Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2023 – 03:15 AM EDT

PDB ID	:	3A13
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:

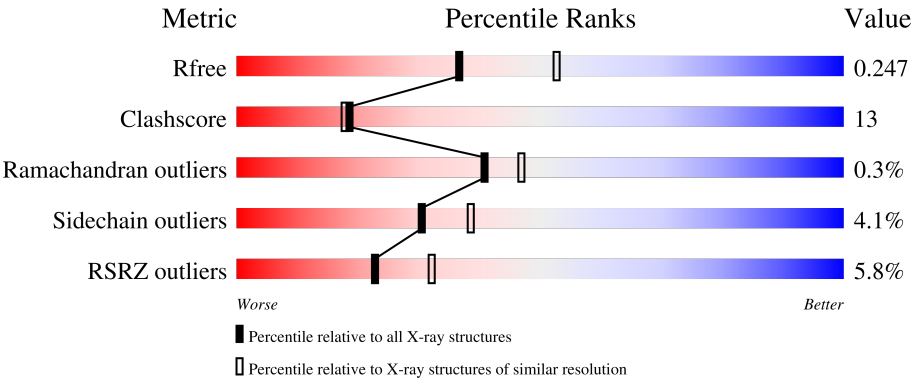
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (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 <=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% 74% 23%
1	B	444	6% 76% 20%
1	C	444	8% 76% 20%
1	D	444	7% 77% 20%

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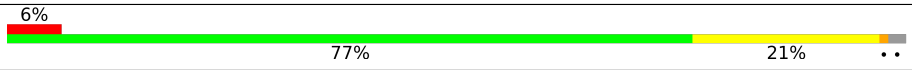
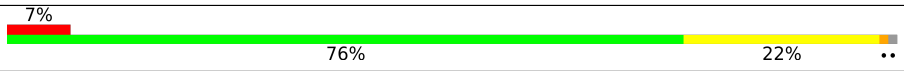
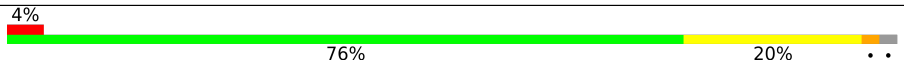
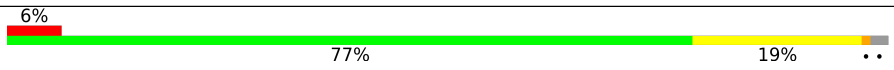
Mol	Chain	Length	Quality of chain
1	E	444	
1	F	444	
1	G	444	
1	H	444	
1	I	444	
1	J	444	

2 Entry composition (i)

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 bisphosphate 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

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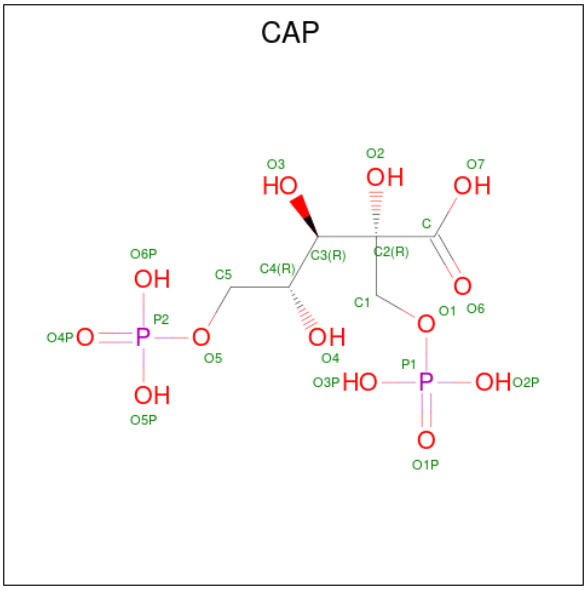
Chain	Residue	Modelled	Actual	Comment	Reference
B	330	THR	VAL	engineered mutation	UNP O93627
C	326	GLU	GLY	engineered mutation	UNP O93627
C	327	ARG	LYS	engineered mutation	UNP O93627
C	328	ASP	TRP	engineered mutation	UNP O93627
C	329	ILE	ASP	engineered mutation	UNP O93627
C	330	THR	VAL	engineered mutation	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 (three-letter code: 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 (three-letter code: 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

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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 (three-letter code: 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		

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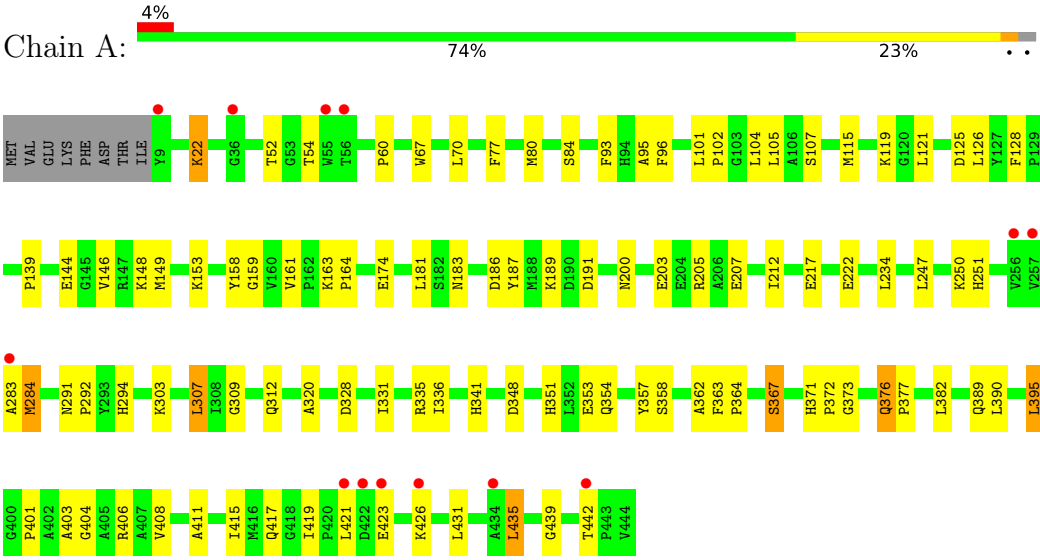
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	212	Total O 212 212	0	0
5	J	194	Total O 194 194	0	0

3 Residue-property plots (i)

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.

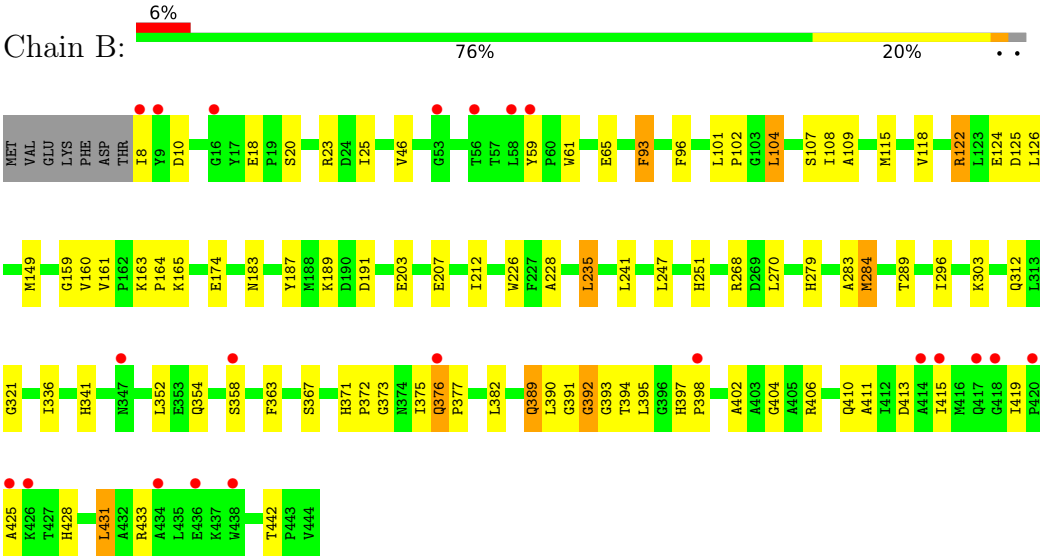
• Molecule 1: Ribulose bisphosphate carboxylase

Chain A:



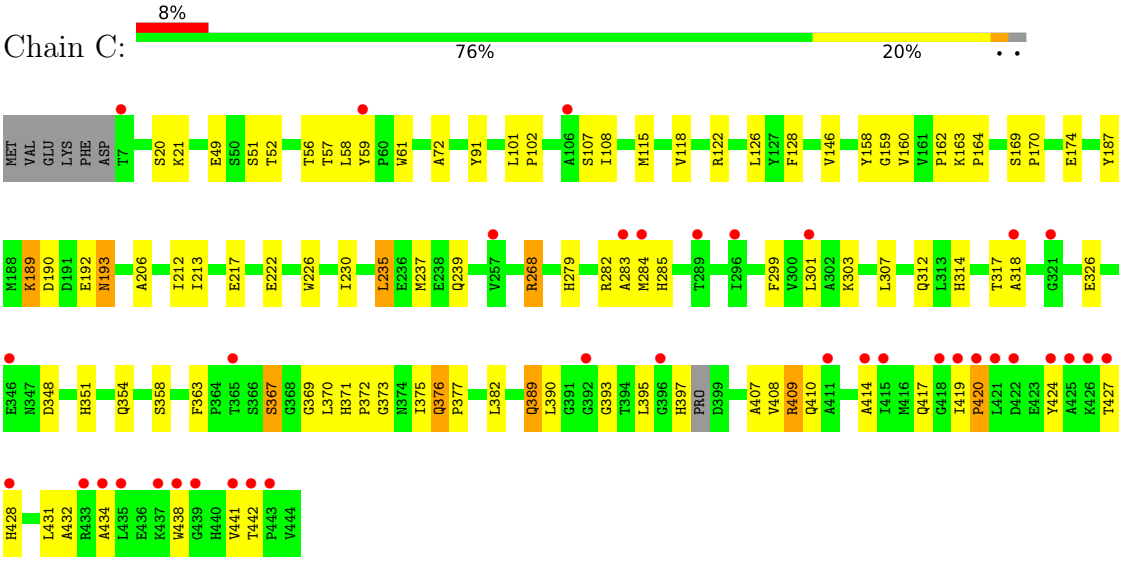
• Molecule 1: Ribulose bisphosphate carboxylase

Chain B:



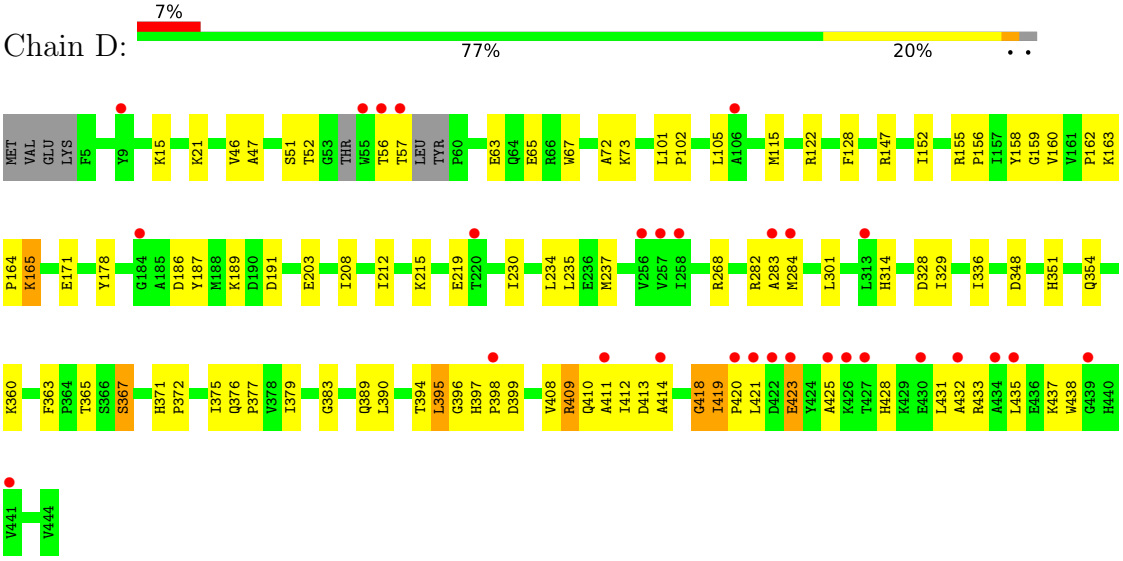
• Molecule 1: Ribulose bisphosphate carboxylase

Chain C:



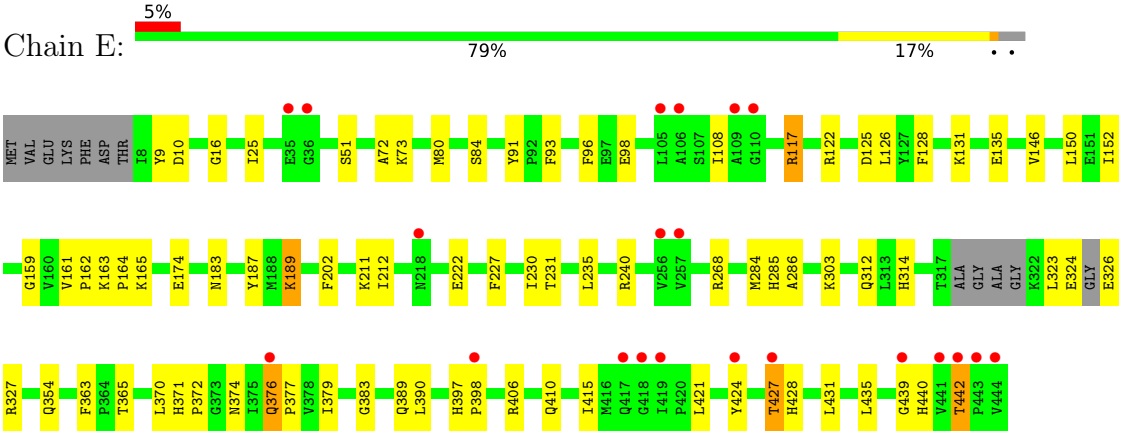
• Molecule 1: Ribulose bisphosphate carboxylase

Chain D:



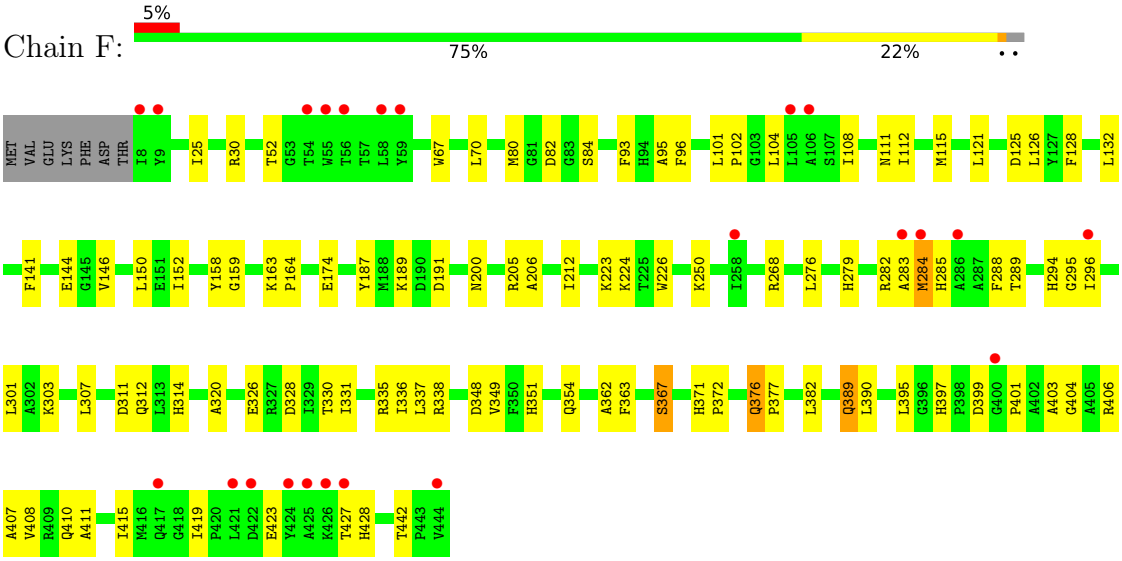
• Molecule 1: Ribulose bisphosphate carboxylase

Chain E:



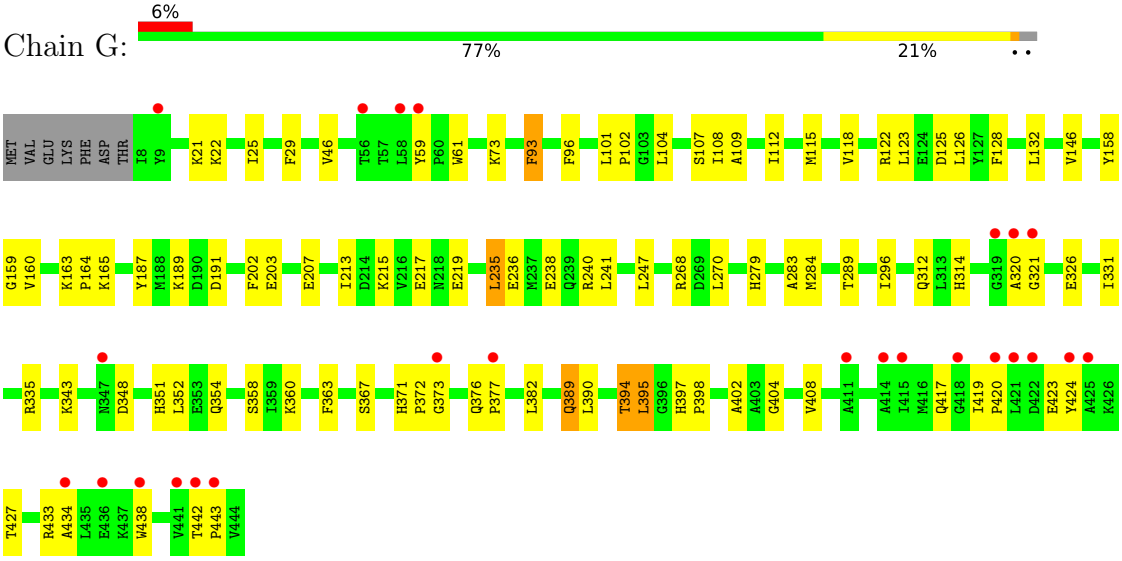
• Molecule 1: Ribulose bisphosphate carboxylase

Chain F:



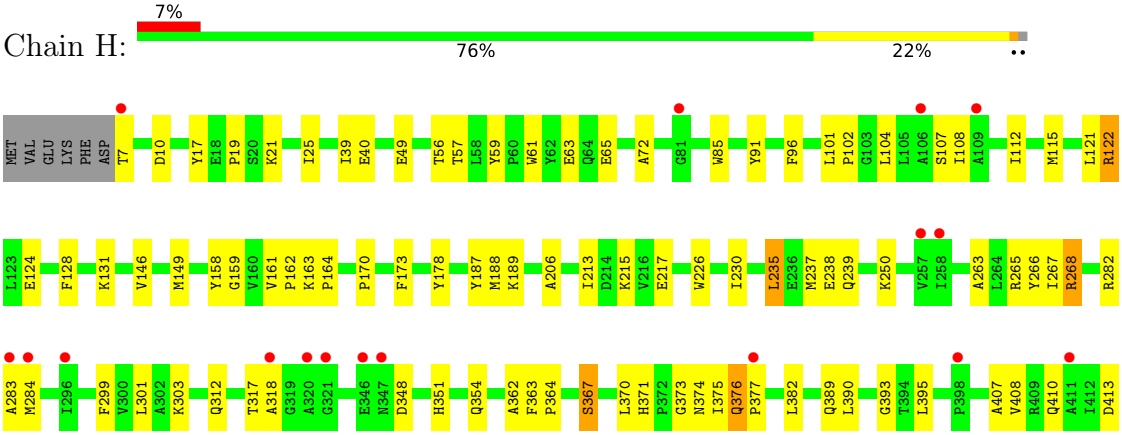
• Molecule 1: Ribulose bisphosphate carboxylase

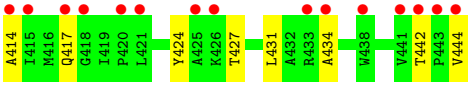
Chain G:



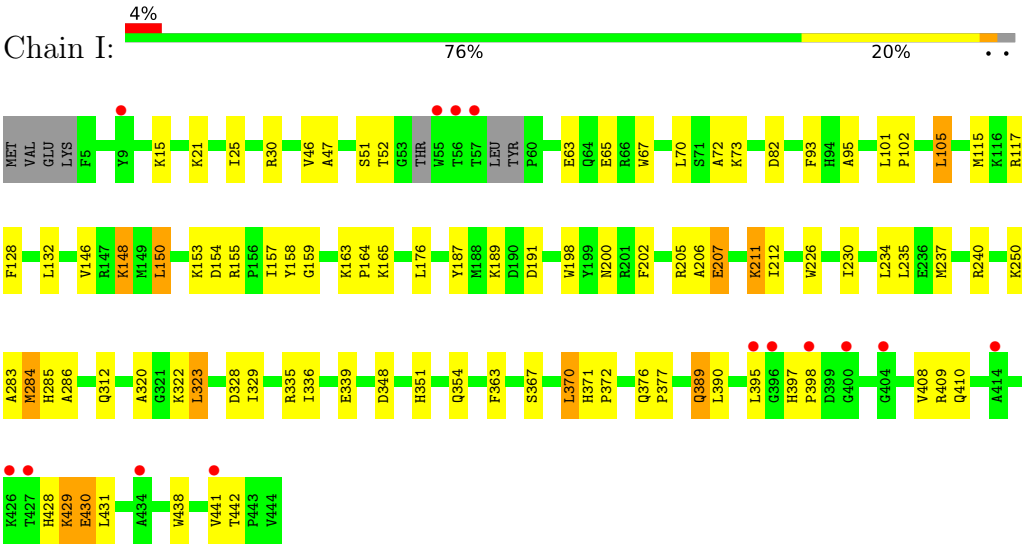
• Molecule 1: Ribulose bisphosphate carboxylase

Chain H:

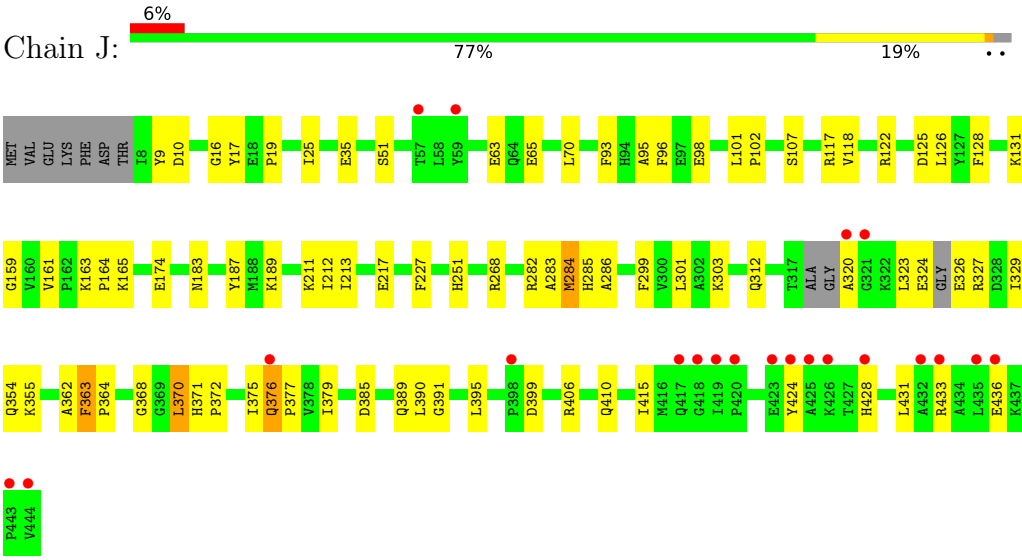




• Molecule 1: Ribulose bisphosphate carboxylase



• Molecule 1: Ribulose bisphosphate carboxylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 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) 99.4 (42.22-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.34Å)	Xtriage
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 (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CAP, CA, KCX

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	0.36	0/3482	0.51	0/4722
1	B	0.37	0/3486	0.52	0/4729
1	C	0.35	0/3472	0.50	0/4711
1	D	0.38	0/3463	0.51	0/4695
1	E	0.37	0/3451	0.51	0/4680
1	F	0.35	0/3479	0.50	0/4719
1	G	0.37	0/3488	0.51	0/4732
1	H	0.37	0/3486	0.51	0/4729
1	I	0.39	0/3495	0.53	0/4735
1	J	0.38	0/3451	0.51	0/4679
All	All	0.37	0/34753	0.51	0/47131

