1	H	335/356 (94%)	325 (97%)	10 (3%)	36	47
1	I	339/356 (95%)	318 (94%)	21 (6%)	16	19
1	J	329/356 (92%)	316 (96%)	13 (4%)	28	36
All	All	3341/3560 (94%)	3207 (96%)	134 (4%)	28	36

All (134) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LYS
1	A	105	LEU
1	A	144	GLU
1	A	148	LYS
1	A	181	LEU
1	A	211	LYS
1	A	234	LEU
1	A	247	LEU
1	A	301	LEU
1	A	307	LEU
1	A	328	ASP
1	A	363	PHE
1	A	367	SER
1	A	382	LEU
1	A	395	LEU
1	A	409	ARG
1	A	435	LEU
1	B	18	GLU
1	B	104	LEU
1	B	107	SER
1	B	122	ARG
1	B	211	LYS
1	B	235	LEU
1	B	247	LEU
1	B	352	LEU
1	B	358	SER
1	B	363	PHE
1	B	376	GLN
1	B	382	LEU
1	B	423	GLU
1	B	431	LEU
1	C	58	LEU
1	C	118	VAL
1	C	193	ASN
1	C	235	LEU
1	C	301	LEU
1	C	307	LEU
1	C	326	GLU
1	C	363	PHE
1	C	382	LEU
1	C	409	ARG
1	D	7	THR
1	D	15	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	65	GLU
1	D	105	LEU
1	D	122	ARG
1	D	165	LYS
1	D	234	LEU
1	D	235	LEU
1	D	301	LEU
1	D	323	LEU
1	D	328	ASP
1	D	363	PHE
1	D	367	SER
1	D	395	LEU
1	D	409	ARG
1	D	419	ILE
1	D	435	LEU
1	E	10	ASP
1	E	104	LEU
1	E	117	ARG
1	E	122	ARG
1	E	165	LYS
1	E	235	LEU
1	E	363	PHE
1	E	376	GLN
1	E	427	THR
1	E	440	HIS
1	E	442	THR
1	F	144	GLU
1	F	301	LEU
1	F	307	LEU
1	F	328	ASP
1	F	363	PHE
1	F	367	SER
1	F	419	ILE
1	F	427	THR
1	G	21	LYS
1	G	107	SER
1	G	122	ARG
1	G	211	LYS
1	G	235	LEU
1	G	236	GLU
1	G	247	LEU
1	G	352	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	358	SER
1	G	363	PHE
1	G	382	LEU
1	G	394	THR
1	G	395	LEU
1	H	65	GLU
1	H	98	GLU
1	H	107	SER
1	H	122	ARG
1	H	131	LYS
1	H	235	LEU
1	H	301	LEU
1	H	363	PHE
1	H	367	SER
1	H	382	LEU
1	I	7	THR
1	I	15	LYS
1	I	64	GLN
1	I	65	GLU
1	I	104	LEU
1	I	105	LEU
1	I	122	ARG
1	I	148	LYS
1	I	150	LEU
1	I	207	GLU
1	I	211	LYS
1	I	234	LEU
1	I	235	LEU
1	I	301	LEU
1	I	323	LEU
1	I	328	ASP
1	I	363	PHE
1	I	370	LEU
1	I	429	LYS
1	I	430	GLU
1	I	431	LEU
1	J	10	ASP
1	J	35	GLU
1	J	65	GLU
1	J	107	SER
1	J	122	ARG
1	J	165	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	211	LYS
1	J	236	GLU
1	J	301	LEU
1	J	363	PHE
1	J	370	LEU
1	J	376	GLN
1	J	440	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	294	HIS
1	A	312	GLN
1	A	341	HIS
1	A	351	HIS
1	A	354	GLN
1	A	376	GLN
1	B	239	GLN
1	B	279	HIS
1	B	312	GLN
1	B	354	GLN
1	B	376	GLN
1	C	64	GLN
1	C	193	ASN
1	C	239	GLN
1	C	312	GLN
1	C	347	ASN
1	C	351	HIS
1	C	354	GLN
1	C	376	GLN
1	C	410	GLN
1	D	312	GLN
1	D	351	HIS
1	D	354	GLN
1	E	218	ASN
1	E	312	GLN
1	E	332	GLN
1	E	354	GLN
1	E	410	GLN
1	E	440	HIS
1	F	294	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	312	GLN
1	F	351	HIS
1	F	354	GLN
1	F	376	GLN
1	G	239	GLN
1	G	279	HIS
1	G	312	GLN
1	G	351	HIS
1	G	354	GLN
1	H	239	GLN
1	H	312	GLN
1	H	351	HIS
1	H	354	GLN
1	H	376	GLN
1	H	389	GLN
1	H	410	GLN
1	H	417	GLN
1	H	440	HIS
1	I	64	GLN
1	I	312	GLN
1	I	351	HIS
1	I	354	GLN
1	J	312	GLN
1	J	354	GLN
1	J	410	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	B	189	2,1	10,11,12	0.99	0	6,12,14	1.39	1 (16%)
1	KCX	E	189	4,1	10,11,12	0.93	0	6,12,14	1.36	1 (16%)
1	KCX	C	189	2,1	10,11,12	0.95	0	6,12,14	1.65	2 (33%)
1	KCX	A	189	2,1	10,11,12	0.89	0	6,12,14	1.24	1 (16%)
1	KCX	H	189	2,1	10,11,12	1.01	0	6,12,14	1.36	1 (16%)
1	KCX	J	189	4,1	10,11,12	0.96	0	6,12,14	1.66	1 (16%)
1	KCX	G	189	2,1	10,11,12	1.06	1 (10%)	6,12,14	1.19	1 (16%)
1	KCX	D	189	2,1	10,11,12	0.79	0	6,12,14	1.64	1 (16%)
1	KCX	F	189	2,1	10,11,12	0.93	0	6,12,14	1.40	1 (16%)
1	KCX	I	189	2,1	10,11,12	0.89	0	6,12,14	1.34	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	B	189	2,1	-	0/9/10/12	-
1	KCX	E	189	4,1	-	0/9/10/12	-
1	KCX	C	189	2,1	-	0/9/10/12	-
1	KCX	A	189	2,1	-	1/9/10/12	-
1	KCX	H	189	2,1	-	2/9/10/12	-
1	KCX	J	189	4,1	-	0/9/10/12	-
1	KCX	G	189	2,1	-	1/9/10/12	-
1	KCX	D	189	2,1	-	0/9/10/12	-
1	KCX	F	189	2,1	-	1/9/10/12	-
1	KCX	I	189	2,1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	189	KCX	OQ1-CX	2.24	1.25	1.21

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	189	KCX	OQ1-CX-NZ	-3.82	119.11	124.92
1	D	189	KCX	OQ1-CX-NZ	-3.77	119.19	124.92
1	F	189	KCX	OQ1-CX-NZ	-3.26	119.97	124.92

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	189	KCX	OQ1-CX-NZ	-3.07	120.26	124.92
1	C	189	KCX	OQ1-CX-NZ	-3.06	120.27	124.92
1	I	189	KCX	OQ1-CX-NZ	-2.92	120.48	124.92
1	B	189	KCX	OQ1-CX-NZ	-2.72	120.78	124.92
1	H	189	KCX	OQ1-CX-NZ	-2.70	120.81	124.92
1	A	189	KCX	OQ1-CX-NZ	-2.67	120.86	124.92
1	C	189	KCX	CE-NZ-CX	-2.55	117.66	121.98
1	G	189	KCX	OQ1-CX-NZ	-2.31	121.42	124.92

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	189	KCX	C-CA-CB-CG
1	G	189	KCX	C-CA-CB-CG
1	H	189	KCX	C-CA-CB-CG
1	H	189	KCX	O-C-CA-CB
1	F	189	KCX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	189	KCX	1	0
1	C	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	446	2	18,20,20	1.00	1 (5%)	23,31,31	1.16	2 (8%)
3	CAP	F	446	2	18,20,20	1.05	1 (5%)	23,31,31	1.07	1 (4%)
3	CAP	I	446	2	18,20,20	0.92	0	23,31,31	1.24	2 (8%)
3	CAP	D	446	2	18,20,20	0.91	0	23,31,31	1.25	2 (8%)
3	CAP	H	446	2	18,20,20	0.97	0	23,31,31	1.45	4 (17%)
3	CAP	C	446	2	18,20,20	1.01	1 (5%)	23,31,31	1.50	3 (13%)
3	CAP	G	446	2	18,20,20	1.01	1 (5%)	23,31,31	1.27	2 (8%)
3	CAP	J	446	4	18,20,20	0.98	1 (5%)	23,31,31	1.01	2 (8%)
3	CAP	B	446	2	18,20,20	1.02	1 (5%)	23,31,31	1.28	3 (13%)
3	CAP	E	446	4	18,20,20	0.92	1 (5%)	23,31,31	1.13	2 (8%)

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	446	2	-	15/29/29/29	-
3	CAP	F	446	2	-	15/29/29/29	-
3	CAP	I	446	2	-	11/29/29/29	-
3	CAP	D	446	2	-	9/29/29/29	-
3	CAP	H	446	2	-	6/29/29/29	-
3	CAP	C	446	2	-	6/29/29/29	-
3	CAP	G	446	2	-	6/29/29/29	-
3	CAP	J	446	4	-	0/29/29/29	-
3	CAP	B	446	2	-	3/29/29/29	-
3	CAP	E	446	4	-	0/29/29/29	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	446	CAP	C2-C	-2.33	1.51	1.53
3	B	446	CAP	C4-C3	-2.29	1.51	1.54
3	C	446	CAP	C4-C3	-2.25	1.51	1.54
3	G	446	CAP	C4-C3	-2.17	1.51	1.54
3	J	446	CAP	C2-C	-2.13	1.51	1.53
3	F	446	CAP	C4-C3	-2.08	1.52	1.54
3	A	446	CAP	C4-C3	-2.02	1.52	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	446	CAP	O7-C-C2	4.19	121.08	114.06
3	H	446	CAP	O7-C-C2	4.13	120.98	114.06
3	B	446	CAP	O7-C-C2	3.60	120.10	114.06
3	D	446	CAP	O7-C-C2	3.48	119.88	114.06
3	I	446	CAP	O7-C-C2	3.41	119.78	114.06
3	G	446	CAP	O7-C-C2	3.40	119.75	114.06
3	A	446	CAP	O7-C-C2	3.31	119.60	114.06
3	F	446	CAP	O7-C-C2	3.18	119.38	114.06
3	C	446	CAP	C2-C3-C4	-2.96	108.13	114.03
3	H	446	CAP	C2-C3-C4	-2.91	108.23	114.03
3	E	446	CAP	O7-C-C2	2.89	118.89	114.06
3	I	446	CAP	O6P-P2-O5	2.88	114.17	106.67
3	J	446	CAP	C2-C3-C4	-2.63	108.78	114.03
3	A	446	CAP	O6P-P2-O5	2.61	113.47	106.67
3	E	446	CAP	C2-C3-C4	-2.60	108.84	114.03
3	D	446	CAP	O6P-P2-O5	2.51	113.20	106.67
3	H	446	CAP	O6-C-C2	-2.37	117.91	122.32
3	C	446	CAP	O1-P1-O1P	2.25	112.51	106.44
3	G	446	CAP	O6P-P2-O5	2.14	112.25	106.67
3	B	446	CAP	O1-P1-O1P	2.14	112.22	106.44
3	B	446	CAP	O6P-P2-O5	2.03	111.96	106.67
3	H	446	CAP	O1-P1-O1P	2.01	111.88	106.44
3	J	446	CAP	O7-C-C2	2.01	117.42	114.06

