Full wwPDB X-ray Structure Validation Report (i)

Dec 7, 2023 – 12:13 pm GMT

PDB ID	:	1UZD
Title	:	Chlamydomonas,Spinach Chimeric Rubisco
Authors	:	Karkehabadi, S.; Spreitzer, R.J.; Andersson, I.
Deposited on	:	2004-03-11
Resolution	:	2.40 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 (i) 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 (i)) were used in the production of this report:

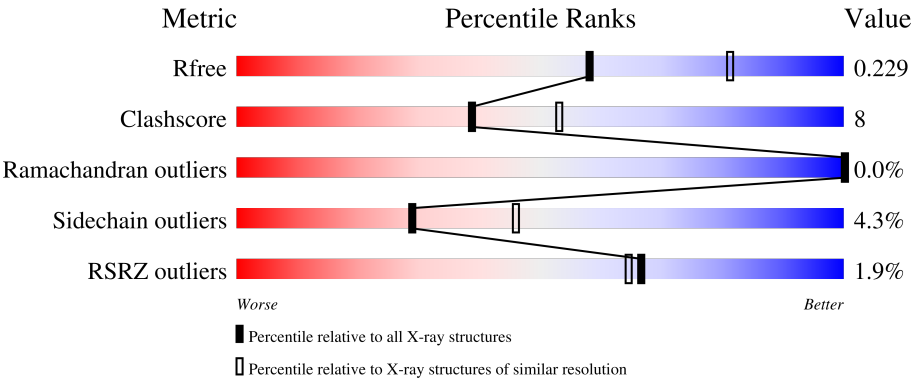
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	475	85% 11%
1	B	475	82% 14%
1	E	475	83% 15%
1	H	475	83% 14%
1	K	475	86% 12%

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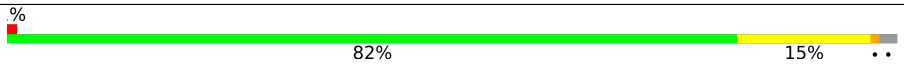
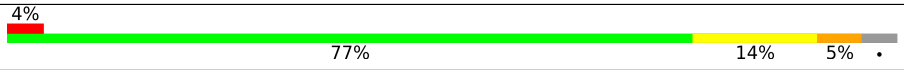
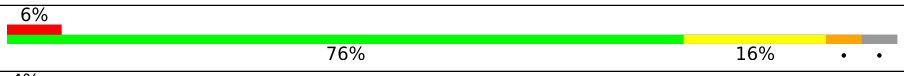
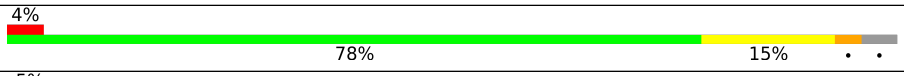
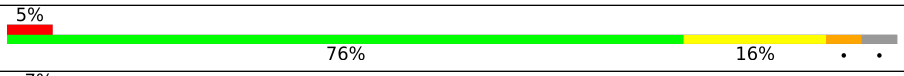
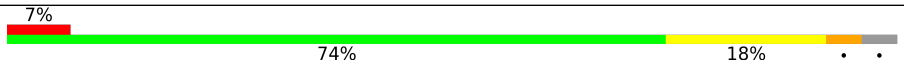
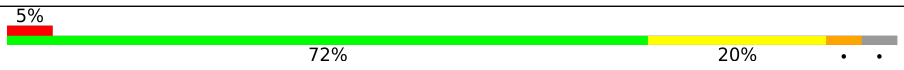
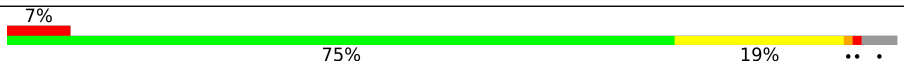
Mol	Chain	Length	Quality of chain
1	O	475	
1	R	475	
1	V	475	
2	C	134	
2	F	134	
2	I	134	
2	J	134	
2	M	134	
2	P	134	
2	T	134	
2	W	134	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	K	1482	-	-	-	X
5	EDO	O	1483	-	-	X	-
5	EDO	R	1484	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 40055 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 large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	465	Total	C	N	O	S	0	2	0
			3637	2299	641	673	24			
1	B	467	Total	C	N	O	S	0	1	0
			3641	2302	640	675	24			
1	E	465	Total	C	N	O	S	0	3	0
			3640	2300	641	675	24			
1	H	469	Total	C	N	O	S	0	1	0
			3657	2312	643	678	24			
1	K	469	Total	C	N	O	S	0	4	0
			3669	2319	646	680	24			
1	O	469	Total	C	N	O	S	0	2	0
			3661	2313	646	678	24			
1	R	465	Total	C	N	O	S	0	2	0
			3637	2299	641	673	24			
1	V	466	Total	C	N	O	S	0	2	0
			3641	2301	642	674	24			