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3408	0	3311	86	0
1	B	3412	0	3307	119	0
1	C	3399	0	3284	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3392	0	3267	91	0
1	E	3379	0	3253	74	0
1	F	3405	0	3301	73	0
1	G	3413	0	3303	86	0
1	H	3412	0	3315	95	0
1	I	3423	0	3330	83	0
1	J	3379	0	3235	81	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
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	15	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	14	0
5	H	180	0	0	6	0
5	I	212	0	0	14	0
5	J	194	0	0	10	0
All	All	36193	0	32982	885	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 (885) 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:J:174:GLU:HG3	1:J:212:ILE:HD11	1.29	1.13
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
1:H:149:MET:HE3	1:H:250:LYS:HD2	1.15	1.09
3:C:446:CAP:H4	3:C:446:CAP:O6	1.50	1.09
1:B:104:LEU:HD23	1:B:104:LEU:C	1.72	1.09
1:A:358:SER:HB2	5:A:678:HOH:O	1.48	1.08
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
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: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: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:49:GLU:HG3	1:C:115:MET:HE3	1.56	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:H:149:MET:HE3	1:H:250:LYS:CD	2.04	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:LEU:C	1:B:104:LEU:CD2	2.46	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:G:104:LEU:HD23	1:G:104:LEU:C	1.98	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
1:D:155:ARG:CZ	1:D:409:ARG:NH2	2.43	0.82
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: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:G:417:GLN:C	5:G:564:HOH:O	2.23	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:B:423:GLU:HG3	1:B:424:TYR:N	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:348:ASP:OD2	1:C:351:HIS:HD2	1.70	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: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
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: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:A:389:GLN:C	1:A:390:LEU:HD12	2.12	0.69
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:I:389:GLN:C	1:I:390:LEU:HD12	2.13	0.69
1:A:320:ALA:O	1:A:442:THR:HG23	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:F:389:GLN:C	1:F:390:LEU:HD12	2.16	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:65:GLU:OE1	1:B:65:GLU:HA	1.96	0.65
1:B:149:MET:HE2	1:B:251:HIS:HE1	1.61	0.65
1:B:367:SER:HB2	1:B:389:GLN:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:J:163:LYS:HA	1:J:164:PRO:C	2.17	0.64
1:C:427:THR:O	1:C:427:THR:HG22	1.97	0.64
1:E:25:ILE:HD12	1:E:96:PHE:CE2	2.33	0.64
1:H:427:THR:O	1:H:427:THR:HG22	1.96	0.64
1:B:149:MET:CE	1:B:251:HIS:CE1	2.81	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:H:56:THR:OG1	1:H:57:THR:N	2.31	0.64
1:A:397:HIS:CG	1:A:398:PRO:HD2	2.33	0.64
1:E:162:PRO:O	1:E:163:LYS:HD3	1.98	0.64
1:G:165:LYS:NZ	1:G:191:ASP:OD2	2.26	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:A:149:MET:HE3	1:A:250:LYS:HE3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:J:389:GLN:C	1:J:390:LEU:HD12	2.20	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:G:73:LYS:HG3	5:G:683:HOH:O	1.99	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: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: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:46:VAL:HG22	1:B:115:MET:HE1	1.83	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
1:B:149:MET:HE1	1:B:251:HIS:CE1	2.37	0.59
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:A:376:GLN:N	1:A:377:PRO:CD	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:149:MET:CE	1:H:250:LYS:HB3	2.33	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: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:G:163:LYS:HA	1:G:164:PRO:C	2.23	0.58
1:D:418:GLY:C	1:D:419:ILE:HD12	2.23	0.57
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: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: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:J:391:GLY:C	1:J:395:LEU:HD12	2.25	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:B:373:GLY:C	5:B:608:HOH:O	2.43	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: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:A:419:ILE:HD12	1:A:419:ILE:H	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:ILE:HD12	1:B:108:ILE:C	2.25	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: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:B:419:ILE:HG22	1:B:423:GLU:HG3	1.88	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: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:D:163:LYS:HA	1:D:164:PRO:C	2.26	0.55
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:E:371:HIS:HB2	1:E:372:PRO:HD2	1.89	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:93:PHE:CD1	1:G:93:PHE:C	2.80	0.55
1:G:343:LYS:HE3	5:G:588:HOH:O	2.06	0.55
1:B:402:ALA:CB	5:B:550:HOH:O	2.54	0.55
1:C:56:THR:OG1	1:C:57:THR:N	2.40	0.55
1:E:323:LEU:O	1:E:324:GLU:C	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:VAL:HG22	1:D:115:MET:HE1	1.90	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: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:A:104:LEU:HD13	1:A:104:LEU:C	2.28	0.54
1:A:200:ASN:OD1	1:A:205:ARG:HD3	2.07	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: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:A:389:GLN:O	1:A:390:LEU:HD12	2.08	0.54
1:B:25:ILE:HD12	1:B:96:PHE:CE2	2.43	0.54
1:B:163:LYS:HA	1:B:164:PRO:C	2.29	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:G:108:ILE:C	1:G:108:ILE:HD12	2.27	0.54
1:G:389:GLN:C	1:G:390:LEU:HD12	2.29	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:G:46:VAL:HG22	1:G:115:MET:HE1	1.90	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
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: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:A:121:LEU:N	1:A:294:HIS:HD2	2.05	0.53
1:B:391:GLY:O	1:B:392:GLY:C	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:397:HIS:CG	1:I:398:PRO:HD2	2.43	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: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: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: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: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:419:ILE:CG2	1:B:423:GLU:CD	2.78	0.52
1:B:163:LYS:H	1:B:395:LEU:HD22	1.73	0.52
1:G:235:LEU:HD12	1:G:238:GLU:OE1	2.10	0.52
1:I:163:LYS:HA	1:I:164:PRO:C	2.30	0.52
1:I:250:LYS:HD3	5:I:667:HOH:O	2.08	0.52
1:A:163:LYS:HA	1:A:164:PRO:C	2.30	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: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:E:163:LYS:HA	1:E:164:PRO:C	2.30	0.52
1:H:371:HIS:O	1:H:375:ILE:HG23	2.09	0.52
1:H:389:GLN:C	1:H:390:LEU:HD12	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:125:ASP:OD1	1:G:126:LEU:N	2.42	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:F:146:VAL:HG21	1:F:312:GLN:HE21	1.76	0.51
1:A:161:VAL:HG23	1:A:389:GLN:CD	2.30	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:I:206:ALA:HA	1:I:226:TRP:CZ3	2.46	0.51
1:H:65:GLU:CD	1:H:65:GLU:H	2.11	0.51
1:B:159:GLY:HA3	1:B:187:TYR:CE1	2.45	0.51
1:F:163:LYS:HA	1:F:164:PRO:C	2.30	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
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:G:104:LEU:C	1:G:104:LEU:CD2	2.73	0.50
1:G:395:LEU:C	1:G:395:LEU:HD12	2.32	0.50
1:F:330:THR:HG22	1:F:382:LEU:HD21	1.92	0.50
1:I:431:LEU:HD12	1:I:431:LEU:C	2.31	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:I:46:VAL:HG22	1:I:115:MET:HE1	1.94	0.50
1:B:93:PHE:CD1	1:B:93:PHE:C	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:I:72:ALA:O	1:I:73:LYS:HD3	2.11	0.50
1:J:65:GLU:CD	1:J:65:GLU:H	2.14	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: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:H:149:MET:CE	1:H:250:LYS:CB	2.91	0.49
1:B:419:ILE:HG23	1:B:423:GLU:CD	2.33	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
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:442:THR:O	1:H:444:VAL:HG23	2.11	0.49
1:E:439:GLY:C	1:E:440:HIS:CD2	2.86	0.49
1:F:289:THR:HG22	1:F:296:ILE:O	2.12	0.49
1:I:65:GLU:H	1:I:65:GLU:CD	2.16	0.49
1:J:93:PHE:CD1	1:J:93:PHE:C	2.86	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:397:HIS:ND1	1:D:398:PRO:CD	2.74	0.48
1:B:389:GLN:C	1:B:390:LEU:HD12	2.33	0.48
1:D:65:GLU:HG3	5:D:648:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:419:ILE:O	1:G:420:PRO:C	2.51	0.48
1:J:440:HIS:ND1	5:J:694:HOH:O	2.33	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:C:432:ALA:C	1:C:434:ALA:H	2.15	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:D:65:GLU:H	1:D:65:GLU:CD	2.16	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:I:371:HIS:HB2	1:I:372:PRO:HD2	1.94	0.48
1:C:389:GLN:C	1:C:390:LEU:HD12	2.33	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:F:108:ILE:C	1:F:108:ILE:HD12	2.34	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: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
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:46:VAL:CG2	1:B:115:MET:HE1	2.43	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:149:MET:HE1	1:H:250:LYS:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:351:HIS:HE1	5:G:526:HOH:O	1.97	0.47
1:A:93:PHE:C	1:A:93:PHE:CD1	2.88	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: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:E:439:GLY:C	5:E:691:HOH:O	2.53	0.47
1:J:323:LEU:O	1:J:324:GLU:C	2.52	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:D:282:ARG:O	1:D:283:ALA:C	2.53	0.47
1:G:101:LEU:HB3	1:G:102:PRO:HD3	1.97	0.47
1:H:104:LEU:C	1:H:104:LEU:HD23	2.35	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: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
1:G:331:ILE:O	1:G:335:ARG:HG3	2.15	0.47
1:H:282:ARG:O	1:H:283:ALA:C	2.53	0.47
1:I:117:ARG:HG3	1:I:117:ARG:NH1	2.30	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:A:149:MET:HE2	1:A:251:HIS:CE1	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:149:MET:HE1	1:A:251:HIS:ND1	2.29	0.46
1:D:412:ILE:C	5:D:594:HOH:O	2.53	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: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:I:93:PHE:CD1	1:I:93:PHE:C	2.89	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: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
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: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:419:ILE:O	1:C:420:PRO:C	2.54	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:VAL:HG21	1:C:312:GLN:HE21	1.81	0.45
1:F:112:ILE:O	1:F:115:MET:HE2	2.16	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:C:193:ASN:N	1:C:193:ASN:ND2	2.59	0.45
1:D:208:ILE:O	1:D:212:ILE:HG12	2.16	0.45
1:H:72:ALA:HB2	1:H:91:TYR:CD1	2.51	0.45
1:A:115:MET:HB2	1:A:115:MET:HE2	1.72	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:G:46:VAL:HG22	1:G:115:MET:CE	2.46	0.45
1:J:326:GLU:OE1	1:J:329:ILE:CD1	2.64	0.45
1:A:149:MET:HE1	1:A:251:HIS:CE1	2.52	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:C:371:HIS:HB2	1:C:372:PRO:HD2	1.99	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
1:H:149:MET:HE1	1:H:250:LYS:CB	2.46	0.44
1:J:370:LEU:N	1:J:370:LEU:CD1	2.79	0.44
1:J:391:GLY:C	1:J:395:LEU:CD1	2.84	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: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:HG23	1:B:118:VAL:O	2.17	0.44
1:F:191:ASP:HB2	5:F:536:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:268:ARG:HD3	1:H:268:ARG:C	2.38	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:163:LYS:HA	1:C:164:PRO:C	2.37	0.44
1:C:279:HIS:NE2	1:C:314:HIS:NE2	2.59	0.44
1:E:303:LYS:HZ3	1:E:354:GLN:HE21	1.66	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
1:J:399:ASP:OD1	1:J:433:ARG:NH2	2.45	0.44
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:56:THR:OG1	1:D:57:THR:N	2.50	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: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: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:H:371:HIS:ND1	1:H:373:GLY:HA3	2.29	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
1:I:150:LEU:HD23	1:I:157:ILE:HD13	1.99	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:163:LYS:HA	1:H:164:PRO:C	2.39	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:A:149:MET:HE2	1:A:251:HIS:HE1	1.82	0.42
1:C:268:ARG:HD3	1:C:268:ARG:C	2.39	0.42
1:D:351:HIS:HE1	5:D:548:HOH:O	2.02	0.42
1:F:115:MET:HE2	1:F:115:MET:HB2	1.79	0.42
1:J:333:ASN:OD1	5:J:543:HOH:O	2.21	0.42
1:B:391:GLY:O	1:B:393:GLY:N	2.52	0.42
1:H:283:ALA:O	1:H:284:MET:HB3	2.18	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:J:336:ILE:HD12	1:J:336:ILE:HA	1.91	0.42
1:B:371:HIS:CE1	1:B:373:GLY:C	2.92	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:E:389:GLN:C	1:E:390:LEU:HD12	2.40	0.42
1:F:52:THR:HB	1:F:67:TRP:NE1	2.35	0.42
1:J:285:HIS:CG	1:J:286:ALA:N	2.87	0.42
1:A:284:MET:O	1:A:284:MET:HG2	2.20	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: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:I:285:HIS:CG	1:I:286:ALA:N	2.88	0.42
1:J:439:GLY:C	1:J:440:HIS:ND1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:108:ILE:C	1:B:108:ILE:CD1	2.88	0.41
1:D:101:LEU:HB3	1:D:102:PRO:HD3	2.01	0.41
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:HG23	1:J:118:VAL:O	2.20	0.41
1:J:159:GLY:CA	1:J:187:TYR:CZ	3.02	0.41
1:C:192:GLU:HG3	1:C:283:ALA:HB2	2.01	0.41
1:E:230:ILE:O	1:E:231:THR:C	2.59	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: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: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: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:D:178:TYR:OH	1:D:219:GLU:OE1	2.32	0.41
1:F:279:HIS:NE2	1:F:314:HIS:NE2	2.67	0.41
1:I:200:ASN:OD1	1:I:205:ARG:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:432:ALA:C	1:C:434:ALA:N	2.74	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:H:149:MET:HE3	1:H:250:LYS:CB	2.51	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
1:D:410:GLN:OE1	1:D:431:LEU:N	2.54	0.41
1:E:222:GLU:CD	5:E:586:HOH:O	2.59	0.41
1:F:93:PHE:CD1	1:F:93:PHE:C	2.94	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:C:169:SER:HB2	1:C:170:PRO:HD2	2.02	0.41
1:F:111:ASN:HA	5:F:621:HOH:O	2.21	0.41
1:G:213:ILE:O	1:G:217:GLU:HG3	2.21	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:F:82:ASP:C	1:F:82:ASP:OD1	2.60	0.40
1:G:108:ILE:C	1:G:108:ILE:CD1	2.89	0.40
1:I:25:ILE:HD11	1:I:132:LEU:HD21	2.03	0.40
1:B:122:ARG:HG3	1:B:124:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:321:GLY:HA3	5:G:642:HOH:O	2.21	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
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: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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	433/444 (98%)	417 (96%)	13 (3%)	3 (1%)	22	22
1	B	434/444 (98%)	413 (95%)	19 (4%)	2 (0%)	29	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	432/444 (97%)	408 (94%)	23 (5%)	1 (0%)	47 55
1	D	430/444 (97%)	401 (93%)	26 (6%)	3 (1%)	22 22
1	E	425/444 (96%)	410 (96%)	14 (3%)	1 (0%)	47 55
1	F	434/444 (98%)	409 (94%)	23 (5%)	2 (0%)	29 31
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%)	47 55
1	J	427/444 (96%)	407 (95%)	19 (4%)	1 (0%)	47 55
All	All	4314/4440 (97%)	4102 (95%)	198 (5%)	14 (0%)	41 47

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%)	320 (95%)	16 (5%)	25 32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	336/356 (94%)	320 (95%)	16 (5%)	25	32
1	C	332/356 (93%)	315 (95%)	17 (5%)	24	29
1	D	332/356 (93%)	318 (96%)	14 (4%)	30	37
1	E	333/356 (94%)	322 (97%)	11 (3%)	38	46
1	F	334/356 (94%)	324 (97%)	10 (3%)	41	50
1	G	335/356 (94%)	321 (96%)	14 (4%)	30	37
1	H	335/356 (94%)	326 (97%)	9 (3%)	44	55
1	I	339/356 (95%)	322 (95%)	17 (5%)	24	30
1	J	329/356 (92%)	317 (96%)	12 (4%)	35	44
All	All	3341/3560 (94%)	3205 (96%)	136 (4%)	30	38

All (136) 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	234	LEU
1	A	247	LEU
1	A	268	ARG
1	A	307	LEU
1	A	328	ASP
1	A	363	PHE
1	A	367	SER
1	A	376	GLN
1	A	382	LEU
1	A	395	LEU
1	A	435	LEU
1	B	18	GLU
1	B	93	PHE
1	B	104	LEU
1	B	107	SER
1	B	122	ARG
1	B	235	LEU
1	B	247	LEU
1	B	268	ARG
1	B	352	LEU

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Mol	Chain	Res	Type
1	B	358	SER
1	B	363	PHE
1	B	376	GLN
1	B	382	LEU
1	B	389	GLN
1	B	423	GLU
1	B	431	LEU
1	C	20	SER
1	C	58	LEU
1	C	107	SER
1	C	118	VAL
1	C	122	ARG
1	C	193	ASN
1	C	235	LEU
1	C	268	ARG
1	C	301	LEU
1	C	307	LEU
1	C	326	GLU
1	C	363	PHE
1	C	367	SER
1	C	376	GLN
1	C	382	LEU
1	C	389	GLN
1	C	409	ARG
1	D	105	LEU
1	D	122	ARG
1	D	165	LYS
1	D	234	LEU
1	D	235	LEU
1	D	268	ARG
1	D	301	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	117	ARG
1	E	122	ARG
1	E	165	LYS

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Mol	Chain	Res	Type
1	E	211	LYS
1	E	235	LEU
1	E	268	ARG
1	E	363	PHE
1	E	376	GLN
1	E	427	THR
1	E	442	THR
1	F	144	GLU
1	F	268	ARG
1	F	301	LEU
1	F	307	LEU
1	F	328	ASP
1	F	363	PHE
1	F	367	SER
1	F	376	GLN
1	F	389	GLN
1	F	427	THR
1	G	21	LYS
1	G	93	PHE
1	G	107	SER
1	G	122	ARG
1	G	235	LEU
1	G	247	LEU
1	G	268	ARG
1	G	352	LEU
1	G	358	SER
1	G	363	PHE
1	G	382	LEU
1	G	389	GLN
1	G	394	THR
1	G	395	LEU
1	H	107	SER
1	H	122	ARG
1	H	235	LEU
1	H	268	ARG
1	H	301	LEU
1	H	363	PHE
1	H	367	SER
1	H	376	GLN
1	H	382	LEU
1	I	15	LYS
1	I	105	LEU

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Mol	Chain	Res	Type
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	268	ARG
1	I	323	LEU
1	I	328	ASP
1	I	363	PHE
1	I	370	LEU
1	I	389	GLN
1	I	429	LYS
1	I	430	GLU
1	J	10	ASP
1	J	35	GLU
1	J	107	SER
1	J	122	ARG
1	J	165	LYS
1	J	211	LYS
1	J	268	ARG
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 (55) 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

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Mol	Chain	Res	Type
1	B	376	GLN
1	B	417	GLN
1	C	64	GLN
1	C	193	ASN
1	C	239	GLN
1	C	312	GLN
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	D	428	HIS
1	E	218	ASN
1	E	312	GLN
1	E	354	GLN
1	E	410	GLN
1	E	440	HIS
1	F	294	HIS
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	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

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Mol	Chain	Res	Type
1	J	354	GLN
1	J	410	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	1,2	9,11,12	0.95	0	5,12,14	1.52	1 (20%)
1	KCX	E	189	1,4	9,11,12	0.88	0	5,12,14	1.47	1 (20%)
1	KCX	H	189	1,2	9,11,12	0.96	0	5,12,14	1.48	1 (20%)
1	KCX	D	189	1,2	9,11,12	0.72	0	5,12,14	1.77	1 (20%)
1	KCX	I	189	1,2	9,11,12	0.82	0	5,12,14	1.46	1 (20%)
1	KCX	J	189	1,4	9,11,12	0.92	0	5,12,14	1.80	1 (20%)
1	KCX	G	189	1,2	9,11,12	1.04	1 (11%)	5,12,14	1.30	1 (20%)
1	KCX	A	189	1,2	9,11,12	0.82	0	5,12,14	1.35	1 (20%)
1	KCX	C	189	1,2	9,11,12	0.91	0	5,12,14	1.82	2 (40%)
1	KCX	F	189	1,2	9,11,12	0.86	0	5,12,14	1.52	1 (20%)