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	446	CAP	O1-C1-C2-C3
3	A	446	CAP	O1-C1-C2-C
3	A	446	CAP	O1-C1-C2-O2
3	A	446	CAP	O3-C3-C4-O4
3	A	446	CAP	C1-O1-P1-O2P
3	A	446	CAP	C1-O1-P1-O3P
3	B	446	CAP	O4-C4-C5-O5
3	C	446	CAP	O1-C1-C2-C
3	C	446	CAP	O1-C1-C2-O2
3	C	446	CAP	O2-C2-C3-C4
3	C	446	CAP	C2-C3-C4-O4
3	C	446	CAP	O3-C3-C4-O4
3	D	446	CAP	O6-C-C2-C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	446	CAP	O7-C-C2-C1
3	D	446	CAP	O6-C-C2-O2
3	D	446	CAP	O7-C-C2-O2
3	D	446	CAP	C2-C3-C4-O4
3	D	446	CAP	O3-C3-C4-O4
3	D	446	CAP	O4-C4-C5-O5
3	F	446	CAP	O1-C1-C2-C3
3	F	446	CAP	O1-C1-C2-C
3	F	446	CAP	O1-C1-C2-O2
3	F	446	CAP	O6-C-C2-C1
3	F	446	CAP	O6-C-C2-C3
3	F	446	CAP	O6-C-C2-O2
3	F	446	CAP	O7-C-C2-O2
3	F	446	CAP	C2-C3-C4-O4
3	F	446	CAP	O3-C3-C4-O4
3	F	446	CAP	C1-O1-P1-O1P
3	F	446	CAP	C1-O1-P1-O2P
3	F	446	CAP	C1-O1-P1-O3P
3	G	446	CAP	O1-C1-C2-O2
3	H	446	CAP	O1-C1-C2-C
3	H	446	CAP	O1-C1-C2-O2
3	H	446	CAP	O2-C2-C3-C4
3	H	446	CAP	O3-C3-C4-O4
3	I	446	CAP	O6-C-C2-C1
3	I	446	CAP	O7-C-C2-C1
3	I	446	CAP	O6-C-C2-C3
3	I	446	CAP	O6-C-C2-O2
3	I	446	CAP	O7-C-C2-O2
3	I	446	CAP	C2-C3-C4-O4
3	I	446	CAP	O3-C3-C4-O4
3	I	446	CAP	O4-C4-C5-O5
3	A	446	CAP	O6-C-C2-C1
3	F	446	CAP	O7-C-C2-C1
3	A	446	CAP	C1-O1-P1-O1P
3	H	446	CAP	O4-C4-C5-O5
3	A	446	CAP	O6-C-C2-O2
3	A	446	CAP	O6-C-C2-C3
3	A	446	CAP	O7-C-C2-C1
3	G	446	CAP	O6-C-C2-C1
3	G	446	CAP	O7-C-C2-C1
3	I	446	CAP	C3-C4-C5-O5
3	B	446	CAP	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

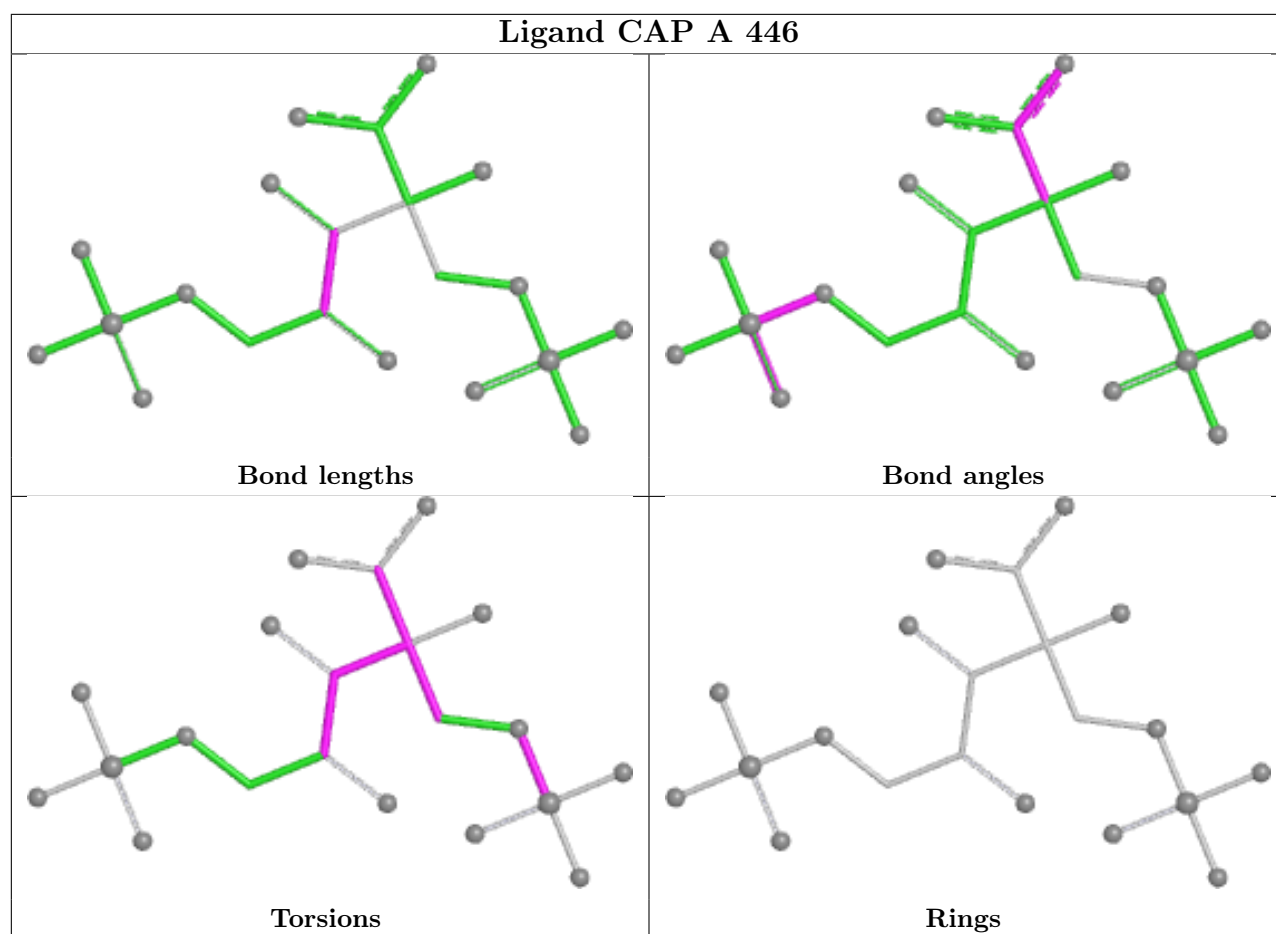
Mol	Chain	Res	Type	Atoms
3	A	446	CAP	O2-C2-C3-C4
3	B	446	CAP	O2-C2-C3-C4
3	D	446	CAP	O2-C2-C3-C4
3	F	446	CAP	O2-C2-C3-C4
3	G	446	CAP	O2-C2-C3-C4
3	H	446	CAP	C2-C3-C4-O4
3	I	446	CAP	O2-C2-C3-C4
3	C	446	CAP	C5-O5-P2-O4P
3	A	446	CAP	O7-C-C2-C3
3	F	446	CAP	O7-C-C2-C3
3	G	446	CAP	O7-C-C2-C3
3	I	446	CAP	O7-C-C2-C3
3	D	446	CAP	C3-C4-C5-O5
3	A	446	CAP	O7-C-C2-O2
3	A	446	CAP	C2-C3-C4-O4
3	G	446	CAP	O6-C-C2-C3

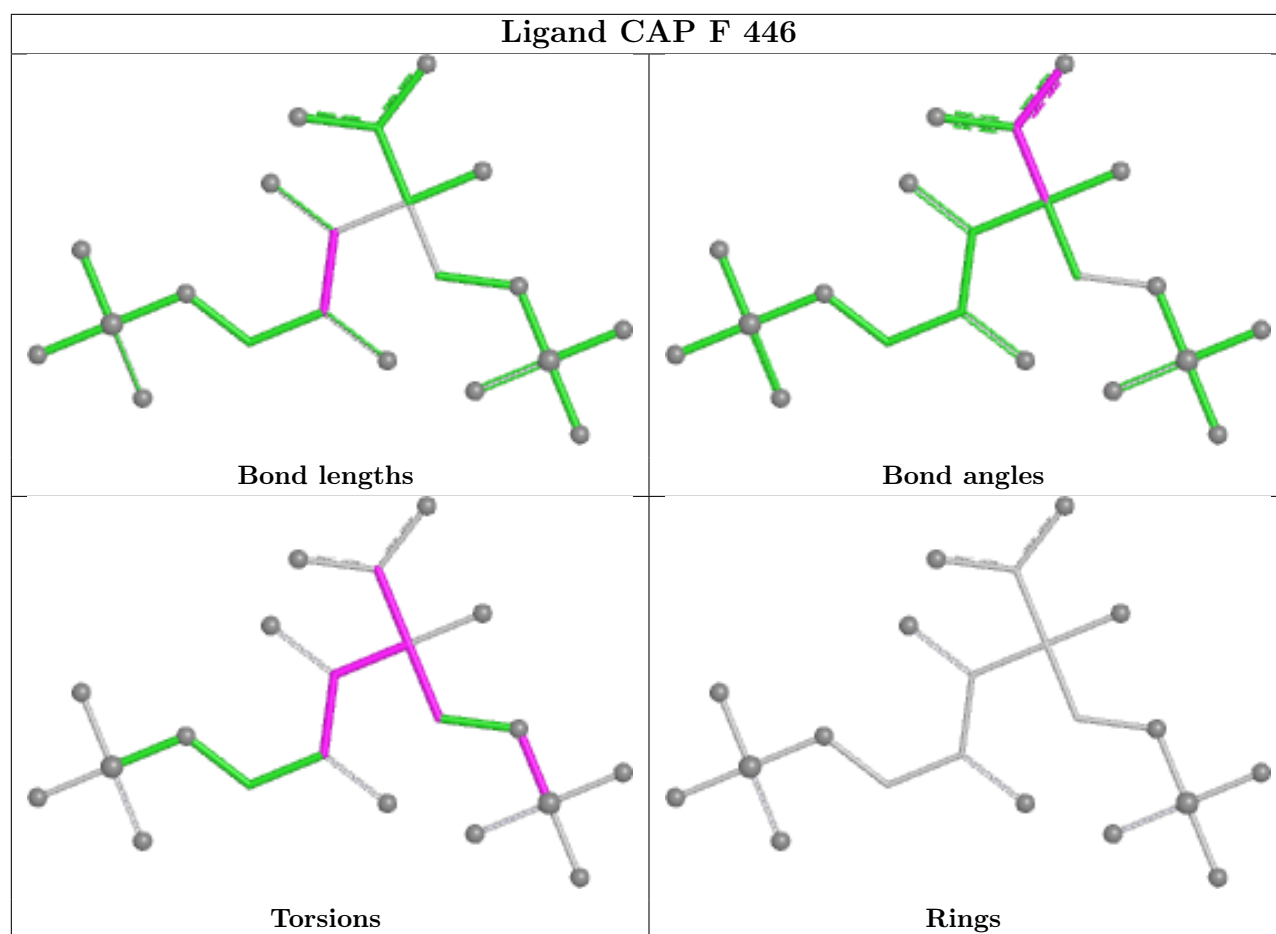
There are no ring outliers.