- Molecule 2 is a protein called Ribulose bisphosphate carboxylase small chain 1, chloroplas tic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	129	Total	C	N	O	S	0	1	0
			1070	694	182	184	10			
2	F	129	Total	C	N	O	S	0	4	0
			1083	703	183	186	11			
2	I	129	Total	C	N	O	S	0	2	0
			1073	695	183	185	10			
2	J	129	Total	C	N	O	S	0	2	0
			1072	695	182	184	11			
2	M	129	Total	C	N	O	S	0	1	0
			1070	694	182	184	10			

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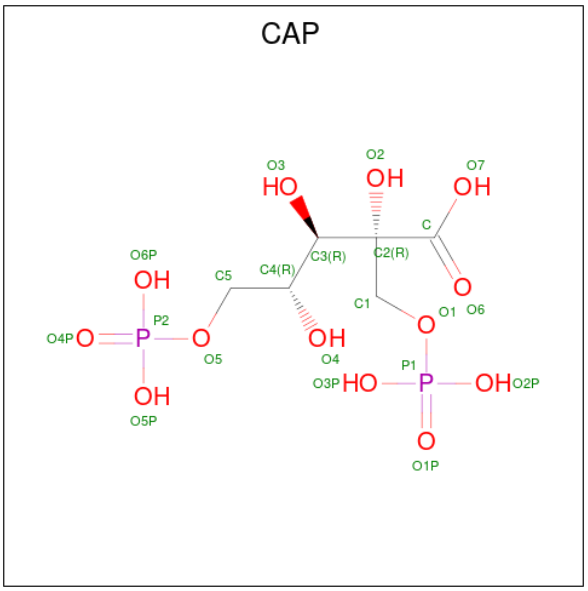
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	129	Total	C	N	O	S	0	1	0
			1070	694	182	184	10			
2	T	129	Total	C	N	O	S	0	2	0
			1078	701	182	185	10			
2	W	129	Total	C	N	O	S	0	3	0
			1073	695	182	185	11			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

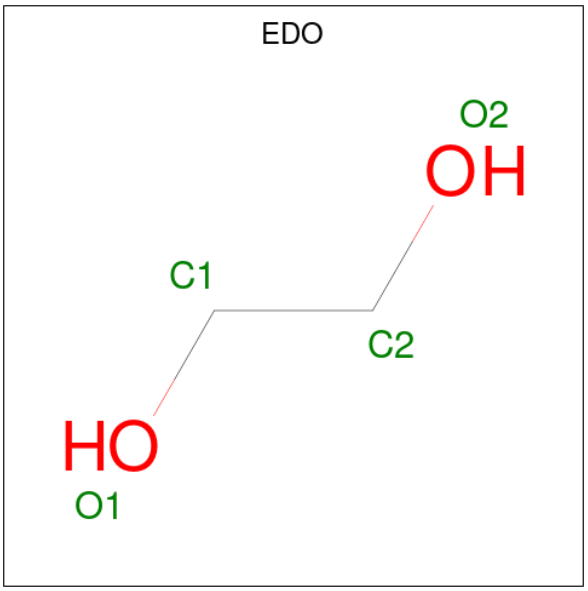
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	O	1	Total	Mg	0	0
			1	1		
3	R	1	Total	Mg	0	0
			1	1		
3	V	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 2-CARBOXYARABINITOL-1,5-DIPHOSPHATE (three-letter code: CAP) (formula: $C_6H_{14}O_{13}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			21	6	13	2		
4	B	1	Total	C	O	P	0	0
			21	6	13	2		
4	E	1	Total	C	O	P	0	0
			21	6	13	2		
4	H	1	Total	C	O	P	0	0
			21	6	13	2		
4	K	1	Total	C	O	P	0	0
			21	6	13	2		
4	O	1	Total	C	O	P	0	0
			21	6	13	2		
4	R	1	Total	C	O	P	0	0
			21	6	13	2		
4	V	1	Total	C	O	P	0	0
			21	6	13	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		
5	I	1	Total	C	O	0	0
			4	2	2		
5	J	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	K	1	Total	C	O	0	0
			4	2	2		
5	M	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		
5	O	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	O	1	Total C O 4 2 2	0	0
5	O	1	Total C O 4 2 2	0	0
5	P	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	R	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	T	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	V	1	Total C O 4 2 2	0	0
5	W	1	Total C O 4 2 2	0	0