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	1,2	-	0/9/10/12	-
1	KCX	E	189	1,4	-	0/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	H	189	1,2	-	2/9/10/12	-
1	KCX	D	189	1,2	-	0/9/10/12	-
1	KCX	I	189	1,2	-	0/9/10/12	-
1	KCX	J	189	1,4	-	0/9/10/12	-
1	KCX	G	189	1,2	-	1/9/10/12	-
1	KCX	A	189	1,2	-	1/9/10/12	-
1	KCX	C	189	1,2	-	0/9/10/12	-
1	KCX	F	189	1,2	-	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	2.22	1.25	1.21

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	189	KCX	OQ1-CX-NZ	-3.77	119.11	124.96
1	D	189	KCX	OQ1-CX-NZ	-3.72	119.19	124.96
1	F	189	KCX	OQ1-CX-NZ	-3.22	119.97	124.96
1	E	189	KCX	OQ1-CX-NZ	-3.03	120.26	124.96
1	C	189	KCX	OQ1-CX-NZ	-3.02	120.27	124.96
1	I	189	KCX	OQ1-CX-NZ	-2.89	120.48	124.96
1	B	189	KCX	OQ1-CX-NZ	-2.69	120.78	124.96
1	H	189	KCX	OQ1-CX-NZ	-2.67	120.81	124.96
1	A	189	KCX	OQ1-CX-NZ	-2.64	120.86	124.96
1	C	189	KCX	CE-NZ-CX	-2.63	117.66	121.89
1	G	189	KCX	OQ1-CX-NZ	-2.28	121.42	124.96

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	189	KCX	C-CA-CB-CG
1	H	189	KCX	C-CA-CB-CG
1	H	189	KCX	O-C-CA-CB
1	G	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 monosaccharides 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	E	446	4	17,20,20	0.75	0	22,31,31	0.92	1 (4%)
3	CAP	C	446	2	17,20,20	0.98	1 (5%)	22,31,31	1.14	2 (9%)
3	CAP	F	446	2	17,20,20	0.98	1 (5%)	22,31,31	0.94	0
3	CAP	G	446	2	17,20,20	1.01	1 (5%)	22,31,31	1.07	1 (4%)
3	CAP	J	446	4	17,20,20	0.85	0	22,31,31	0.94	1 (4%)
3	CAP	A	446	2	17,20,20	1.00	1 (5%)	22,31,31	1.03	1 (4%)
3	CAP	H	446	2	17,20,20	0.90	0	22,31,31	1.07	1 (4%)
3	CAP	D	446	2	17,20,20	0.89	0	22,31,31	1.16	2 (9%)
3	CAP	B	446	2	17,20,20	1.01	1 (5%)	22,31,31	1.06	1 (4%)
3	CAP	I	446	2	17,20,20	0.92	0	22,31,31	1.17	2 (9%)

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	E	446	4	-	0/29/29/29	-
3	CAP	C	446	2	-	7/29/29/29	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CAP	F	446	2	-	15/29/29/29	-
3	CAP	G	446	2	-	9/29/29/29	-
3	CAP	J	446	4	-	0/29/29/29	-
3	CAP	A	446	2	-	15/29/29/29	-
3	CAP	H	446	2	-	7/29/29/29	-
3	CAP	D	446	2	-	9/29/29/29	-
3	CAP	B	446	2	-	3/29/29/29	-
3	CAP	I	446	2	-	11/29/29/29	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
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	F	446	CAP	C4-C3	-2.08	1.52	1.54
3	A	446	CAP	C4-C3	-2.02	1.52	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	446	CAP	C2-C3-C4	-2.89	108.13	114.00
3	H	446	CAP	C2-C3-C4	-2.84	108.23	114.00
3	I	446	CAP	O6P-P2-O5	2.79	114.17	106.73
3	J	446	CAP	C2-C3-C4	-2.57	108.78	114.00
3	E	446	CAP	C2-C3-C4	-2.54	108.84	114.00
3	A	446	CAP	O6P-P2-O5	2.53	113.47	106.73
3	I	446	CAP	P2-O5-C5	2.44	125.02	118.30
3	D	446	CAP	O6P-P2-O5	2.43	113.20	106.73
3	C	446	CAP	O1-P1-O1P	2.15	112.51	106.47
3	D	446	CAP	P2-O5-C5	2.09	124.06	118.30
3	G	446	CAP	O6P-P2-O5	2.07	112.25	106.73
3	B	446	CAP	O1-P1-O1P	2.05	112.22	106.47

There are no chirality outliers.

All (76) 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

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Mol	Chain	Res	Type	Atoms
3	A	446	CAP	O1-C1-C2-O2
3	A	446	CAP	O6-C-C2-C3
3	A	446	CAP	O6-C-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
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

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

There are no ring outliers.

8 monomers are involved in 12 short contacts:

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

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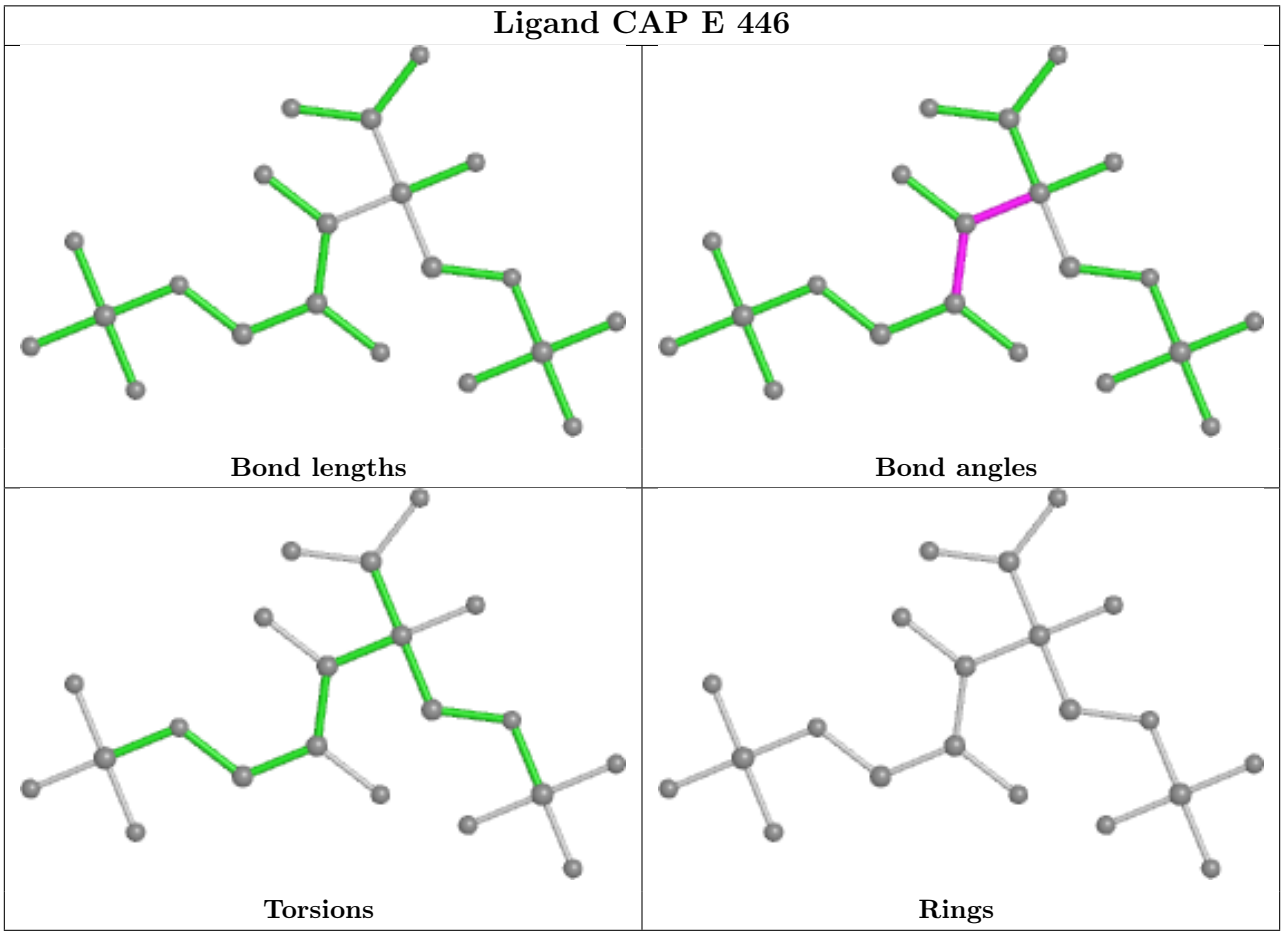
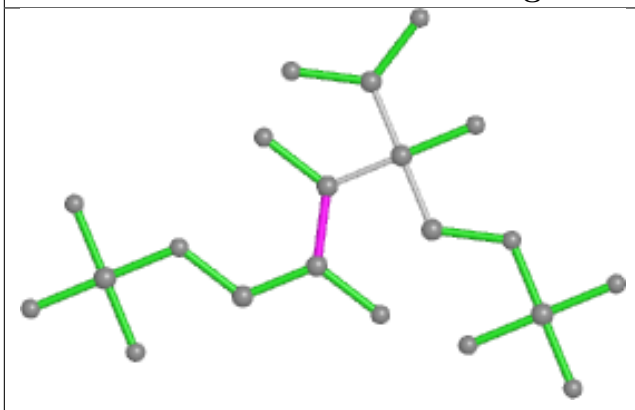
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	446	CAP	1	0
3	H	446	CAP	2	0
3	B	446	CAP	1	0

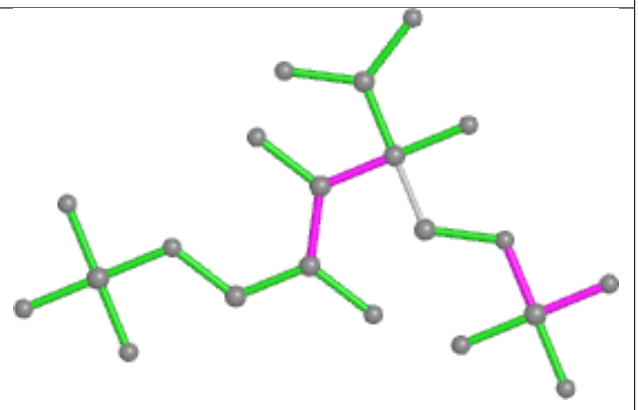
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