8 monomers are involved in 12 short contacts:

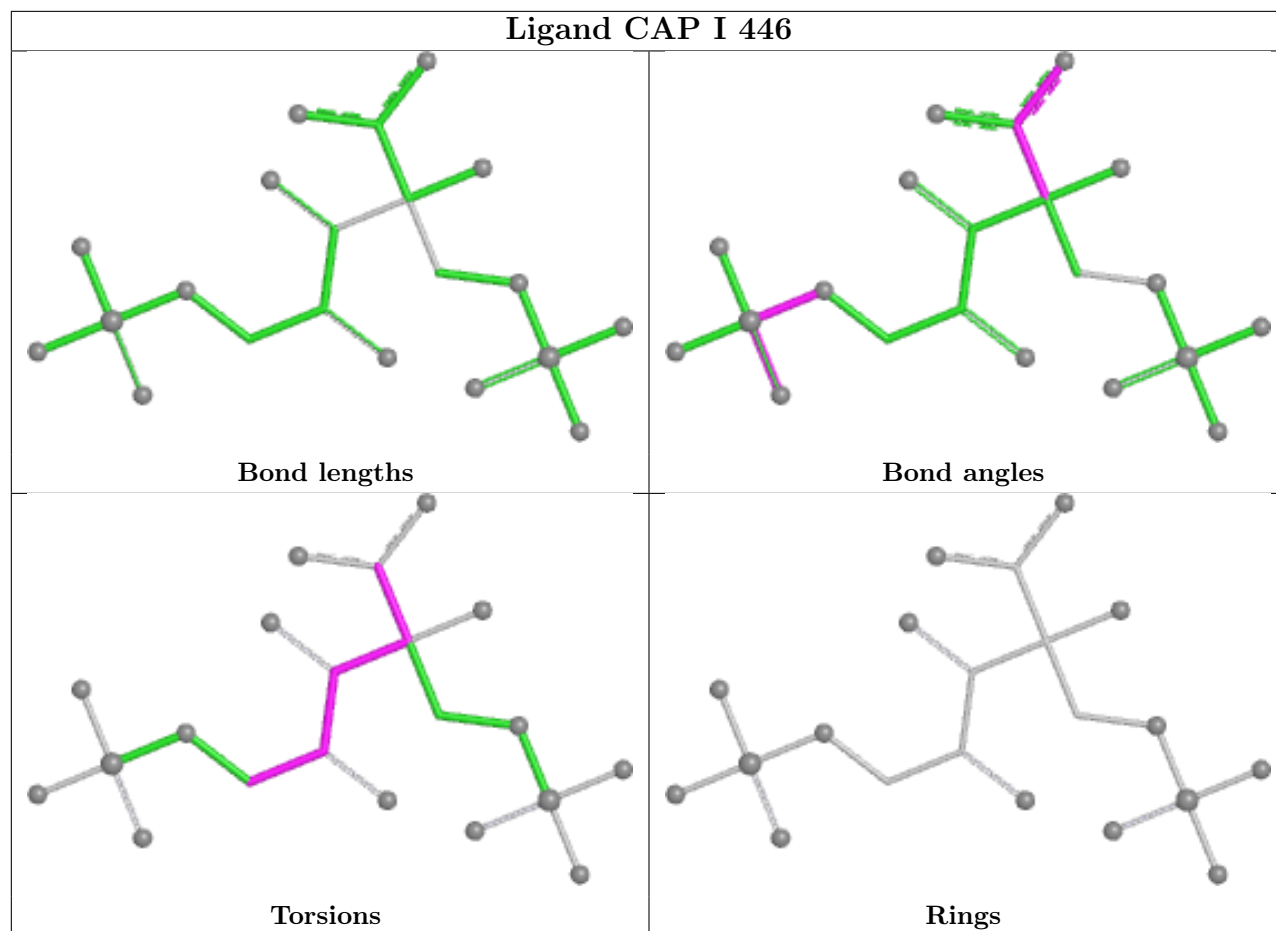
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	446	CAP	1	0
3	F	446	CAP	2	0
3	H	446	CAP	2	0
3	C	446	CAP	3	0
3	G	446	CAP	1	0
3	J	446	CAP	1	0
3	B	446	CAP	1	0
3	E	446	CAP	1	0

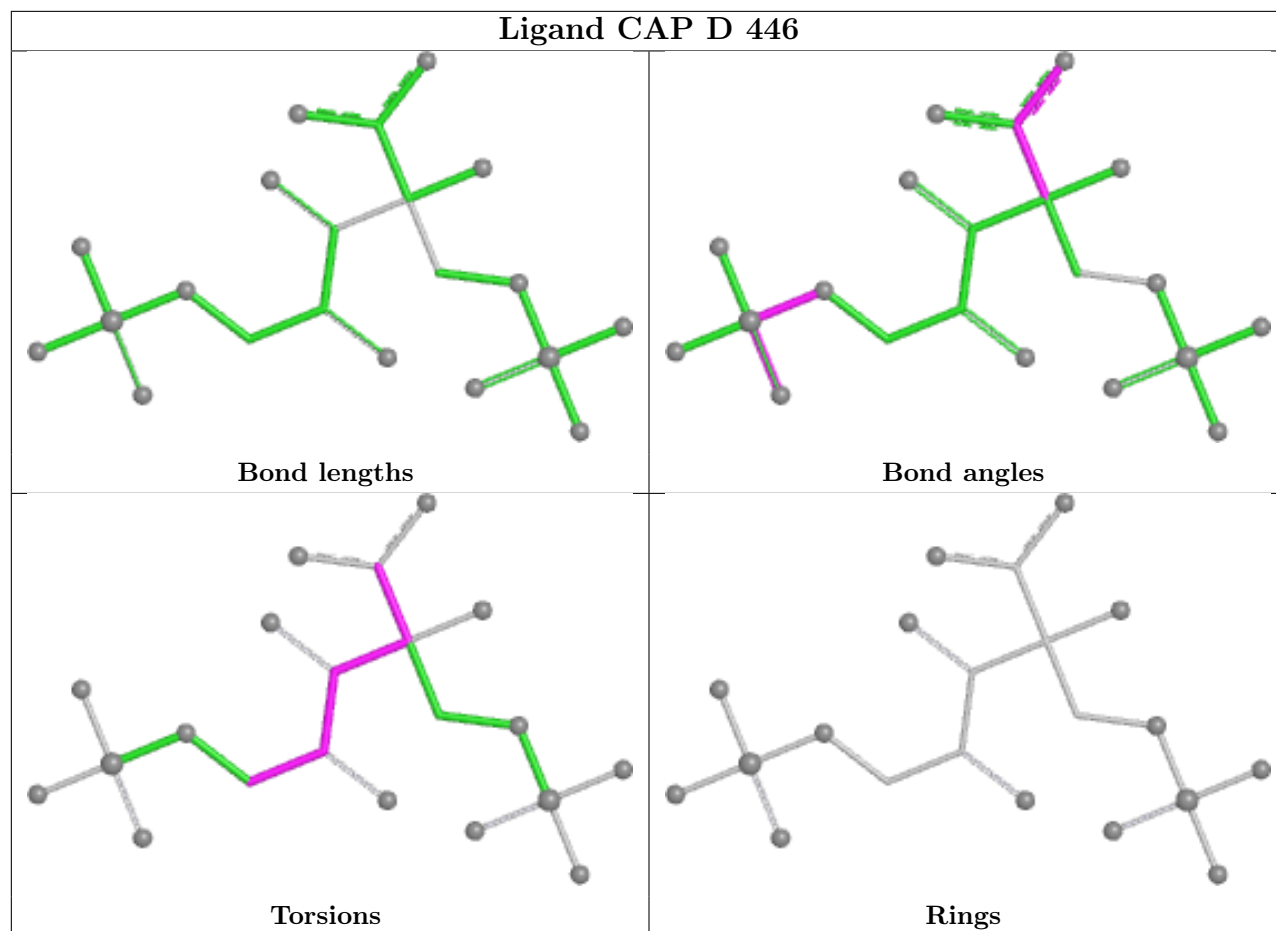
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