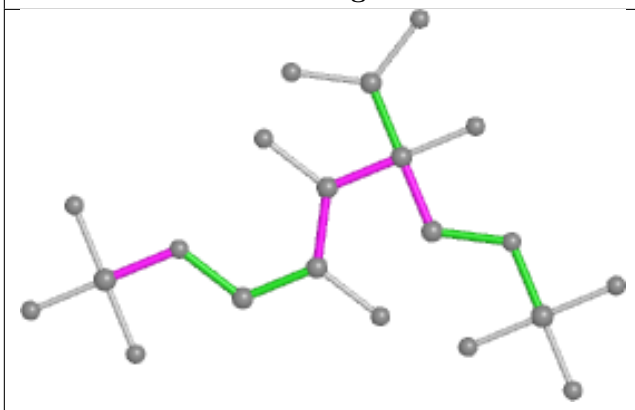
Ligand CAP C 446



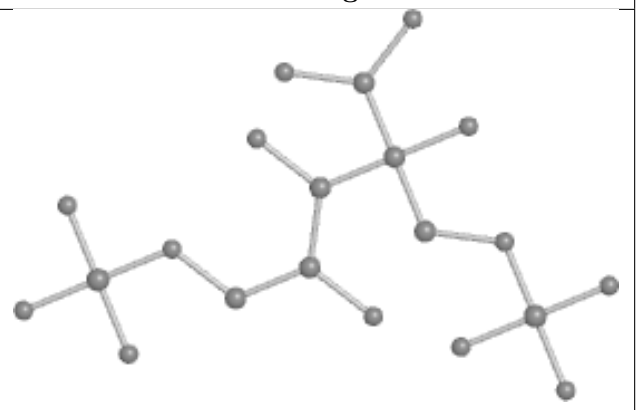
Bond lengths



Bond angles

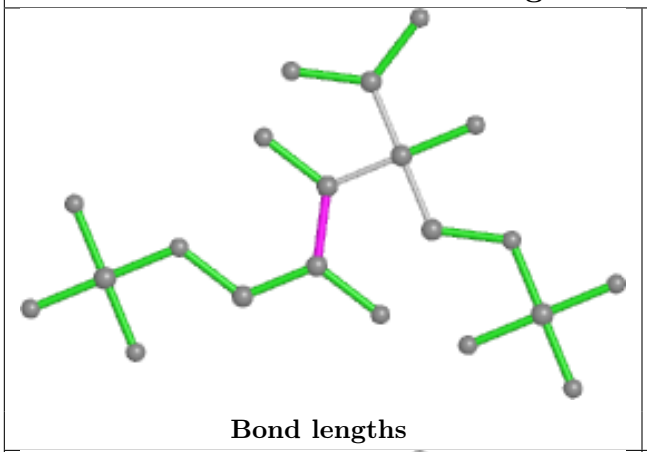


Torsions

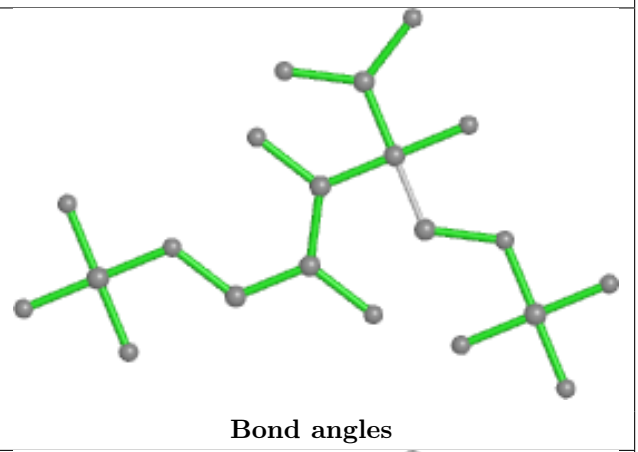


Rings

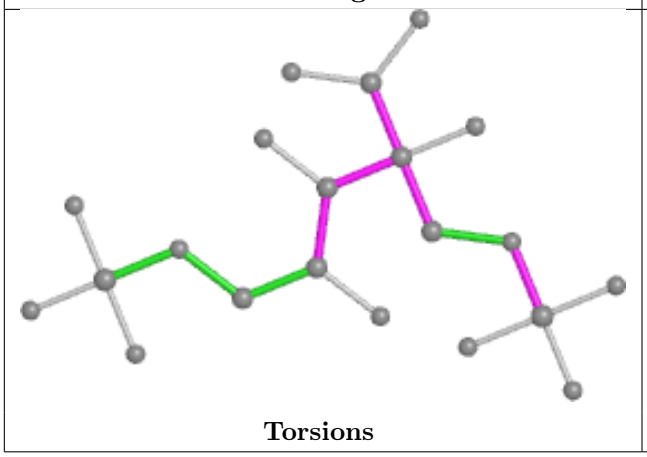
Ligand CAP F 446



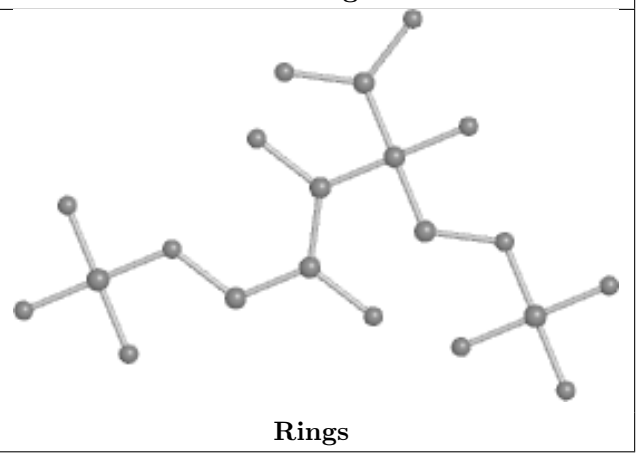
Bond lengths



Bond angles

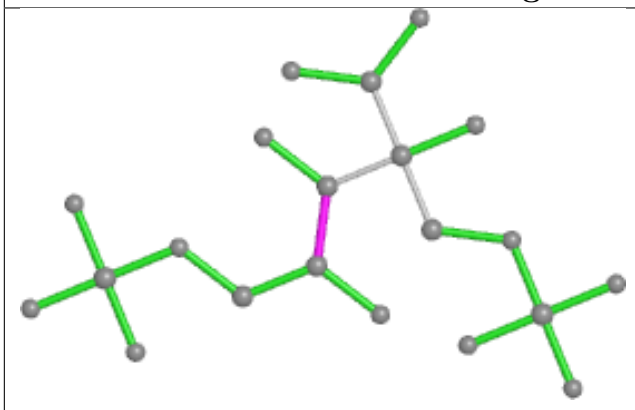


Torsions

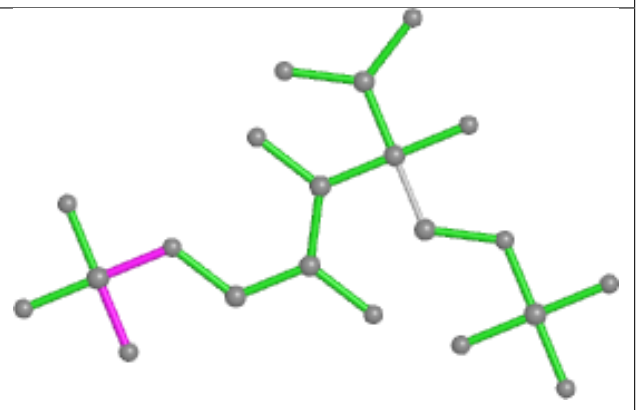


Rings

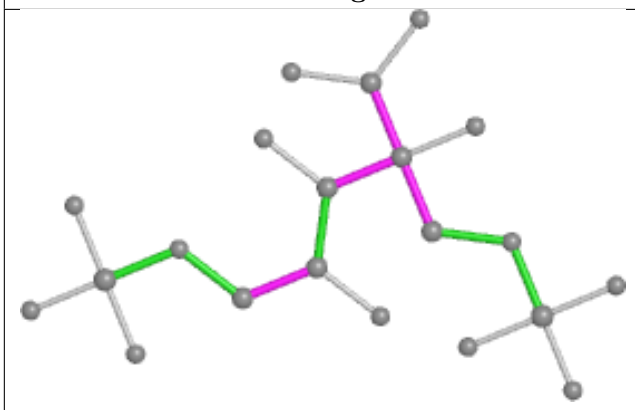
Ligand CAP G 446



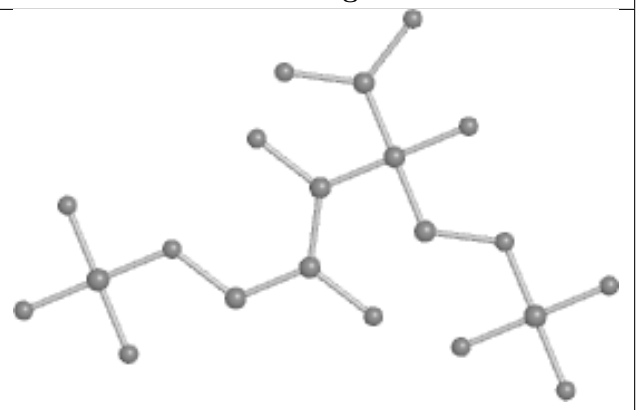
Bond lengths



Bond angles

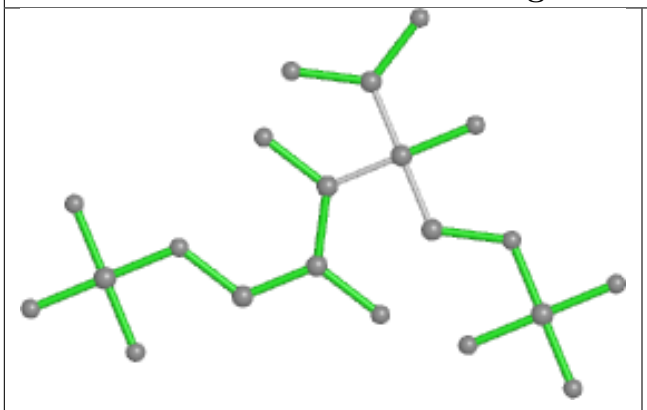


Torsions

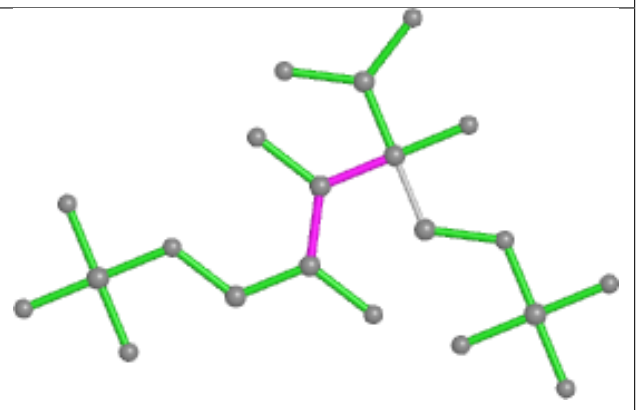


Rings

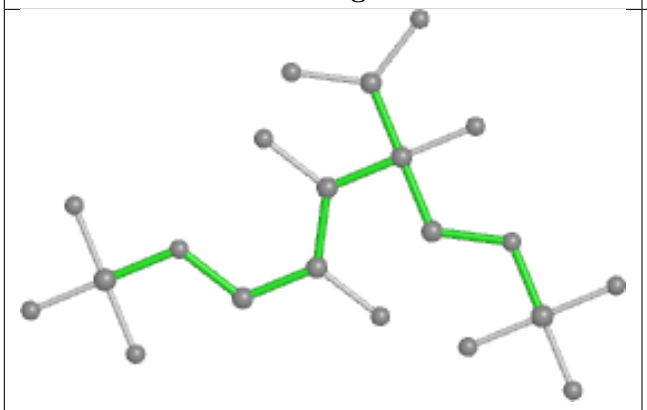
Ligand CAP J 446



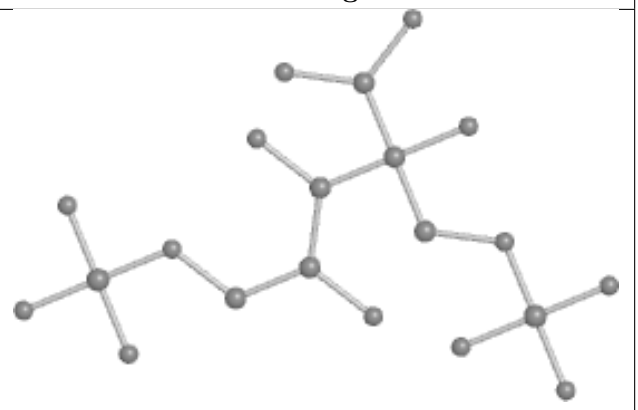
Bond lengths



Bond angles

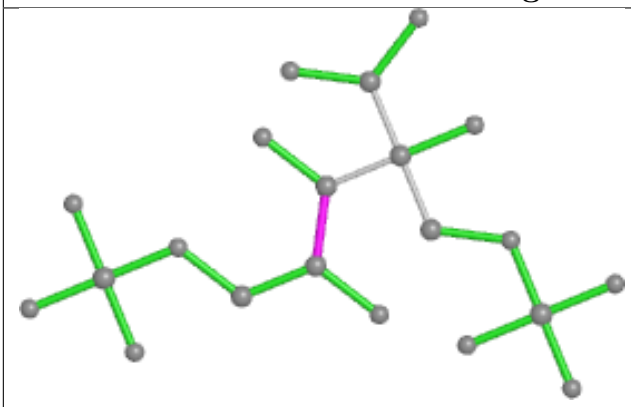


Torsions

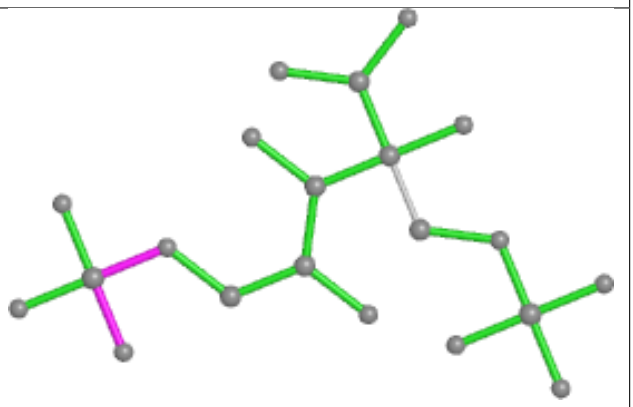


Rings

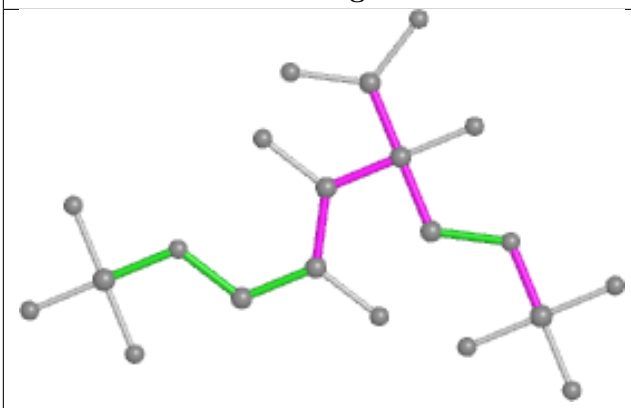
Ligand CAP A 446



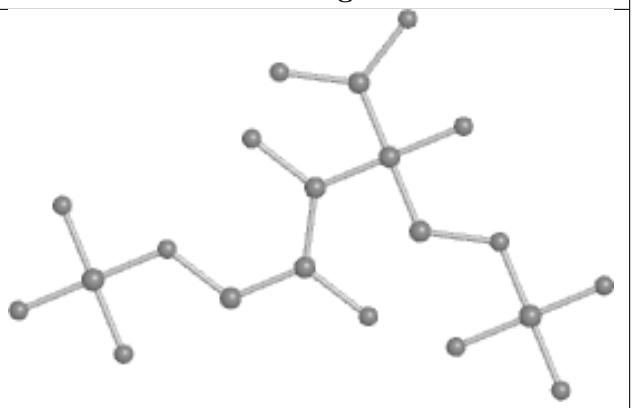
Bond lengths



Bond angles

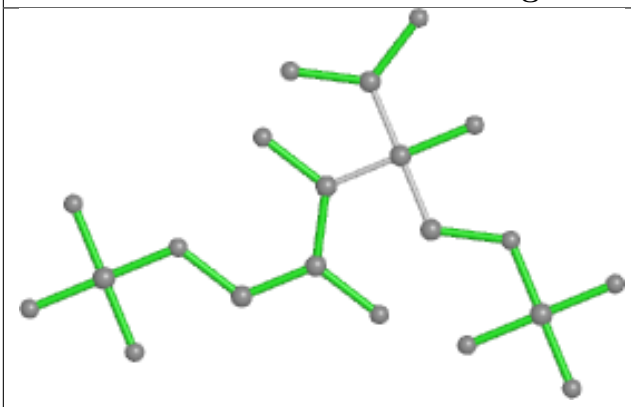


Torsions

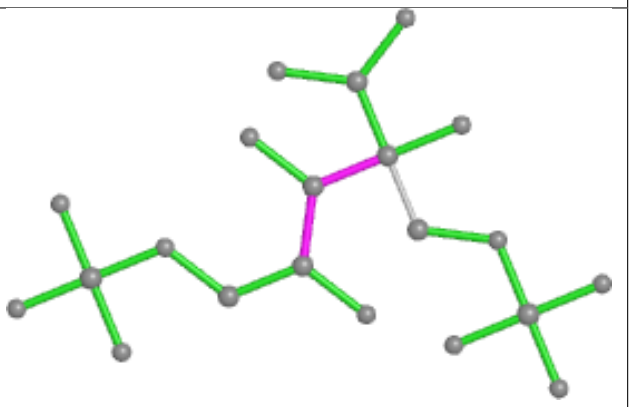


Rings

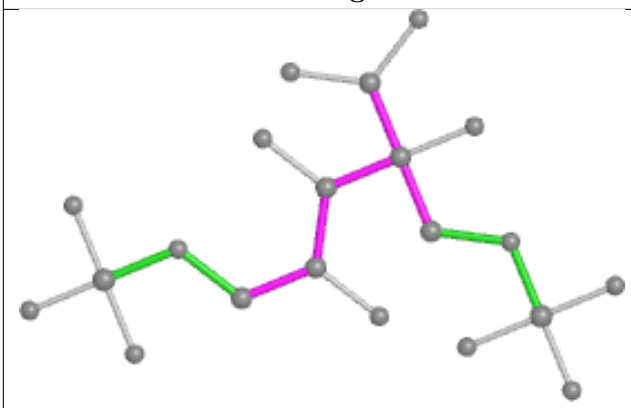
Ligand CAP H 446



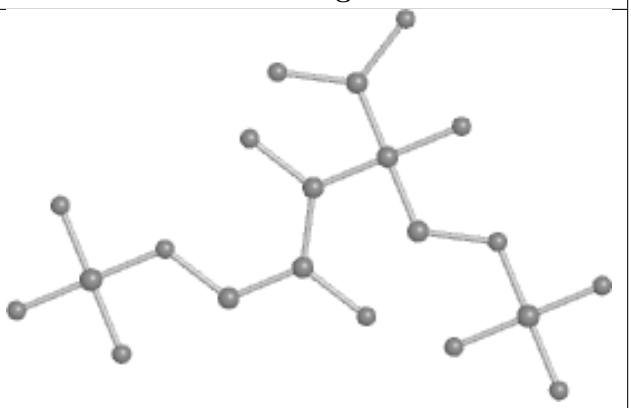
Bond lengths



Bond angles

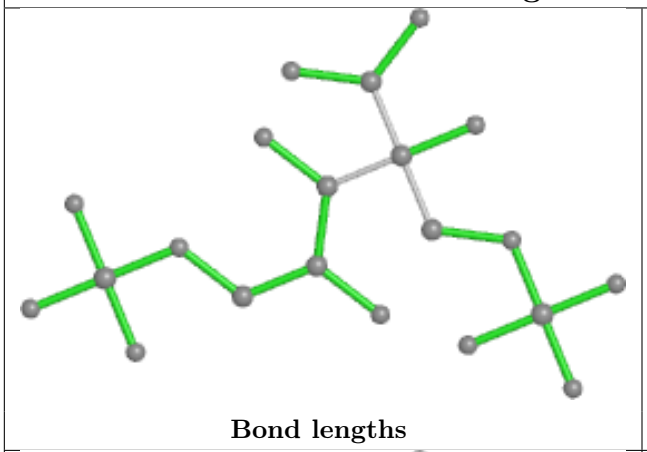


Torsions

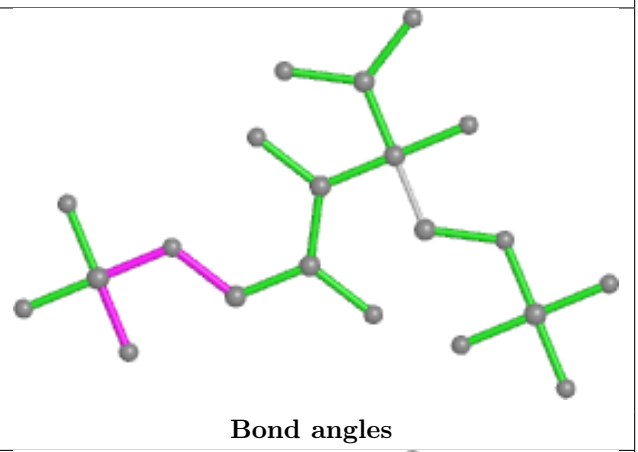


Rings

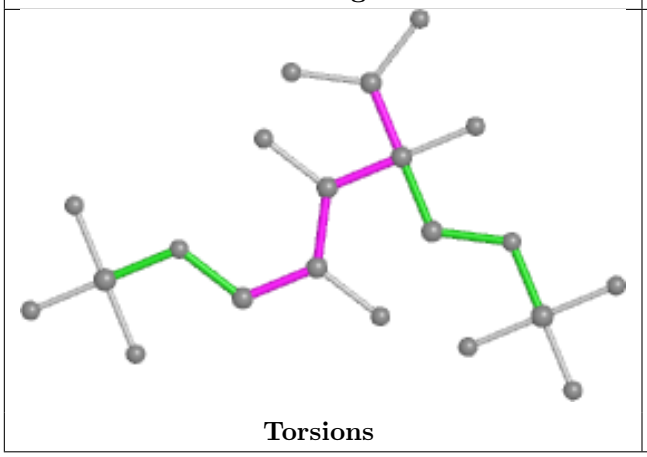
Ligand CAP D 446



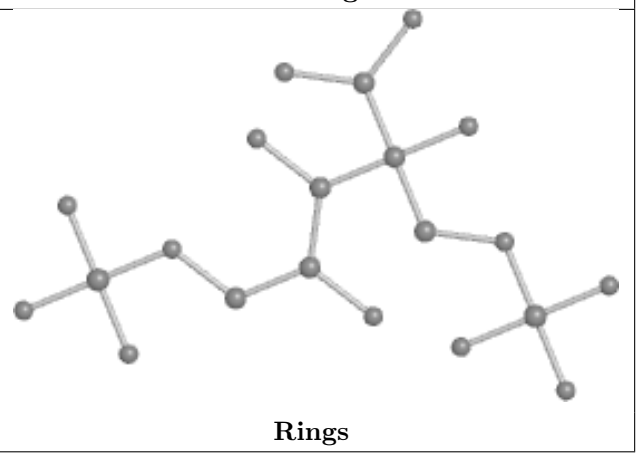
Bond lengths



Bond angles

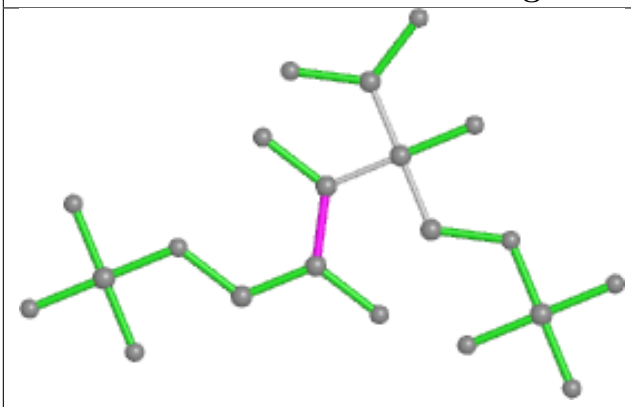


Torsions

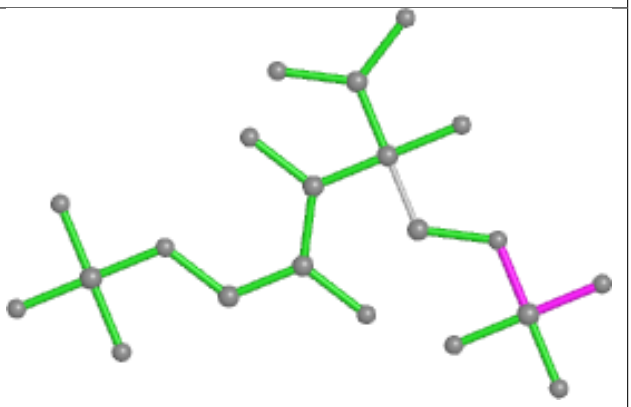


Rings

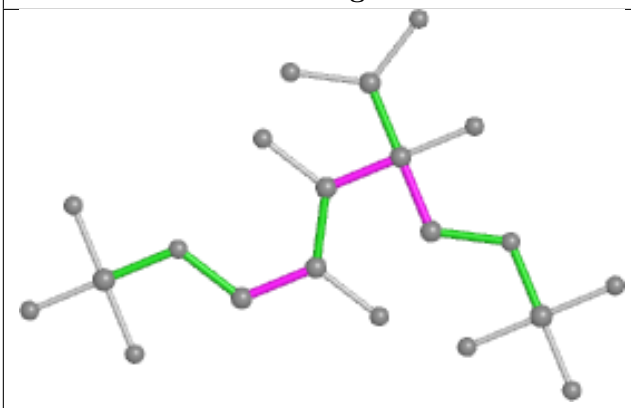
Ligand CAP B 446



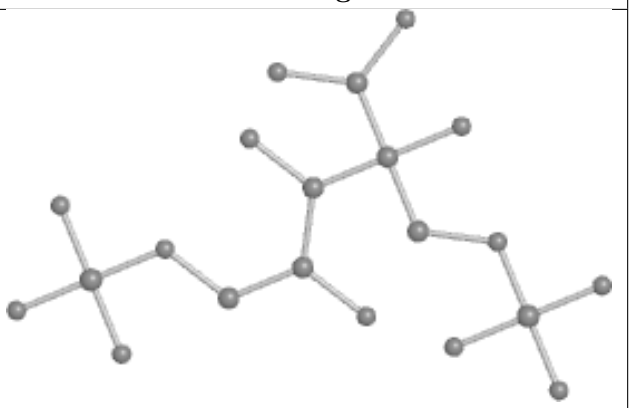
Bond lengths



Bond angles

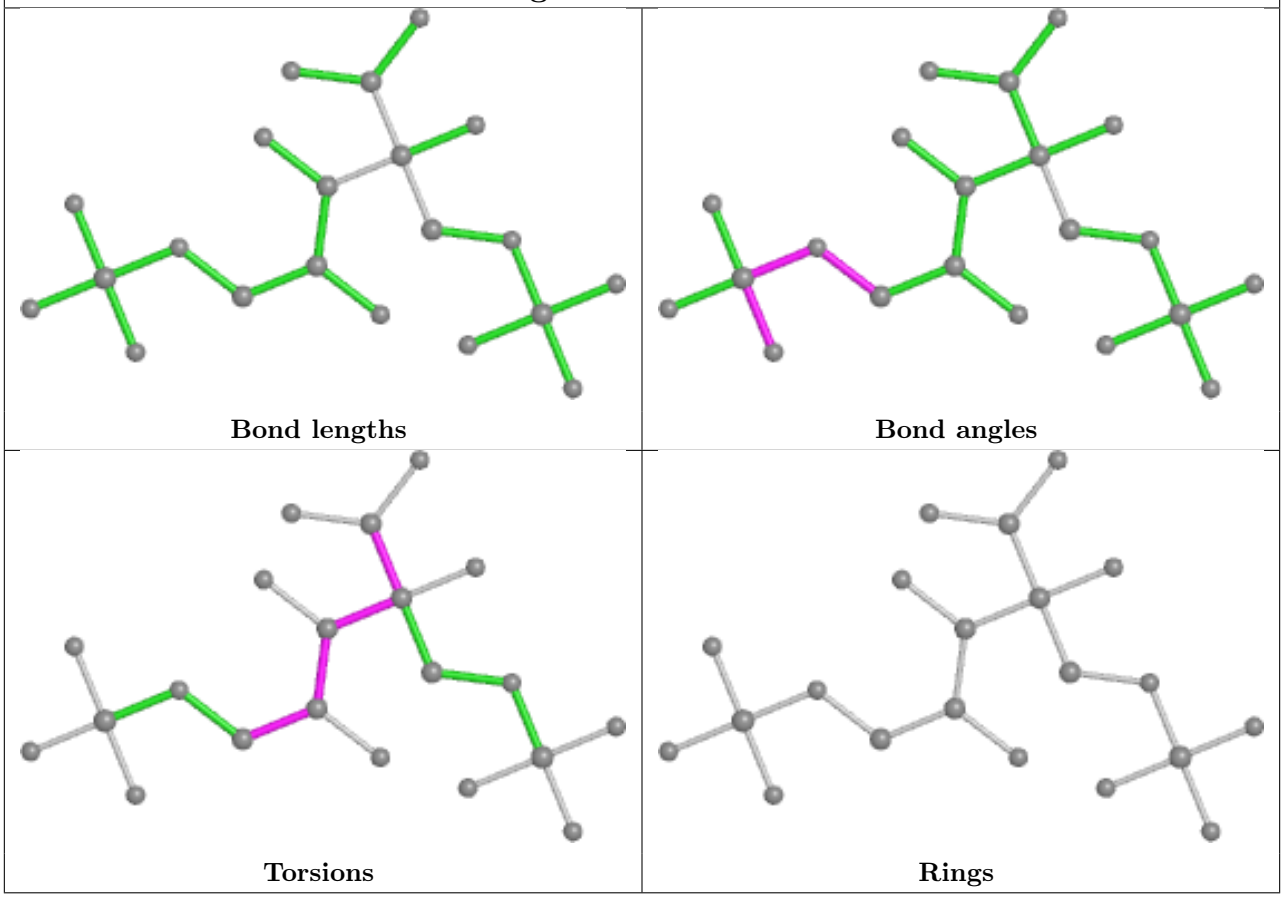


Torsions



Rings

Ligand CAP I 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, 95^{th} 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%)	0.01	16 (3%)	41	52	17, 28, 49, 58	0
1	B	436/444 (98%)	0.09	25 (5%)	23	33	14, 26, 56, 62	0
1	C	436/444 (98%)	0.25	37 (8%)	10	16	16, 27, 60, 66	0
1	D	436/444 (98%)	0.24	29 (6%)	17	25	15, 26, 58, 85	0
1	E	431/444 (97%)	0.03	21 (4%)	29	40	15, 25, 53, 70	0
1	F	436/444 (98%)	0.22	23 (5%)	26	37	17, 30, 57, 64	0
1	G	436/444 (98%)	0.11	25 (5%)	23	33	13, 25, 52, 58	0
1	H	437/444 (98%)	0.21	32 (7%)	15	22	16, 28, 58, 61	0
1	I	436/444 (98%)	-0.03	19 (4%)	34	45	13, 24, 52, 70	0
1	J	433/444 (97%)	0.10	26 (6%)	21	30	14, 25, 57, 74	0
All	All	4352/4440 (98%)	0.12	253 (5%)	23	32	13, 27, 56, 85	0

All (253) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	425	ALA	8.4
1	G	434	ALA	8.1
1	D	421	LEU	7.7
1	C	421	LEU	7.4
1	G	421	LEU	6.6
1	C	434	ALA	6.6
1	J	441	VAL	6.4
1	E	441	VAL	6.3
1	C	425	ALA	6.3
1	F	9	TYR	6.0
1	J	444	VAL	5.8
1	G	59	TYR	5.5
1	J	435	LEU	5.5