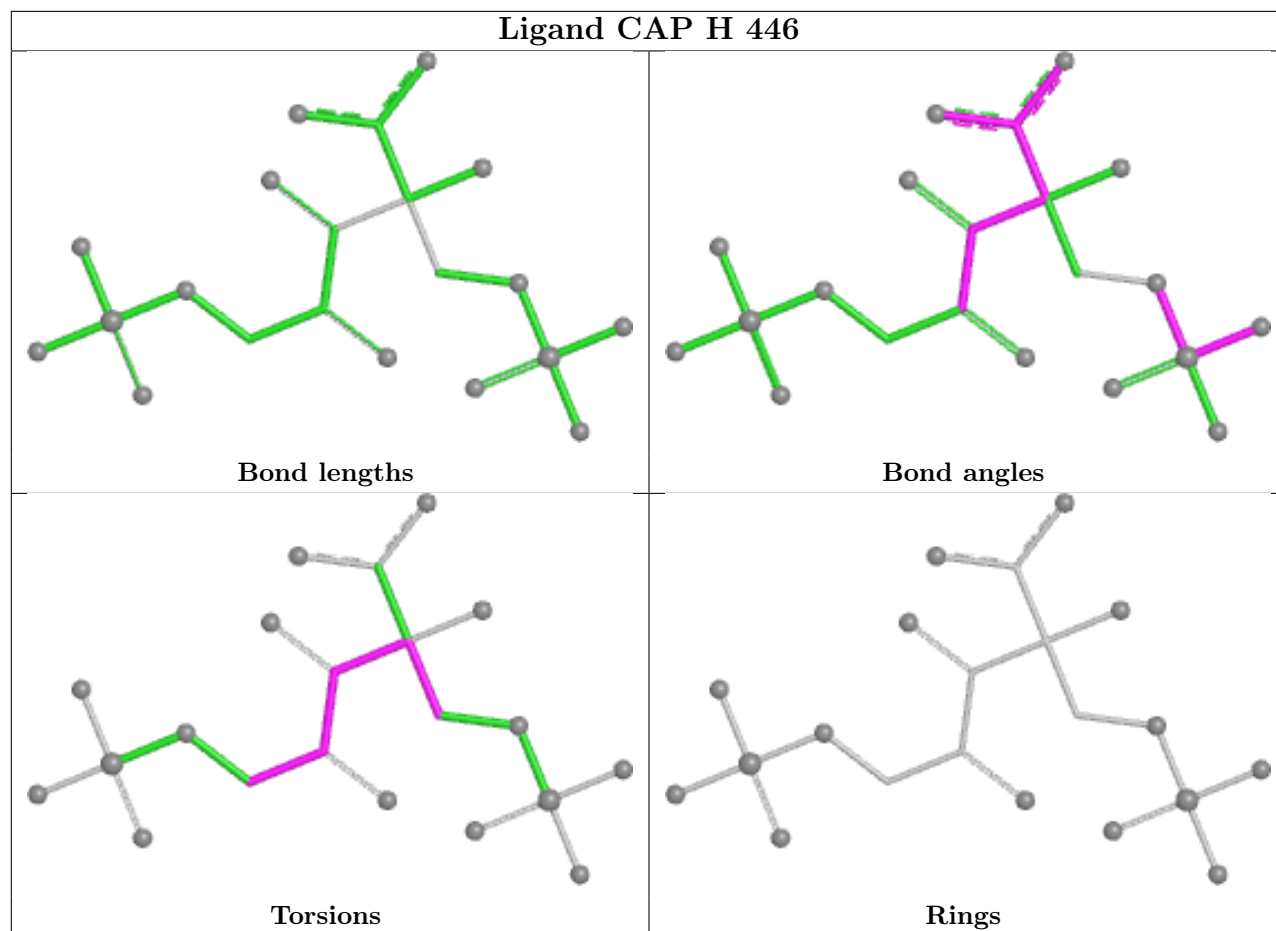


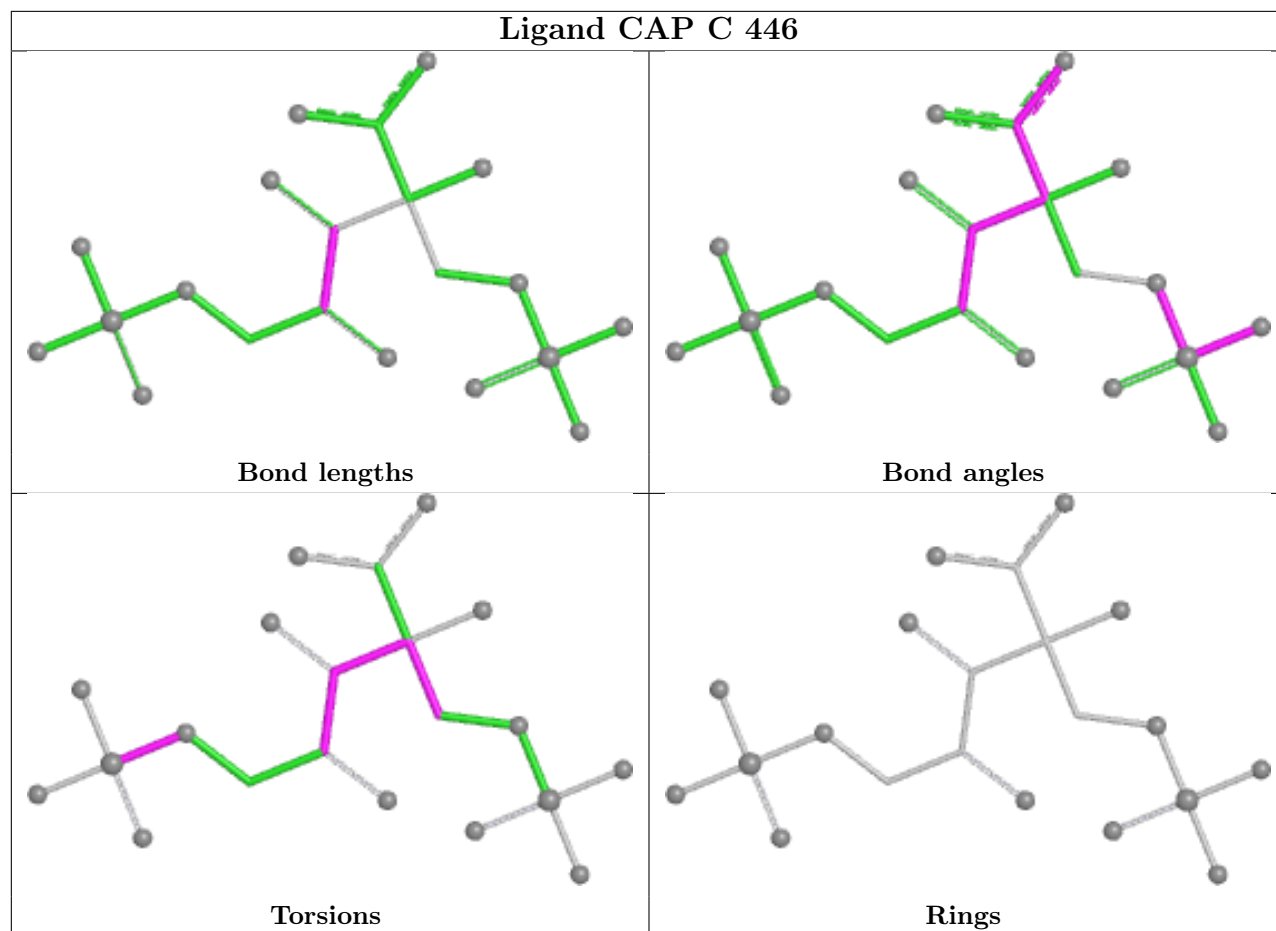


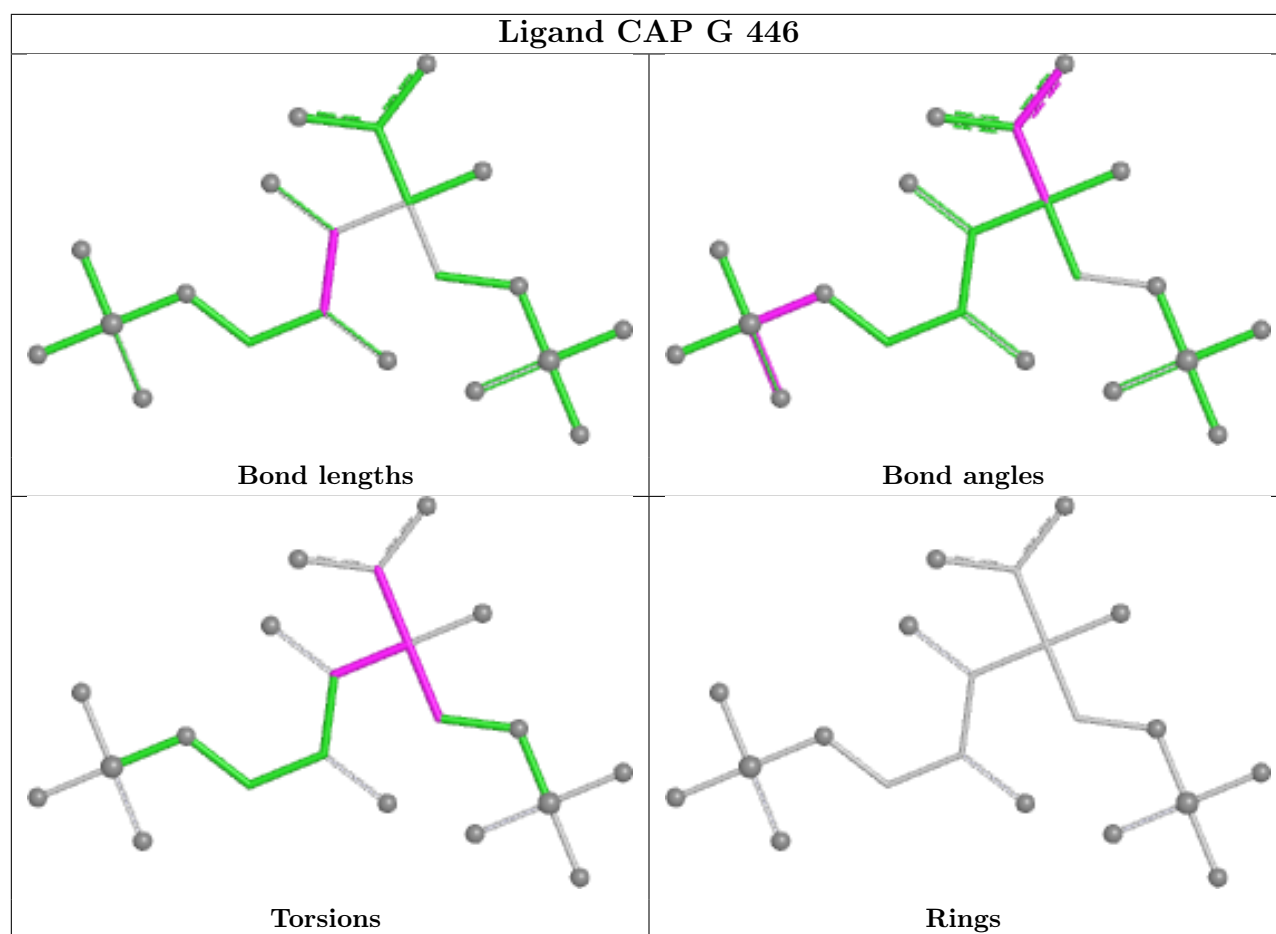
Ligand CAP I 446



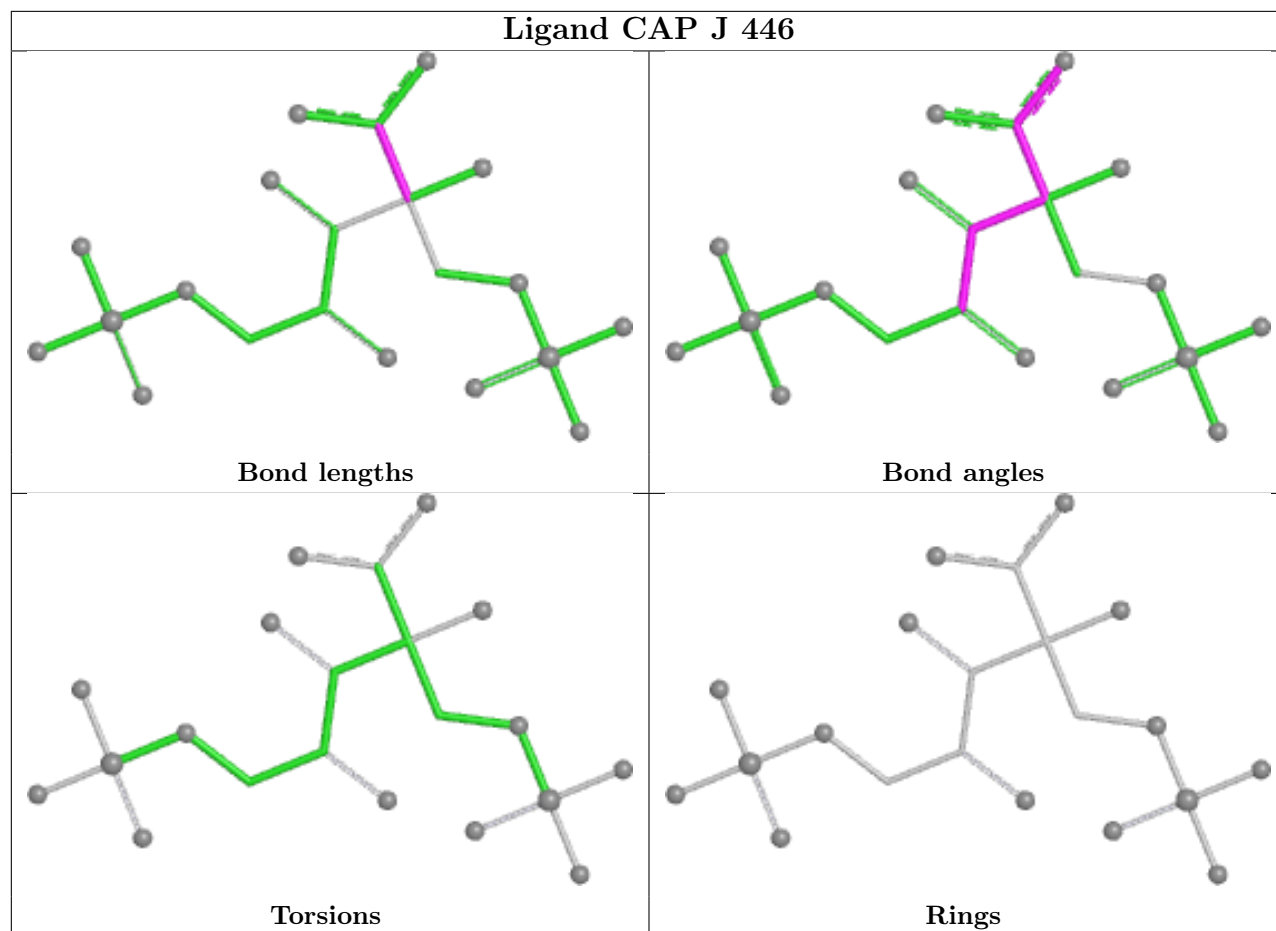


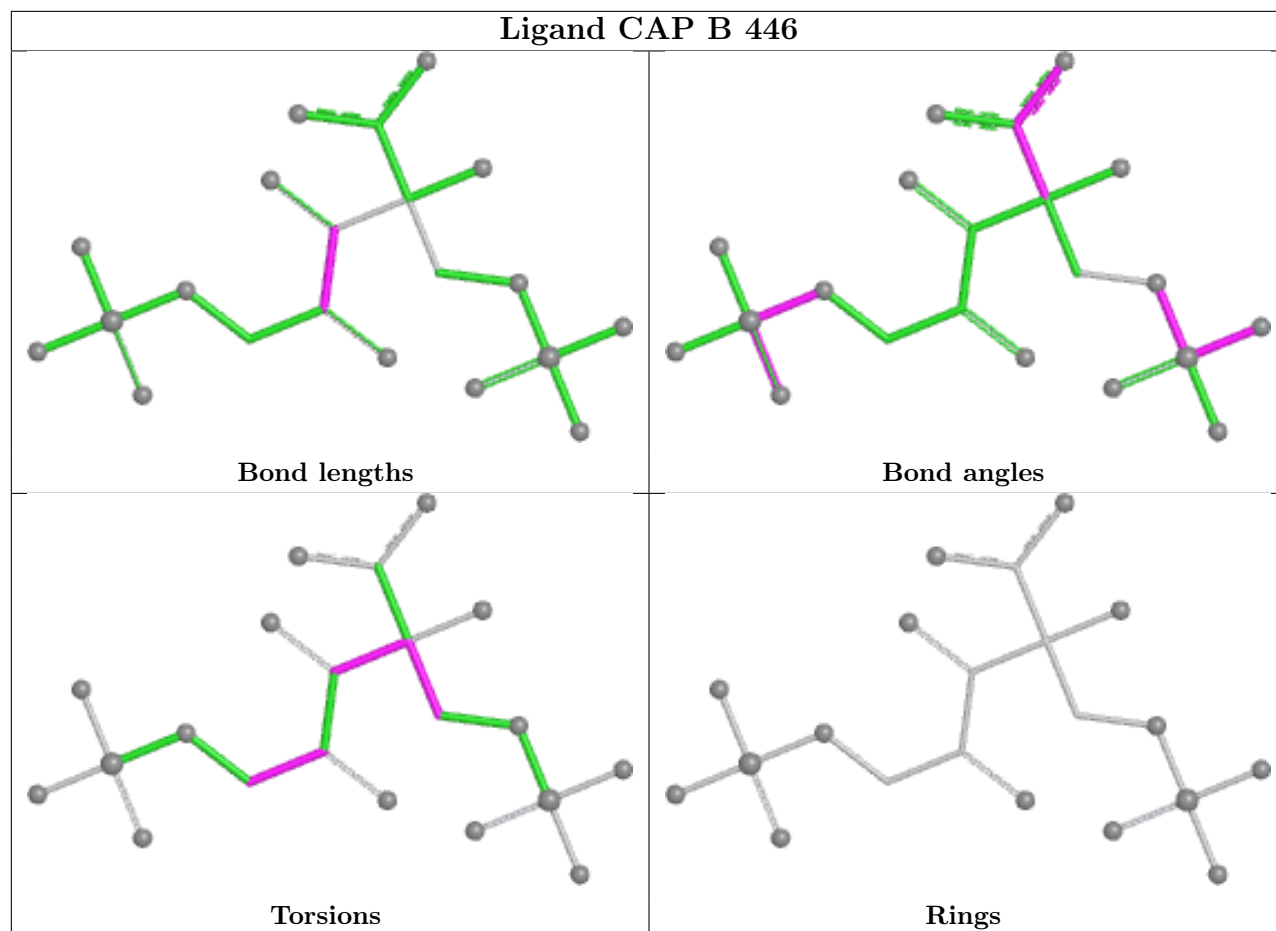


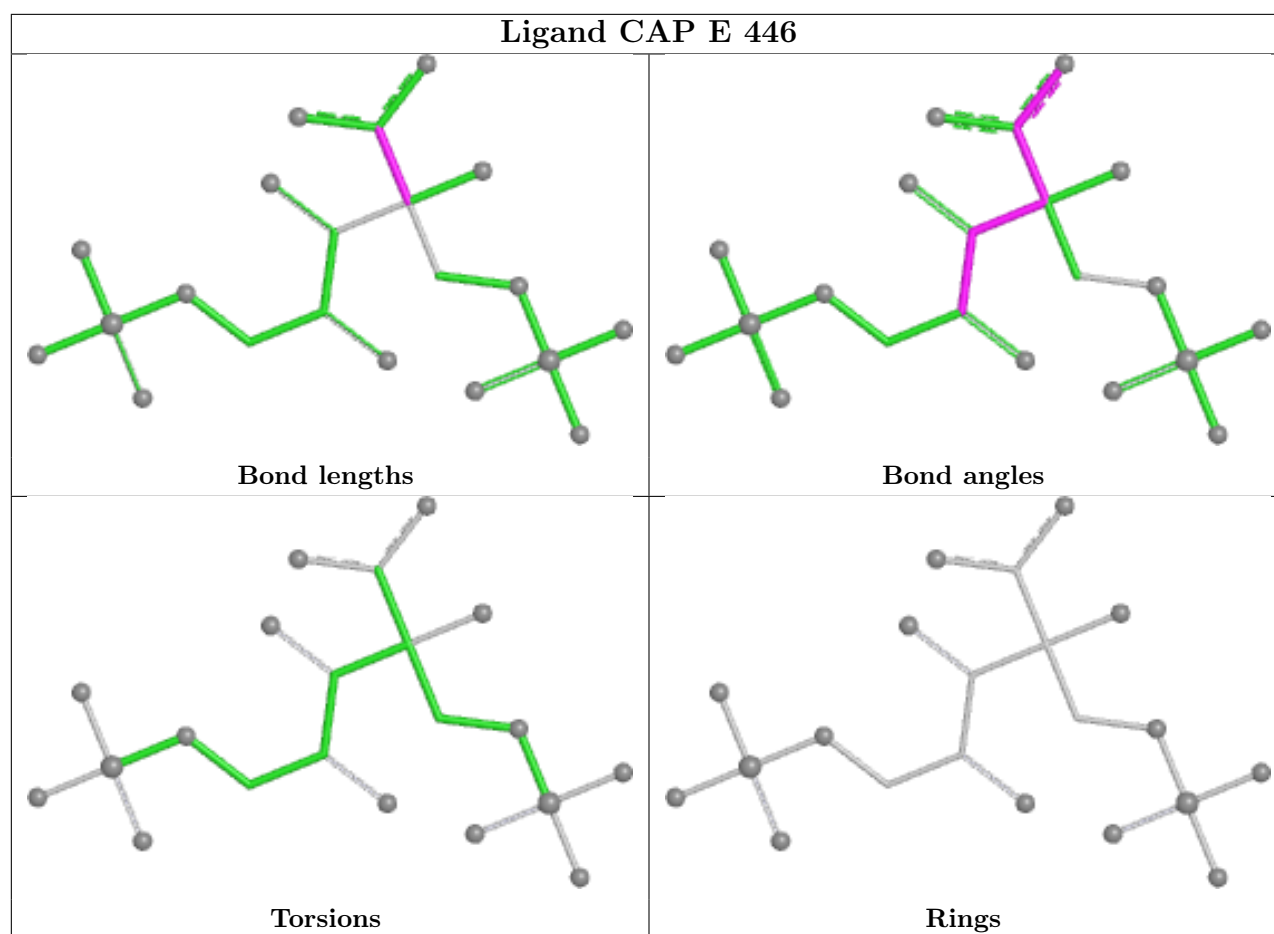




Ligand CAP J 446







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	435/444 (97%)	0.14	19 (4%)	39 45	17, 28, 49, 58	0
1	B	436/444 (98%)	0.23	42 (9%)	13 16	14, 26, 56, 62	0
1	C	436/444 (98%)	0.24	48 (11%)	10 12	16, 27, 60, 66	0
1	D	436/444 (98%)	0.31	56 (12%)	7 9	15, 26, 58, 85	0
1	E	431/444 (97%)	0.07	19 (4%)	39 45	15, 25, 53, 70	0
1	F	436/444 (98%)	0.39	41 (9%)	14 17	17, 30, 57, 64	0
1	G	436/444 (98%)	0.21	38 (8%)	16 19	13, 25, 52, 58	0
1	H	437/444 (98%)	0.27	43 (9%)	13 16	16, 28, 58, 61	0
1	I	436/444 (98%)	0.09	30 (6%)	23 27	13, 24, 52, 70	0
1	J	433/444 (97%)	0.16	33 (7%)	20 24	14, 25, 57, 74	0
All	All	4352/4440 (98%)	0.21	369 (8%)	16 20	13, 27, 56, 85	0

All (369) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	57	THR	8.0
1	G	434	ALA	7.5
1	J	444	VAL	7.3
1	D	421	LEU	6.7
1	E	444	VAL	6.4
1	I	57	THR	6.1
1	E	439	GLY	6.1
1	J	439	GLY	6.0
1	D	425	ALA	5.9
1	D	55	TRP	5.6
1	I	55	TRP	5.5
1	D	411	ALA	5.5
1	D	424	TYR	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	320	ALA	5.2
1	B	8	ILE	5.0
1	C	421	LEU	5.0
1	C	438	TRP	5.0
1	G	8	ILE	5.0
1	D	414	ALA	5.0
1	E	441	VAL	4.9
1	I	56	THR	4.9
1	C	422	ASP	4.9
1	E	442	THR	4.8
1	C	434	ALA	4.7
1	B	59	TYR	4.7
1	F	54	THR	4.6
1	J	442	THR	4.6
1	J	324	GLU	4.6
1	F	9	TYR	4.4
1	F	8	ILE	4.3
1	H	434	ALA	4.3
1	H	441	VAL	4.3
1	D	431	LEU	4.3
1	G	321	GLY	4.2
1	D	56	THR	4.2
1	C	418	GLY	4.2
1	B	54	THR	4.2
1	C	441	VAL	4.1
1	G	59	TYR	4.1
1	C	431	LEU	4.0
1	E	438	TRP	4.0
1	D	415	ILE	4.0
1	G	438	TRP	4.0
1	F	391	GLY	4.0
1	F	59	TYR	4.0
1	H	59	TYR	3.9
1	C	321	GLY	3.9
1	J	59	TYR	3.9
1	B	421	LEU	3.9
1	H	419	ILE	3.9
1	H	320	ALA	3.9
1	G	395	LEU	3.8
1	J	425	ALA	3.8
1	C	419	ILE	3.8
1	H	426	LYS	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	421	LEU	3.8
1	B	438	TRP	3.8
1	F	57	THR	3.8
1	D	9	TYR	3.7
1	H	424	TYR	3.7
1	H	321	GLY	3.6
1	G	441	VAL	3.6
1	H	318	ALA	3.6
1	G	426	LYS	3.6
1	I	5	PHE	3.6
1	B	431	LEU	3.6
1	J	441	VAL	3.6
1	B	434	ALA	3.5
1	C	424	TYR	3.5
1	I	9	TYR	3.5
1	H	422	ASP	3.5
1	E	59	TYR	3.5
1	C	435	LEU	3.5
1	B	358	SER	3.5
1	J	438	TRP	3.5
1	D	418	GLY	3.5
1	H	431	LEU	3.5
1	H	411	ALA	3.4
1	H	438	TRP	3.4
1	B	424	TYR	3.4
1	F	421	LEU	3.4
1	A	56	THR	3.4
1	C	427	THR	3.4
1	F	407	ALA	3.4
1	J	421	LEU	3.4
1	E	322	LYS	3.4
1	H	420	PRO	3.4
1	C	375	ILE	3.4
1	H	421	LEU	3.4
1	F	398	PRO	3.4
1	H	435	LEU	3.3
1	J	427	THR	3.3
1	A	368	GLY	3.3
1	D	419	ILE	3.3
1	E	443	PRO	3.3
1	B	425	ALA	3.3
1	J	321	GLY	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	53	GLY	3.2
1	C	442	THR	3.2
1	A	9	TYR	3.2
1	G	411	ALA	3.2
1	C	392	GLY	3.2
1	F	184	GLY	3.2
1	D	6	ASP	3.2
1	C	426	LYS	3.2
1	H	443	PRO	3.2
1	B	427	THR	3.2
1	H	425	ALA	3.2
1	C	377	PRO	3.2
1	J	58	LEU	3.2
1	B	414	ALA	3.1
1	C	368	GLY	3.1
1	H	427	THR	3.1
1	H	368	GLY	3.1
1	H	414	ALA	3.1
1	I	432	ALA	3.1
1	G	424	TYR	3.1
1	H	398	PRO	3.1
1	I	431	LEU	3.1
1	C	417	GLN	3.1
1	C	432	ALA	3.1
1	G	435	LEU	3.1
1	B	426	LYS	3.1
1	H	429	LYS	3.1
1	I	424	TYR	3.1
1	H	7	THR	3.1
1	D	432	ALA	3.1
1	A	59	TYR	3.0
1	E	425	ALA	3.0
1	A	57	THR	3.0
1	D	426	LYS	3.0
1	H	439	GLY	3.0
1	C	8	ILE	3.0
1	D	427	THR	3.0
1	J	322	LYS	3.0
1	D	321	GLY	3.0
1	I	6	ASP	3.0
1	C	411	ALA	3.0
1	D	375	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	433	ARG	3.0
1	I	427	THR	3.0
1	D	439	GLY	3.0
1	F	368	GLY	3.0
1	F	55	TRP	3.0
1	G	443	PRO	3.0
1	E	58	LEU	2.9
1	C	439	GLY	2.9
1	D	416	MET	2.9
1	E	324	GLU	2.9
1	F	369	GLY	2.9
1	D	5	PHE	2.9
1	I	425	ALA	2.9
1	J	411	ALA	2.9
1	G	54	THR	2.9
1	C	372	PRO	2.9
1	H	377	PRO	2.9
1	I	421	LEU	2.9
1	I	435	LEU	2.9
1	D	376	GLN	2.9
1	B	415	ILE	2.9
1	A	54	THR	2.9
1	B	398	PRO	2.9
1	C	414	ALA	2.9
1	F	58	LEU	2.9
1	J	378	VAL	2.9
1	G	325	GLY	2.8
1	A	58	LEU	2.8
1	H	412	ILE	2.8
1	I	415	ILE	2.8
1	C	429	LYS	2.8
1	B	319	GLY	2.8
1	A	398	PRO	2.8
1	G	9	TYR	2.8
1	H	444	VAL	2.8
1	B	419	ILE	2.8
1	D	60	PRO	2.8
1	C	7	THR	2.8
1	F	415	ILE	2.8
1	J	440	HIS	2.8
1	D	413	ASP	2.8
1	B	9	TYR	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	323	LEU	2.8
1	C	318	ALA	2.8
1	F	432	ALA	2.8
1	H	417	GLN	2.7
1	A	55	TRP	2.7
1	C	320	ALA	2.7
1	C	425	ALA	2.7
1	G	414	ALA	2.7
1	C	420	PRO	2.7
1	C	443	PRO	2.7
1	B	411	ALA	2.7
1	F	425	ALA	2.7
1	F	427	THR	2.7
1	G	422	ASP	2.7
1	B	429	LYS	2.7
1	D	429	LYS	2.7
1	D	428	HIS	2.7
1	D	374	ASN	2.7
1	D	441	VAL	2.7
1	F	444	VAL	2.7
1	C	440	HIS	2.6
1	I	411	ALA	2.6
1	C	326	GLU	2.6
1	D	154	ASP	2.6
1	B	420	PRO	2.6
1	B	435	LEU	2.6
1	D	395	LEU	2.6
1	I	395	LEU	2.6
1	D	422	ASP	2.6
1	C	376	GLN	2.6
1	C	373	GLY	2.6
1	I	396	GLY	2.6
1	J	443	PRO	2.6
1	D	412	ILE	2.6
1	D	410	GLN	2.6
1	D	434	ALA	2.6
1	D	398	PRO	2.6
1	J	8	ILE	2.6
1	I	426	LYS	2.6
1	J	429	LYS	2.6
1	G	417	GLN	2.5
1	C	433	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	432	ALA	2.5
1	F	56	THR	2.5
1	E	440	HIS	2.5
1	F	412	ILE	2.5
1	H	415	ILE	2.5
1	B	58	LEU	2.5
1	G	53	GLY	2.5
1	F	419	ILE	2.5
1	I	423	GLU	2.5
1	F	395	LEU	2.5
1	A	425	ALA	2.5
1	D	405	ALA	2.5
1	C	371	HIS	2.5
1	F	53	GLY	2.5
1	H	442	THR	2.5
1	D	379	ILE	2.5
1	F	408	VAL	2.5
1	C	428	HIS	2.5
1	A	391	GLY	2.5
1	D	409	ARG	2.4
1	G	65	GLU	2.4
1	G	442	THR	2.4
1	G	431	LEU	2.4
1	A	434	ALA	2.4
1	B	392	GLY	2.4
1	G	373	GLY	2.4
1	H	8	ILE	2.4
1	A	438	TRP	2.4
1	C	416	MET	2.4
1	B	376	GLN	2.4
1	G	433	ARG	2.4
1	H	410	GLN	2.4
1	J	413	ASP	2.4
1	A	429	LYS	2.4
1	C	415	ILE	2.4
1	B	417	GLN	2.4
1	C	59	TYR	2.4
1	F	433	ARG	2.4
1	B	222	GLU	2.4
1	E	328	ASP	2.4
1	B	439	GLY	2.4
1	F	414	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	57	THR	2.4
1	G	358	SER	2.4
1	G	415	ILE	2.4
1	J	419	ILE	2.4
1	C	395	LEU	2.4
1	F	218	ASN	2.3
1	F	424	TYR	2.3
1	A	53	GLY	2.3
1	B	321	GLY	2.3
1	F	429	LYS	2.3
1	I	373	GLY	2.3
1	E	434	ALA	2.3
1	E	419	ILE	2.3
1	J	415	ILE	2.3
1	D	371	HIS	2.3
1	E	323	LEU	2.3
1	E	423	GLU	2.3
1	I	404	GLY	2.3
1	H	428	HIS	2.3
1	G	396	GLY	2.3
1	B	432	ALA	2.3
1	H	432	ALA	2.3
1	D	430	GLU	2.3
1	J	53	GLY	2.3
1	D	326	GLU	2.3
1	J	412	ILE	2.3
1	E	421	LEU	2.2
1	F	422	ASP	2.2
1	I	60	PRO	2.2
1	C	409	ARG	2.2
1	D	404	GLY	2.2
1	H	373	GLY	2.2
1	E	427	THR	2.2
1	J	376	GLN	2.2
1	G	58	LEU	2.2
1	J	435	LEU	2.2
1	J	328	ASP	2.2
1	D	377	PRO	2.2
1	A	396	GLY	2.2
1	D	184	GLY	2.2
1	D	396	GLY	2.2
1	B	436	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	318	ALA	2.2
1	G	57	THR	2.2
1	F	431	LEU	2.2
1	B	433	ARG	2.2
1	H	416	MET	2.2
1	D	373	GLY	2.2
1	D	397	HIS	2.2
1	H	376	GLN	2.2
1	D	438	TRP	2.2
1	D	435	LEU	2.2
1	F	435	LEU	2.2
1	I	412	ILE	2.2
1	B	374	ASN	2.2
1	I	398	PRO	2.2
1	J	423	GLU	2.2
1	G	368	GLY	2.2
1	G	418	GLY	2.2
1	C	412	ILE	2.1
1	F	10	ASP	2.1
1	F	401	PRO	2.1
1	G	56	THR	2.1
1	A	421	LEU	2.1
1	C	115	MET	2.1
1	J	424	TYR	2.1
1	G	375	ILE	2.1
1	B	422	ASP	2.1
1	H	374	ASN	2.1
1	F	438	TRP	2.1
1	B	396	GLY	2.1
1	D	369	GLY	2.1
1	F	321	GLY	2.1
1	I	369	GLY	2.1
1	D	384	THR	2.1
1	F	318	ALA	2.1
1	B	412	ILE	2.1
1	I	377	PRO	2.1
1	I	429	LYS	2.1
1	J	35	GLU	2.1
1	H	397	HIS	2.1
1	C	378	VAL	2.1
1	D	408	VAL	2.1
1	B	418	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	392	GLY	2.1
1	C	437	LYS	2.0
1	B	56	THR	2.0
1	G	371	HIS	2.0
1	A	431	LEU	2.0
1	B	328	ASP	2.0
1	F	323	LEU	2.0
1	F	375	ILE	2.0
1	G	419	ILE	2.0
1	H	375	ILE	2.0
1	D	372	PRO	2.0
1	I	408	VAL	2.0
1	J	437	LYS	2.0
1	D	403	ALA	2.0
1	F	411	ALA	2.0
1	I	414	ALA	2.0
1	A	395	LEU	2.0
1	H	413	ASP	2.0
1	D	420	PRO	2.0
1	I	419	ILE	2.0

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

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	B	189	12/13	0.95	0.08	18,20,21,22	0
1	KCX	F	189	12/13	0.95	0.08	23,25,27,27	0
1	KCX	I	189	12/13	0.95	0.08	19,21,25,25	0
1	KCX	G	189	12/13	0.96	0.07	16,19,20,20	0
1	KCX	A	189	12/13	0.96	0.07	20,23,24,24	0
1	KCX	J	189	12/13	0.96	0.08	19,19,24,26	0
1	KCX	D	189	12/13	0.97	0.06	21,22,24,25	0
1	KCX	H	189	12/13	0.97	0.06	20,21,25,26	0
1	KCX	E	189	12/13	0.97	0.07	18,19,23,24	0
1	KCX	C	189	12/13	0.97	0.06	21,22,26,28	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