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Mol	Chain	Res	Type	RSRZ
1	E	444	VAL	5.4
1	C	426	LYS	5.4
1	B	414	ALA	5.2
1	D	414	ALA	5.2
1	C	441	VAL	5.1
1	I	421	LEU	5.1
1	J	439	GLY	4.9
1	H	434	ALA	4.5
1	C	438	TRP	4.4
1	I	398	PRO	4.4
1	C	422	ASP	4.4
1	J	424	TYR	4.4
1	E	443	PRO	4.4
1	D	411	ALA	4.3
1	F	425	ALA	4.2
1	C	418	GLY	4.2
1	I	434	ALA	4.1
1	D	422	ASP	4.1
1	E	439	GLY	4.0
1	J	436	GLU	4.0
1	B	415	ILE	4.0
1	B	421	LEU	3.9
1	G	422	ASP	3.9
1	H	426	LYS	3.9
1	G	441	VAL	3.9
1	H	414	ALA	3.9
1	G	418	GLY	3.9
1	D	398	PRO	3.9
1	C	420	PRO	3.8
1	J	419	ILE	3.7
1	C	427	THR	3.7
1	H	443	PRO	3.7
1	B	434	ALA	3.7
1	A	56	THR	3.7
1	B	426	LYS	3.6
1	I	426	LYS	3.6
1	I	396	GLY	3.6
1	E	419	ILE	3.5
1	E	442	THR	3.5
1	I	56	THR	3.5
1	D	434	ALA	3.5
1	H	442	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	H	441	VAL	3.5
1	J	432	ALA	3.4
1	F	426	LYS	3.4
1	D	56	THR	3.4
1	H	444	VAL	3.4
1	E	417	GLN	3.4
1	A	9	TYR	3.4
1	D	55	TRP	3.3
1	I	55	TRP	3.3
1	G	420	PRO	3.3
1	B	422	ASP	3.3
1	J	321	GLY	3.3
1	J	425	ALA	3.2
1	C	414	ALA	3.2
1	G	443	PRO	3.2
1	F	427	THR	3.2
1	F	417	GLN	3.1
1	J	320	ALA	3.1
1	E	218	ASN	3.1
1	D	441	VAL	3.1
1	C	439	GLY	3.1
1	H	346	GLU	3.1
1	B	425	ALA	3.0
1	D	427	THR	3.0
1	F	421	LEU	3.0
1	J	442	THR	3.0
1	B	59	TYR	3.0
1	C	59	TYR	3.0
1	D	420	PRO	3.0
1	B	438	TRP	3.0
1	D	184	GLY	3.0
1	B	376	GLN	3.0
1	G	424	TYR	3.0
1	F	286	ALA	3.0
1	A	258	ILE	3.0
1	B	420	PRO	3.0
1	B	398	PRO	2.9
1	A	442	THR	2.9
1	G	414	ALA	2.9
1	B	418	GLY	2.9
1	F	56	THR	2.9
1	D	258	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	442	THR	2.9
1	J	417	GLN	2.9
1	D	423	GLU	2.9
1	G	321	GLY	2.8
1	G	442	THR	2.8
1	H	7	THR	2.8
1	C	433	ARG	2.8
1	H	377	PRO	2.8
1	H	421	LEU	2.8
1	D	57	THR	2.8
1	C	419	ILE	2.8
1	C	411	ALA	2.8
1	J	426	LYS	2.8
1	F	59	TYR	2.7
1	H	420	PRO	2.7
1	A	426	LYS	2.7
1	A	421	LEU	2.7
1	I	422	ASP	2.7
1	C	392	GLY	2.7
1	H	398	PRO	2.7
1	G	425	ALA	2.7
1	F	58	LEU	2.7
1	H	258	ILE	2.6
1	H	415	ILE	2.6
1	C	283	ALA	2.6
1	C	435	LEU	2.6
1	B	358	SER	2.6
1	C	296	ILE	2.6
1	F	8	ILE	2.6
1	B	424	TYR	2.6
1	A	422	ASP	2.6
1	I	400	GLY	2.6
1	J	420	PRO	2.6
1	B	9	TYR	2.6
1	F	424	TYR	2.6
1	A	36	GLY	2.6
1	F	422	ASP	2.6
1	A	55	TRP	2.6
1	H	257	VAL	2.6
1	B	16	GLY	2.6
1	F	296	ILE	2.6
1	C	257	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	444	VAL	2.5
1	G	9	TYR	2.5
1	F	283	ALA	2.5
1	J	443	PRO	2.5
1	A	423	GLU	2.5
1	B	436	GLU	2.5
1	G	438	TRP	2.5
1	J	438	TRP	2.5
1	H	433	ARG	2.5
1	C	443	PRO	2.5
1	G	319	GLY	2.5
1	H	320	ALA	2.5
1	F	54	THR	2.5
1	D	430	GLU	2.5
1	D	283	ALA	2.5
1	B	56	THR	2.5
1	E	427	THR	2.5
1	B	8	ILE	2.5
1	F	105	LEU	2.5
1	D	284	MET	2.5
1	C	106	ALA	2.5
1	H	109	ALA	2.5
1	E	376	GLN	2.5
1	E	106	ALA	2.4
1	H	318	ALA	2.4
1	D	426	LYS	2.4
1	E	398	PRO	2.4
1	H	347	ASN	2.4
1	H	321	GLY	2.4
1	C	428	HIS	2.4
1	D	439	GLY	2.4
1	E	110	GLY	2.4
1	C	346	GLU	2.4
1	A	283	ALA	2.4
1	C	424	TYR	2.4
1	C	437	LYS	2.4
1	D	9	TYR	2.4
1	J	59	TYR	2.4
1	J	376	GLN	2.4
1	I	427	THR	2.4
1	H	438	TRP	2.4
1	H	283	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	425	ALA	2.4
1	A	398	PRO	2.3
1	F	284	MET	2.3
1	J	398	PRO	2.3
1	B	58	LEU	2.3
1	G	411	ALA	2.3
1	H	284	MET	2.3
1	A	257	VAL	2.3
1	G	415	ILE	2.3
1	H	425	ALA	2.3
1	G	56	THR	2.3
1	F	55	TRP	2.3
1	C	321	GLY	2.3
1	E	109	ALA	2.3
1	D	257	VAL	2.3
1	E	35	GLU	2.3
1	F	258	ILE	2.3
1	C	318	ALA	2.3
1	D	313	LEU	2.3
1	E	105	LEU	2.3
1	C	284	MET	2.3
1	H	296	ILE	2.3
1	C	7	THR	2.2
1	A	396	GLY	2.2
1	I	404	GLY	2.2
1	H	106	ALA	2.2
1	D	256	VAL	2.2
1	B	53	GLY	2.2
1	J	428	HIS	2.2
1	F	400	GLY	2.2
1	G	373	GLY	2.2
1	C	289	THR	2.2
1	J	423	GLU	2.2
1	J	57	THR	2.2
1	C	415	ILE	2.2
1	A	434	ALA	2.1
1	I	414	ALA	2.1
1	G	58	LEU	2.1
1	I	395	LEU	2.1
1	I	9	TYR	2.1
1	J	440	HIS	2.1
1	H	411	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	396	GLY	2.1
1	G	436	GLU	2.1
1	A	256	VAL	2.1
1	I	57	THR	2.1
1	B	319	GLY	2.1
1	D	106	ALA	2.1
1	D	220	THR	2.1
1	E	256	VAL	2.1
1	G	320	ALA	2.1
1	I	423	GLU	2.1
1	E	418	GLY	2.1
1	G	347	ASN	2.1
1	E	36	GLY	2.1
1	E	424	TYR	2.1
1	H	418	GLY	2.1
1	I	424	TYR	2.1
1	G	377	PRO	2.1
1	E	257	VAL	2.1
1	H	81	GLY	2.1
1	H	417	GLN	2.0
1	D	435	LEU	2.0
1	B	347	ASN	2.0
1	F	106	ALA	2.0
1	I	441	VAL	2.0
1	J	433	ARG	2.0
1	C	301	LEU	2.0
1	J	418	GLY	2.0
1	D	432	ALA	2.0
1	B	417	GLN	2.0
1	C	365	THR	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, 95^{th} 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	0.96	0.20	18,20,21,22	0
1	KCX	F	189	12/13	0.96	0.18	23,25,27,27	0
1	KCX	I	189	12/13	0.96	0.13	19,21,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	KCX	C	189	12/13	0.97	0.16	21,22,26,28	0
1	KCX	G	189	12/13	0.97	0.15	16,19,20,20	0
1	KCX	H	189	12/13	0.97	0.16	20,21,25,26	0
1	KCX	E	189	12/13	0.97	0.14	18,19,23,24	0
1	KCX	J	189	12/13	0.97	0.17	19,19,24,26	0
1	KCX	A	189	12/13	0.98	0.18	20,23,24,24	0
1	KCX	D	189	12/13	0.98	0.20	21,22,24,25	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

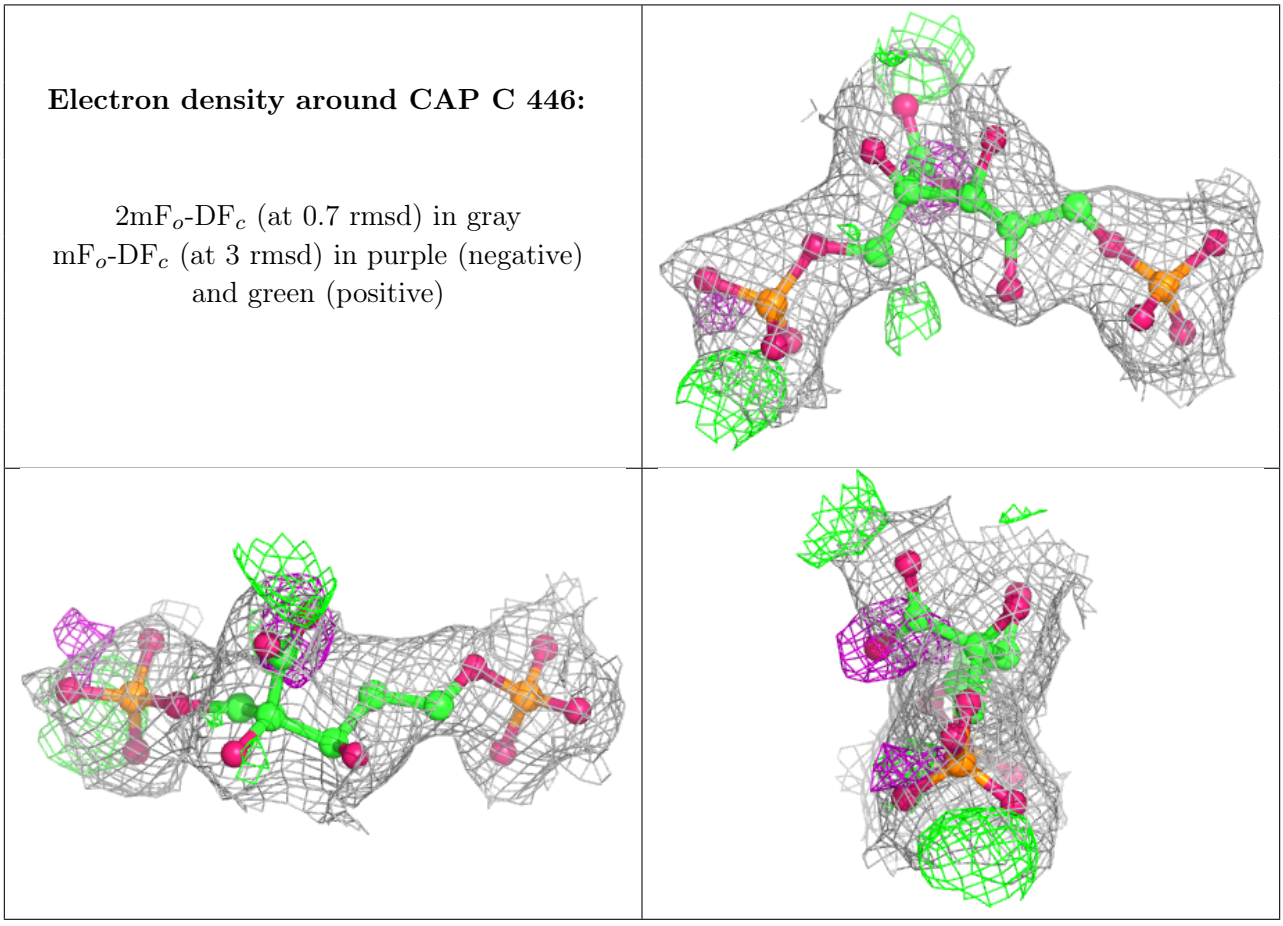
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CAP	C	446	21/21	0.93	0.20	23,34,37,39	0
2	MG	B	445	1/1	0.94	0.16	19,19,19,19	0
3	CAP	H	446	21/21	0.94	0.17	24,35,37,39	0
3	CAP	G	446	21/21	0.95	0.15	16,29,33,34	0
2	MG	C	445	1/1	0.95	0.24	23,23,23,23	0
3	CAP	J	446	21/21	0.95	0.18	20,28,40,40	0
3	CAP	E	446	21/21	0.96	0.15	16,27,37,38	0
3	CAP	F	446	21/21	0.96	0.15	24,33,34,35	0
3	CAP	B	446	21/21	0.96	0.15	18,29,35,36	0
2	MG	G	445	1/1	0.96	0.15	22,22,22,22	0
3	CAP	I	446	21/21	0.96	0.12	15,25,27,28	0
3	CAP	D	446	21/21	0.96	0.15	18,28,31,32	0
2	MG	F	445	1/1	0.97	0.05	36,36,36,36	0
2	MG	A	445	1/1	0.97	0.09	32,32,32,32	0
2	MG	I	445	1/1	0.97	0.07	21,21,21,21	0
4	CA	E	445	1/1	0.97	0.13	27,27,27,27	0
3	CAP	A	446	21/21	0.98	0.12	21,30,31,32	0
4	CA	J	445	1/1	0.98	0.19	27,27,27,27	0
2	MG	H	445	1/1	0.99	0.24	22,22,22,22	0
2	MG	D	445	1/1	0.99	0.12	27,27,27,27	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.

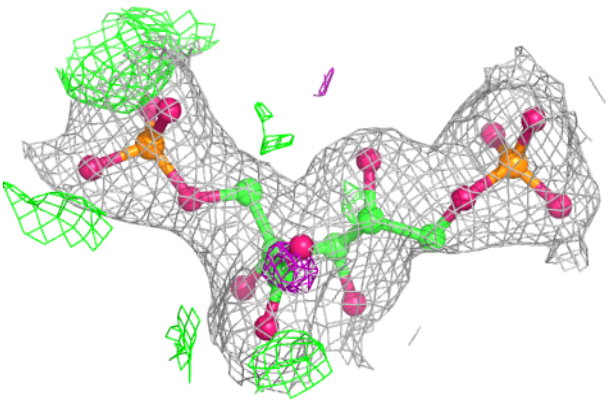
Electron density around CAP C 446:

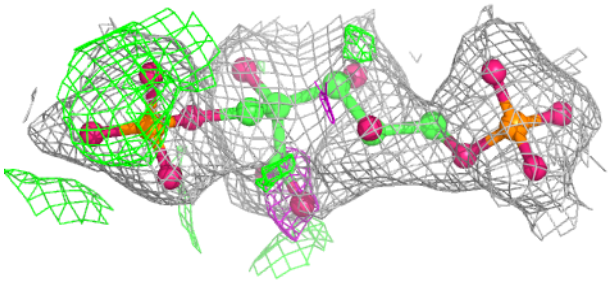
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around CAP H 446:

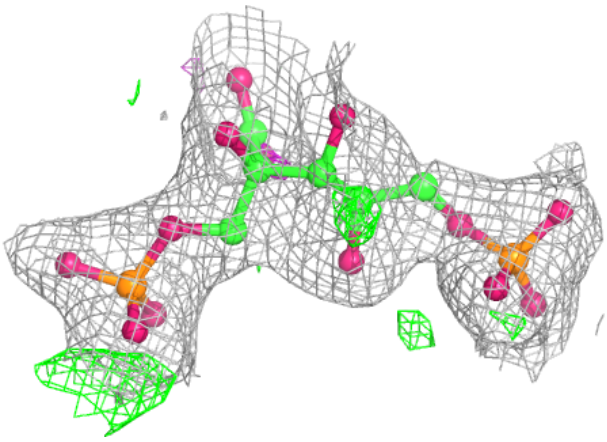
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