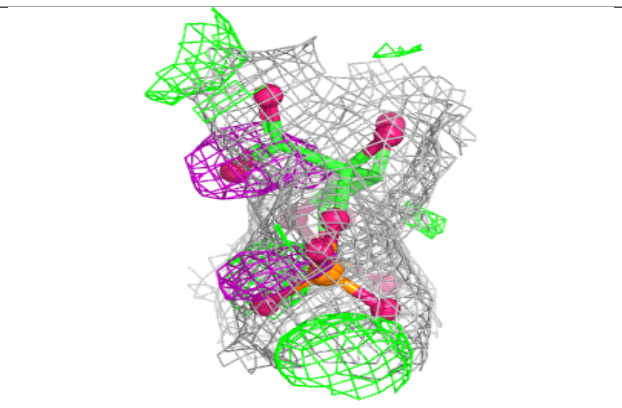
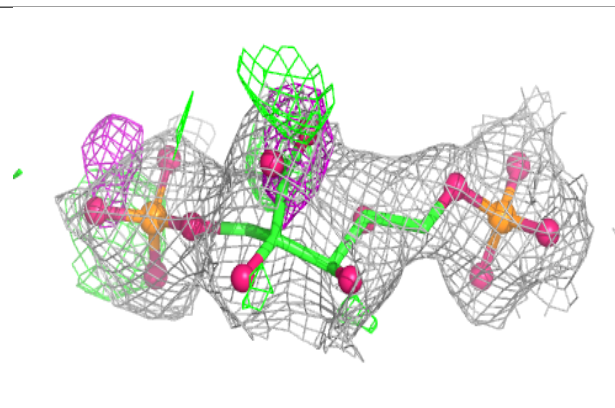
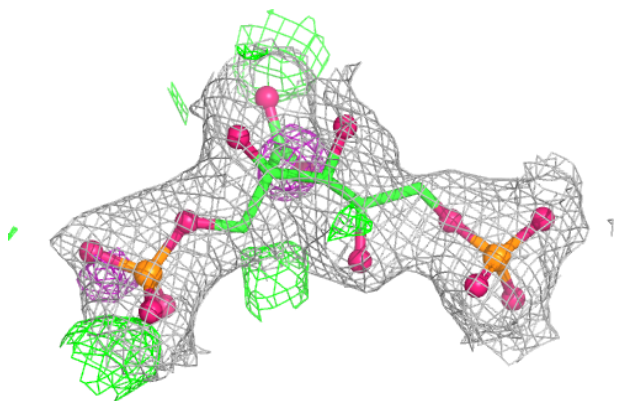
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CAP	C	446	21/21	0.91	0.11	23,34,37,39	0
3	CAP	H	446	21/21	0.93	0.10	24,35,37,39	0
3	CAP	D	446	21/21	0.94	0.09	18,28,31,32	0
3	CAP	F	446	21/21	0.94	0.09	24,33,34,35	0
3	CAP	G	446	21/21	0.94	0.10	16,29,33,34	0
3	CAP	B	446	21/21	0.94	0.09	18,29,35,36	0
3	CAP	J	446	21/21	0.94	0.10	20,28,40,40	0
3	CAP	I	446	21/21	0.95	0.08	15,25,27,28	0
3	CAP	E	446	21/21	0.95	0.09	16,27,37,38	0
2	MG	C	445	1/1	0.96	0.10	23,23,23,23	0
3	CAP	A	446	21/21	0.97	0.07	21,30,31,32	0
4	CA	J	445	1/1	0.97	0.05	27,27,27,27	0
2	MG	H	445	1/1	0.98	0.09	22,22,22,22	0
4	CA	E	445	1/1	0.98	0.03	27,27,27,27	0
2	MG	F	445	1/1	0.98	0.09	36,36,36,36	0
2	MG	G	445	1/1	0.99	0.05	22,22,22,22	0
2	MG	A	445	1/1	0.99	0.03	32,32,32,32	0
2	MG	I	445	1/1	0.99	0.02	21,21,21,21	0
2	MG	D	445	1/1	0.99	0.03	27,27,27,27	0
2	MG	B	445	1/1	0.99	0.05	19,19,19,19	0

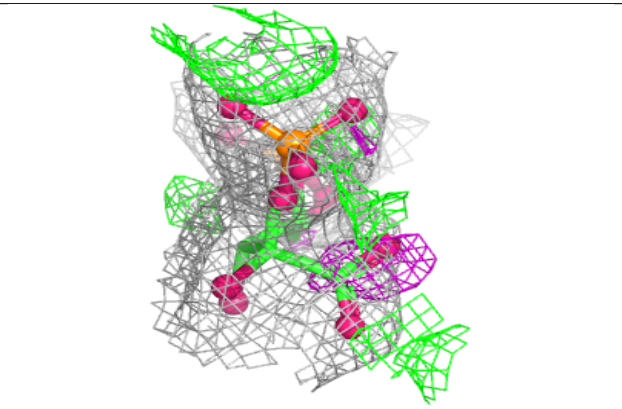
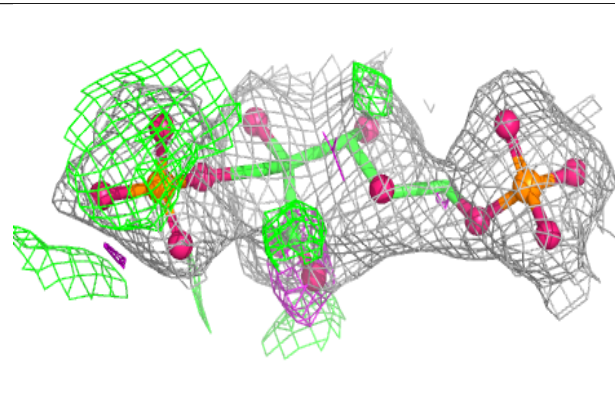
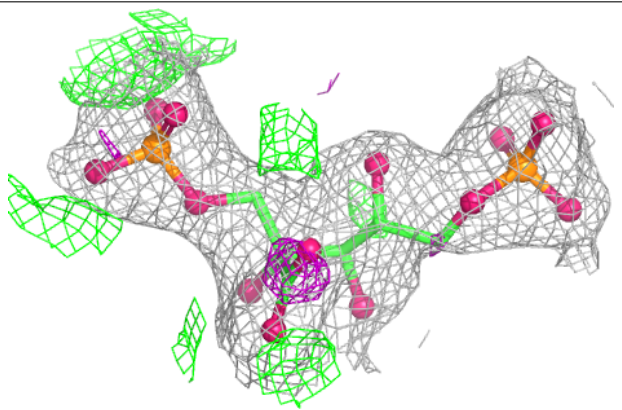
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CAP C 446:

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

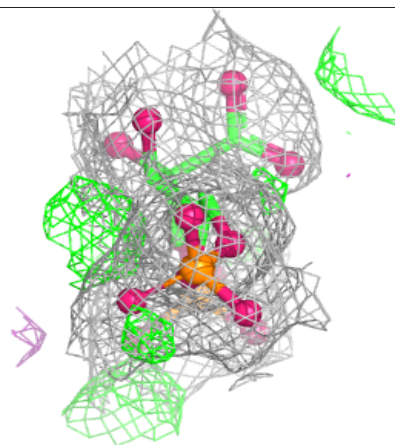
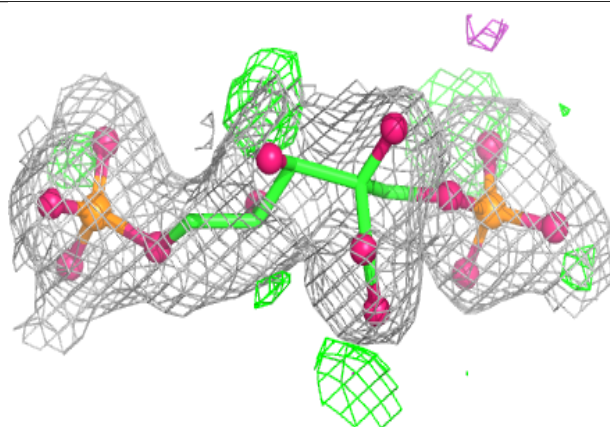
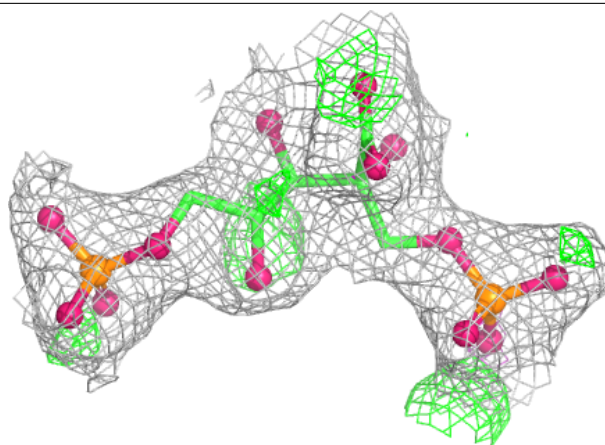
**Electron density around CAP H 446:**

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



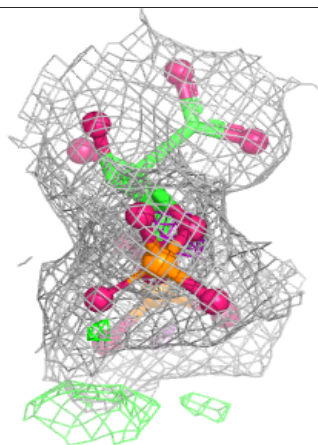
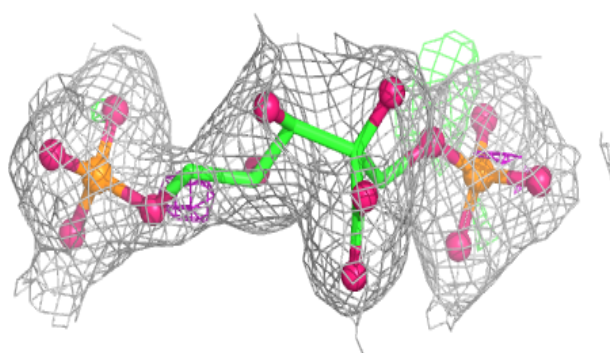
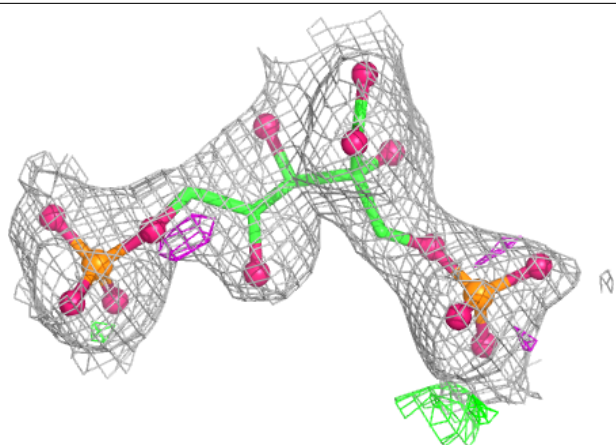
Electron density around CAP D 446:

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



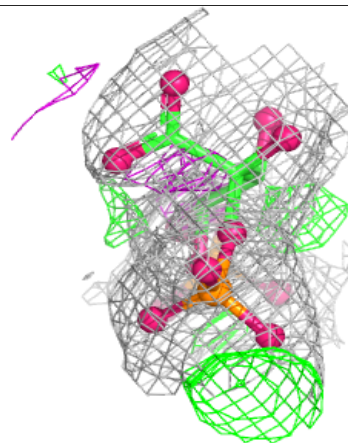
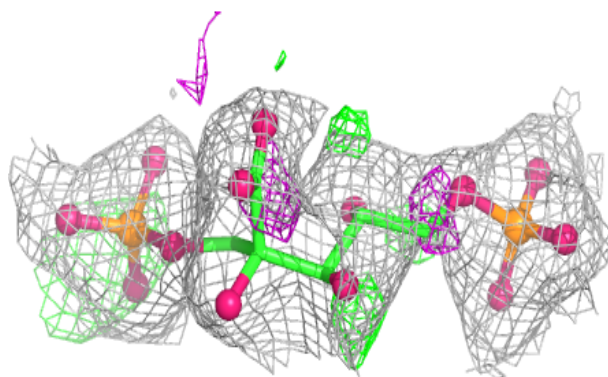
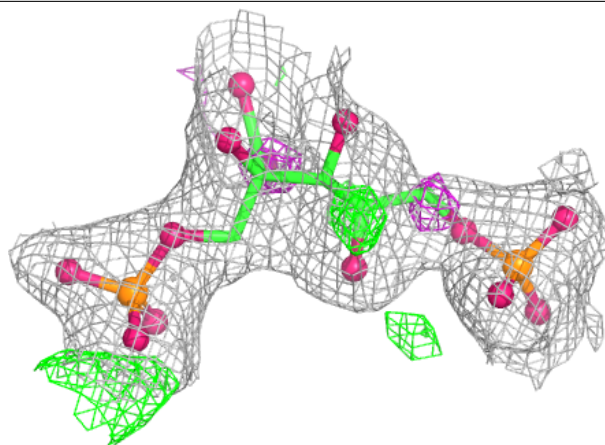
Electron density around CAP F 446:

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



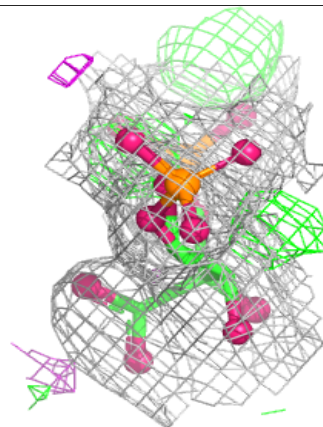
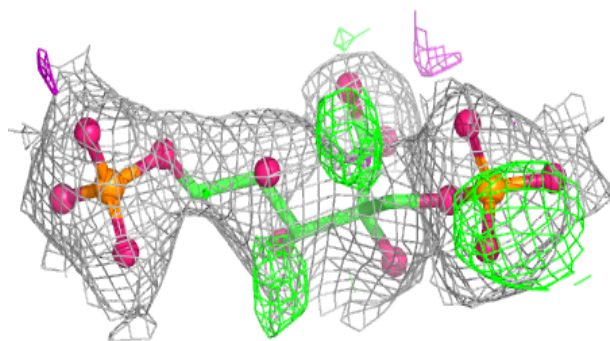
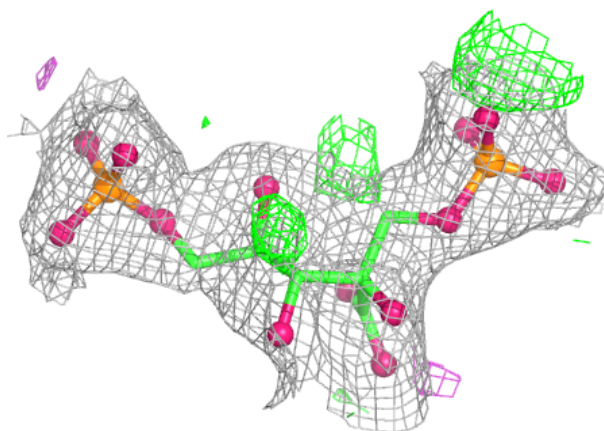
Electron density around CAP G 446:

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

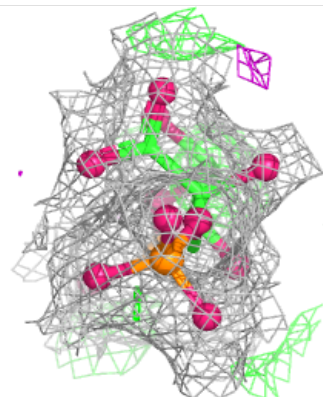
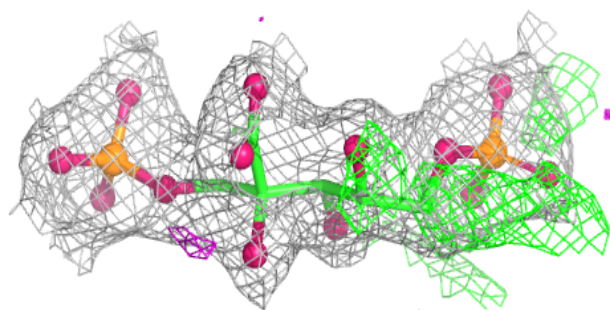
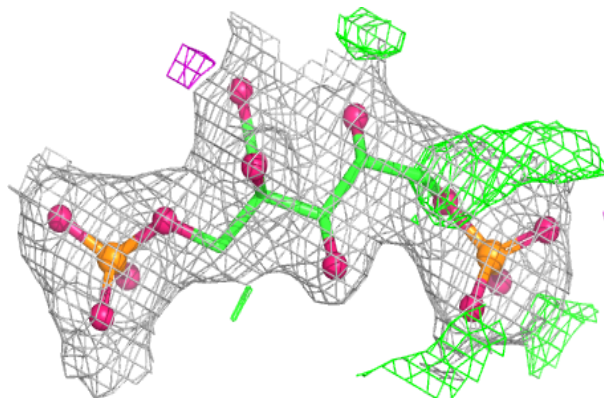


Electron density around CAP B 446:

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

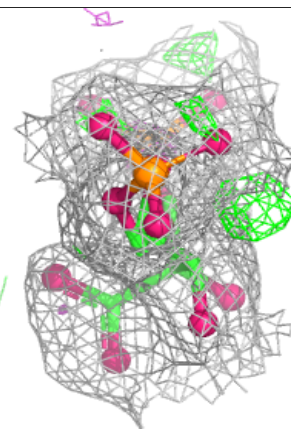
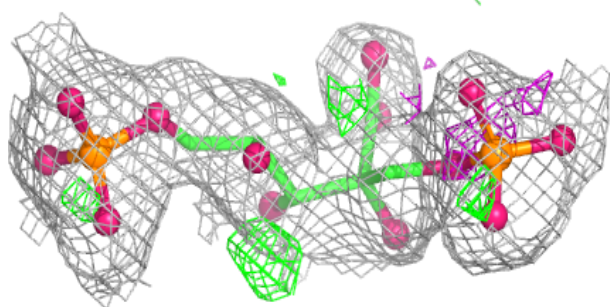
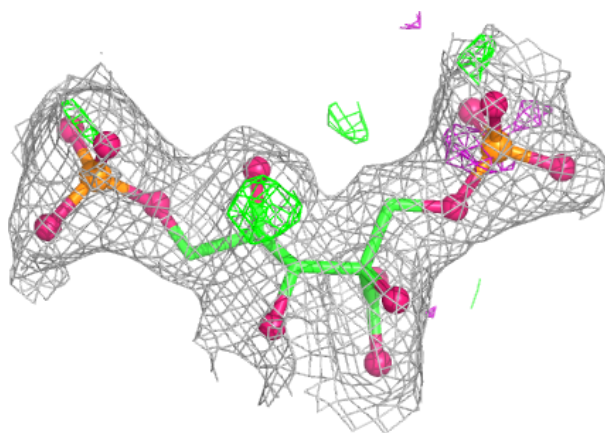
**Electron density around CAP J 446:**

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

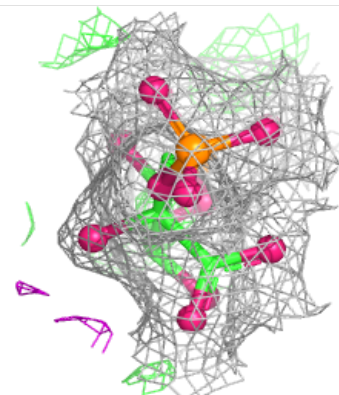
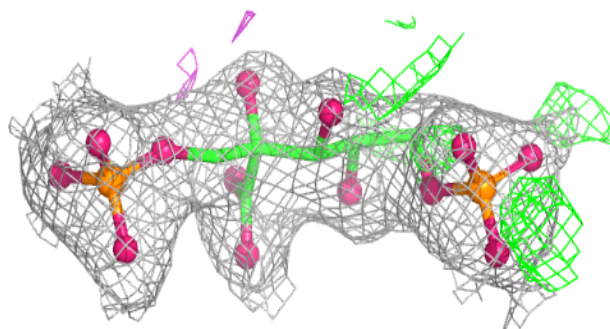
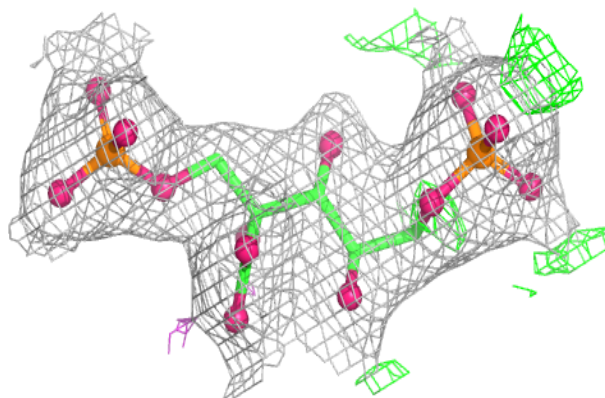


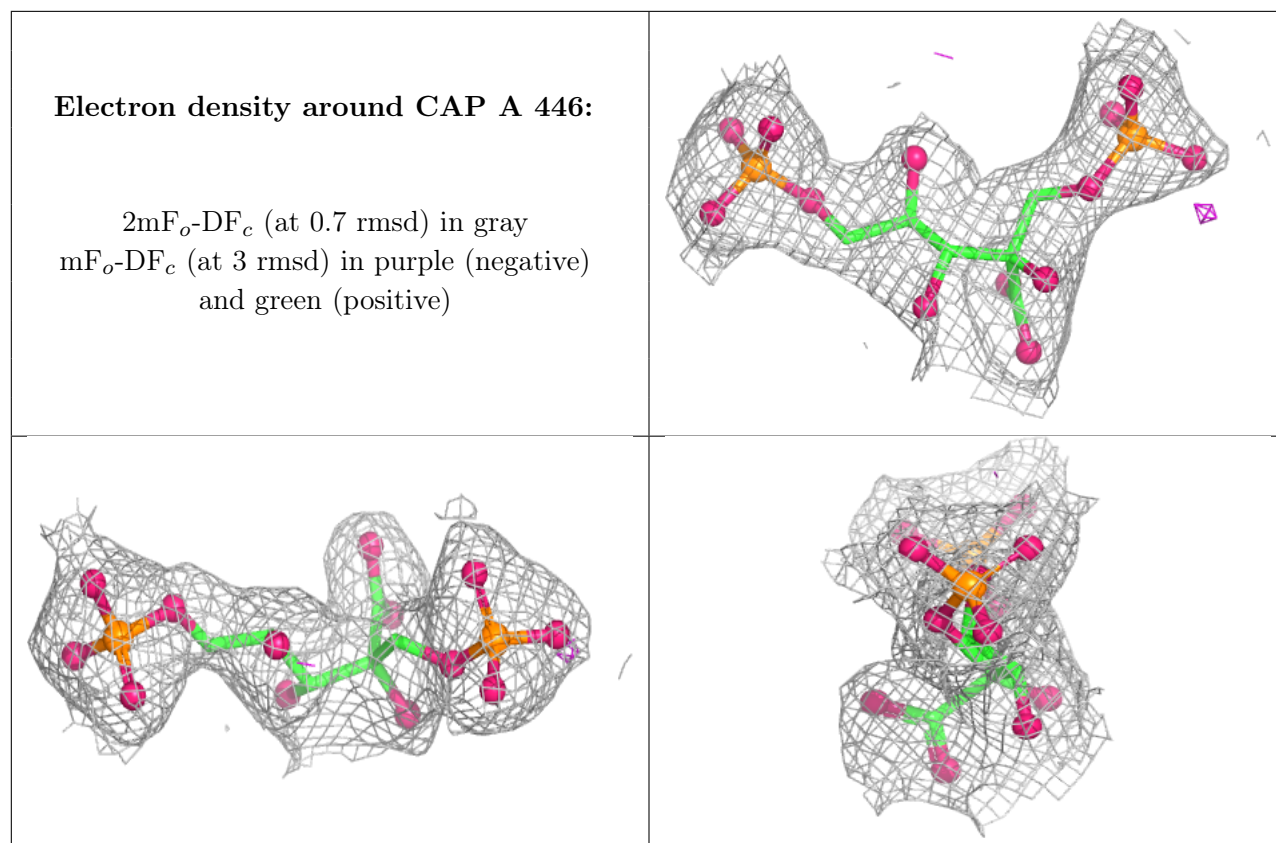
Electron density around CAP I 446:

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

**Electron density around CAP E 446:**

$2mF_o-DF_c$ (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.