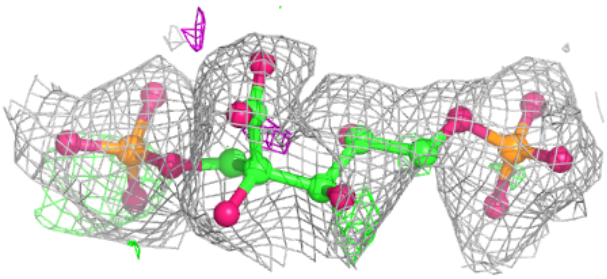




Electron density around CAP G 446:

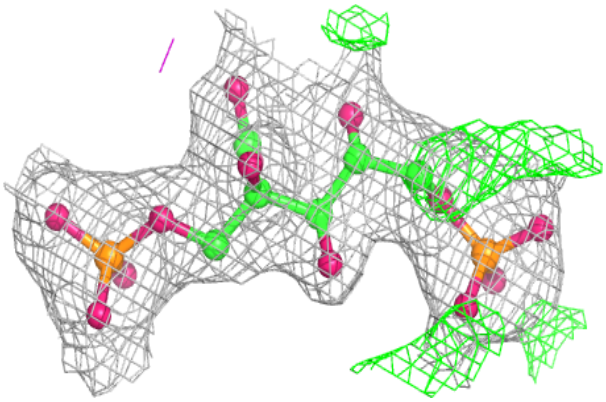
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

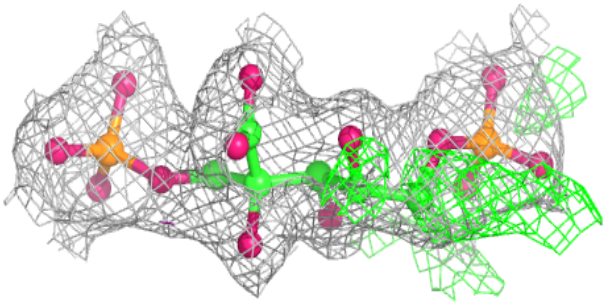


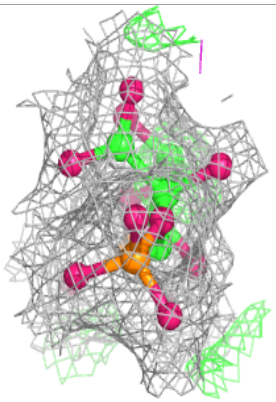


Electron density around CAP J 446:

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

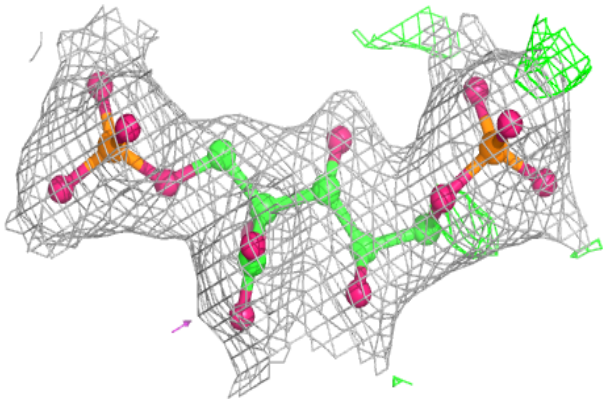


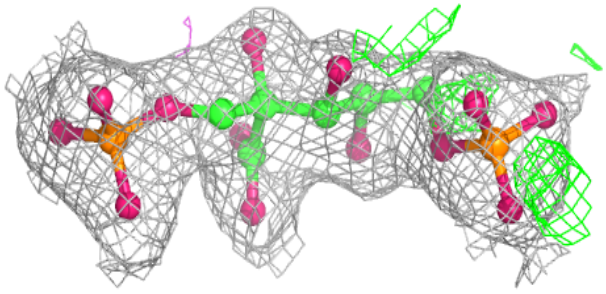


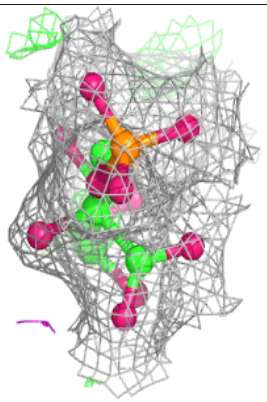


Electron density around CAP E 446:

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

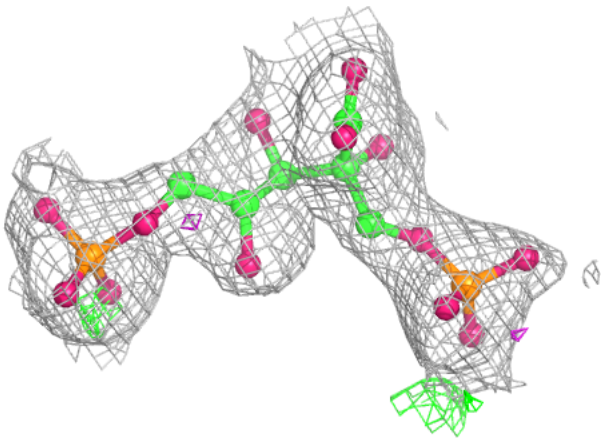


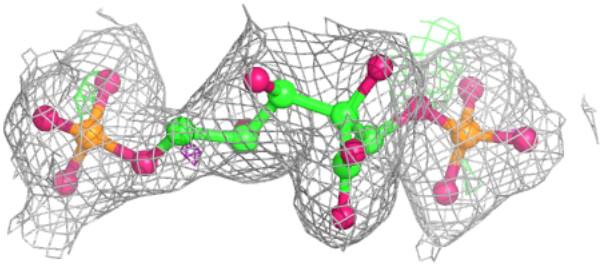


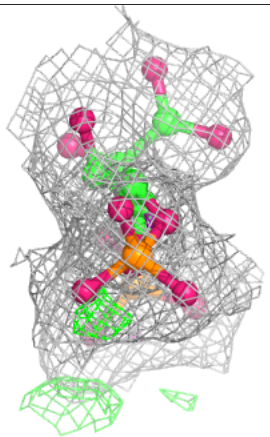


Electron density around CAP F 446:

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

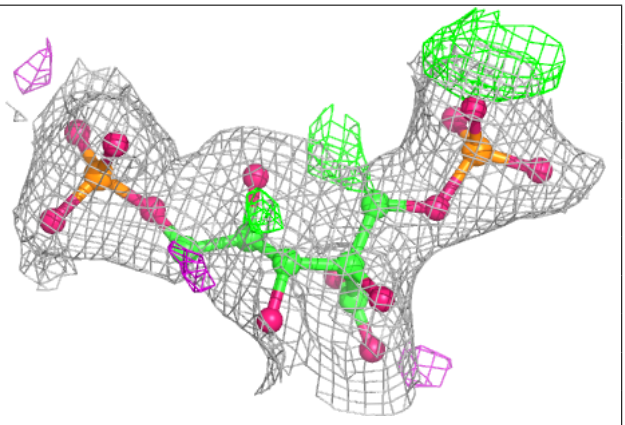


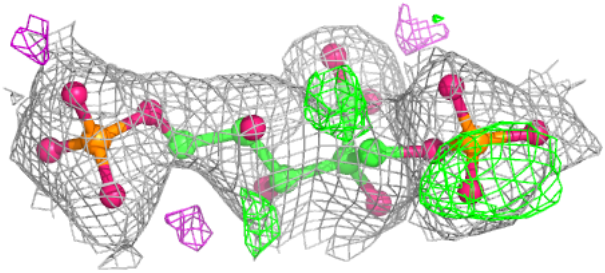


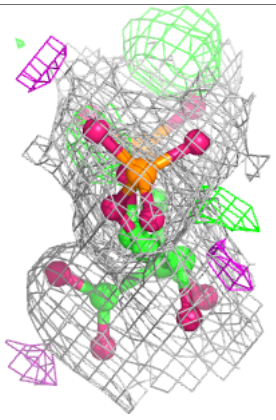


Electron density around CAP B 446:

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

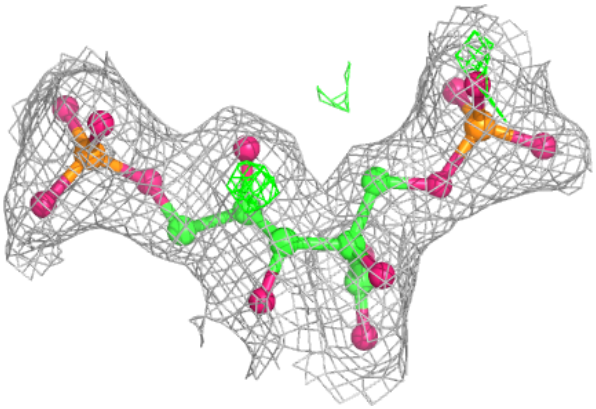


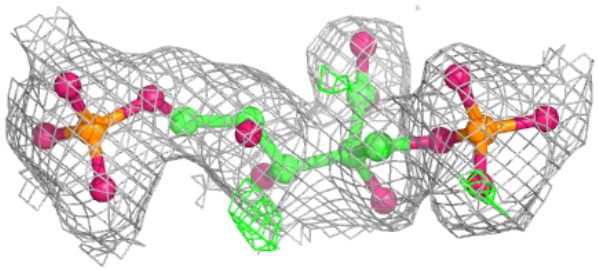


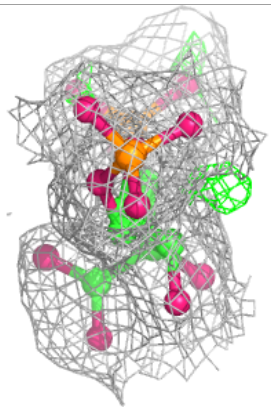


Electron density around CAP I 446:

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

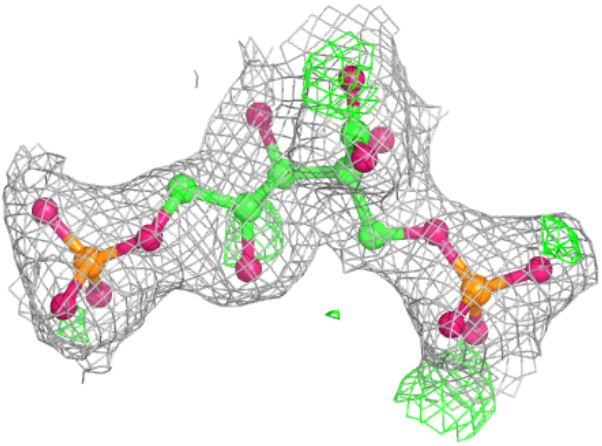


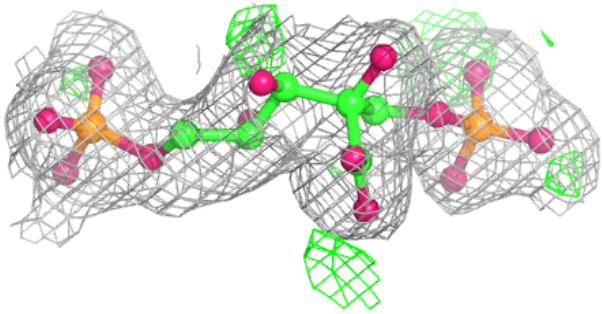


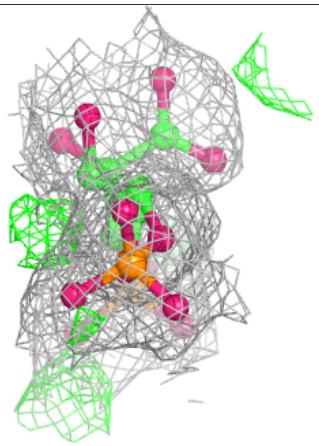


Electron density around CAP D 446:

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

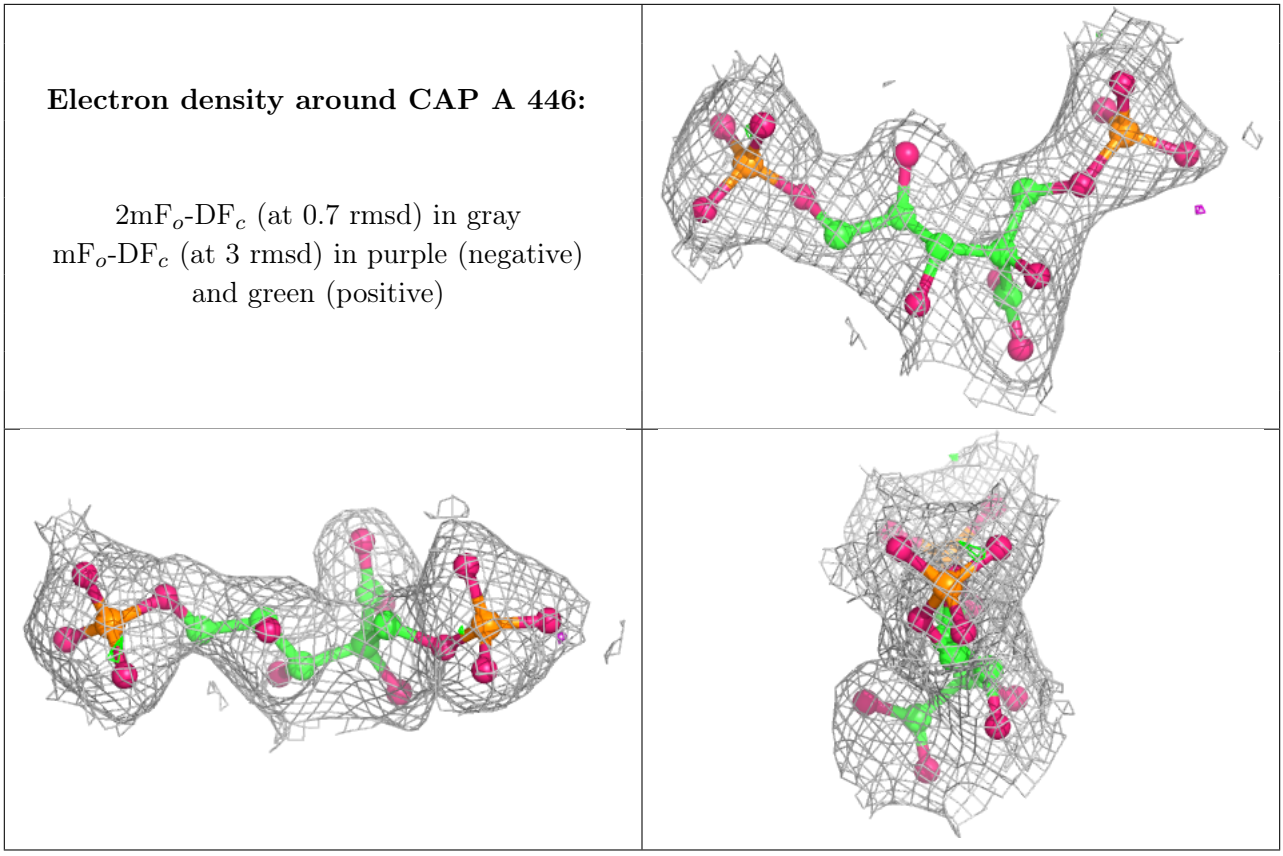






Electron density around CAP A 446:

$2mF_o$-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.