- Molecule 6 is water.

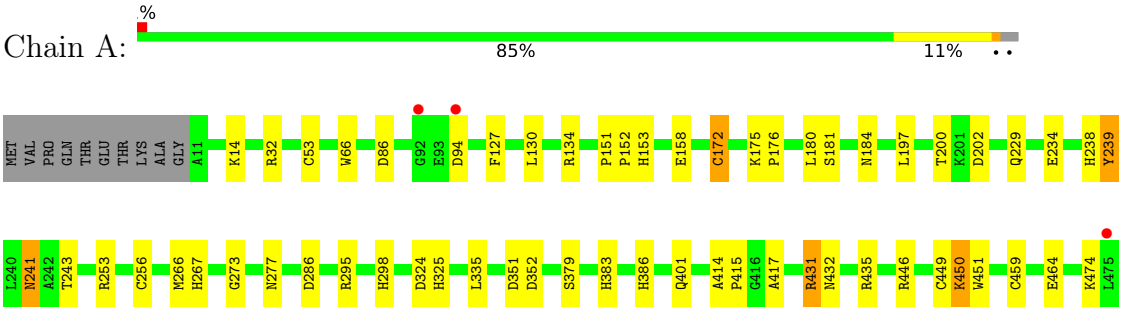
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	178	Total O 178 178	0	0
6	B	201	Total O 201 201	0	0
6	C	55	Total O 55 55	0	0
6	E	186	Total O 186 186	0	0
6	F	52	Total O 52 52	0	0
6	H	166	Total O 166 166	0	0
6	I	68	Total O 68 68	0	0
6	J	31	Total O 31 31	0	0
6	K	192	Total O 192 192	0	0
6	M	47	Total O 47 47	0	0
6	O	188	Total O 188 188	0	0
6	P	51	Total O 51 51	0	0
6	R	183	Total O 183 183	0	0
6	T	48	Total O 48 48	0	0
6	V	195	Total O 195 195	0	0
6	W	50	Total O 50 50	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

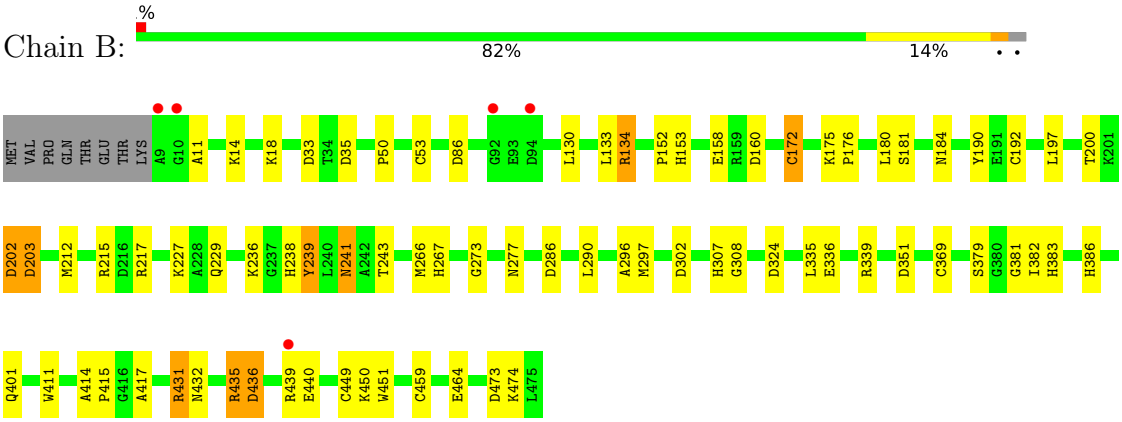
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain A:



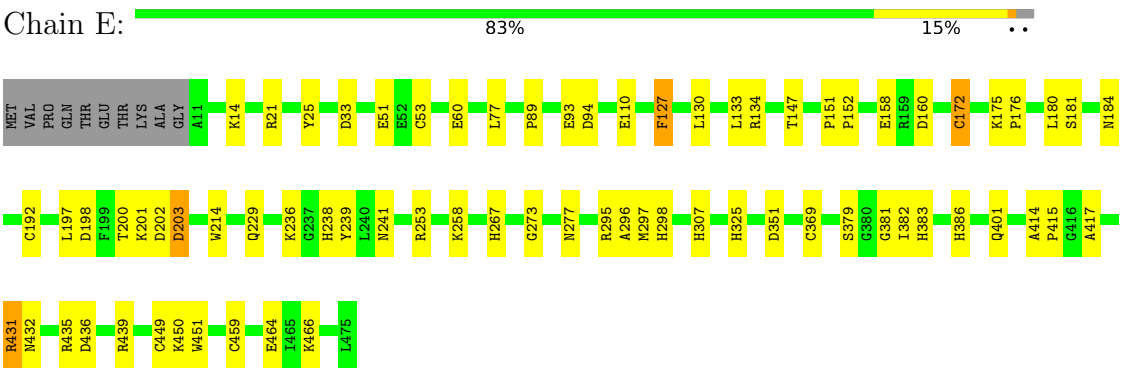
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain B:



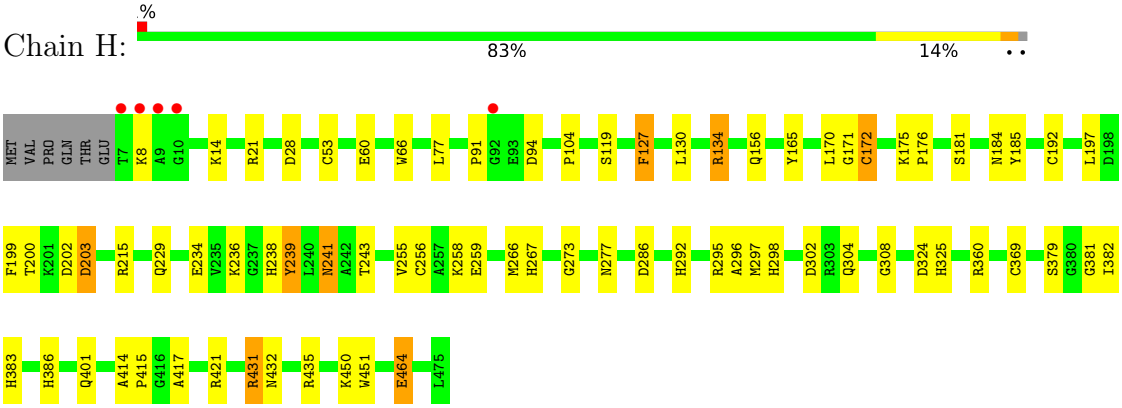
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain E:



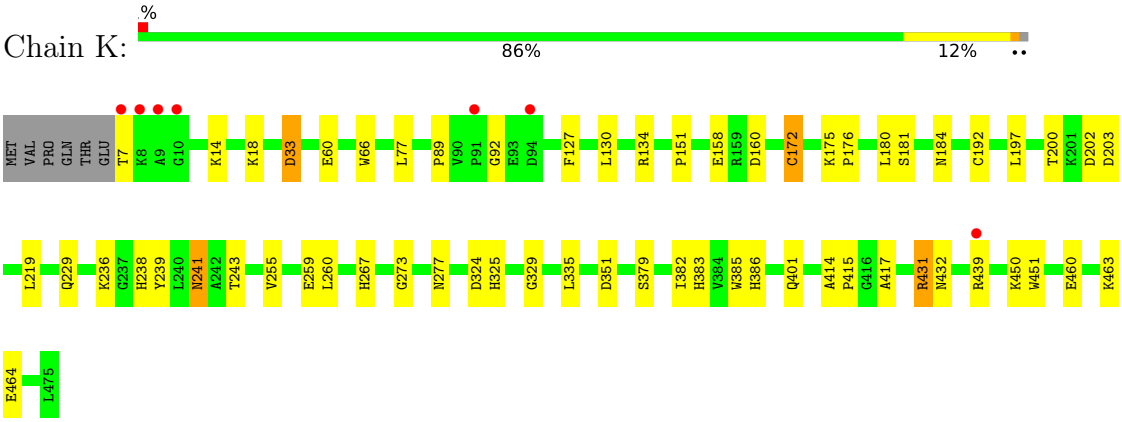
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain H:



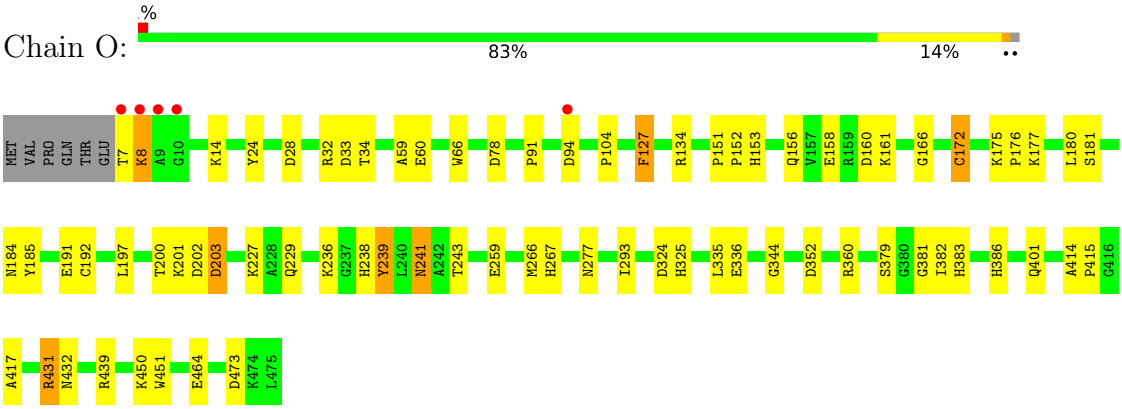
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain K:



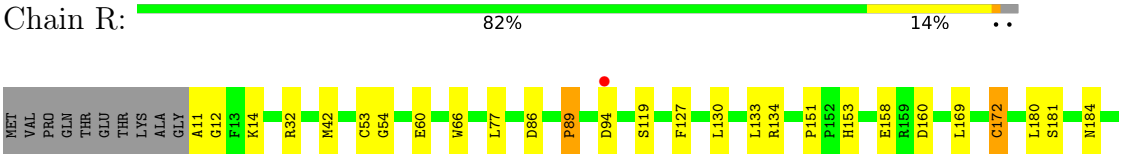
• Molecule 1: Ribulose bisphosphate carboxylase large chain

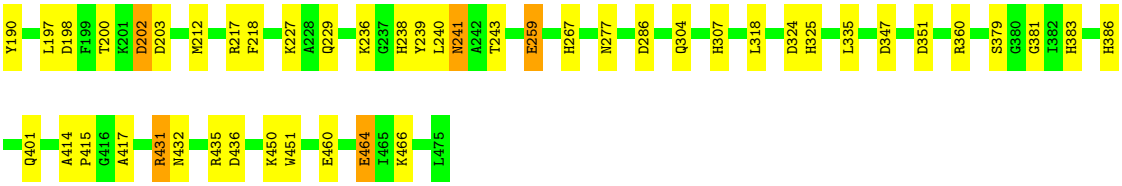
Chain O:



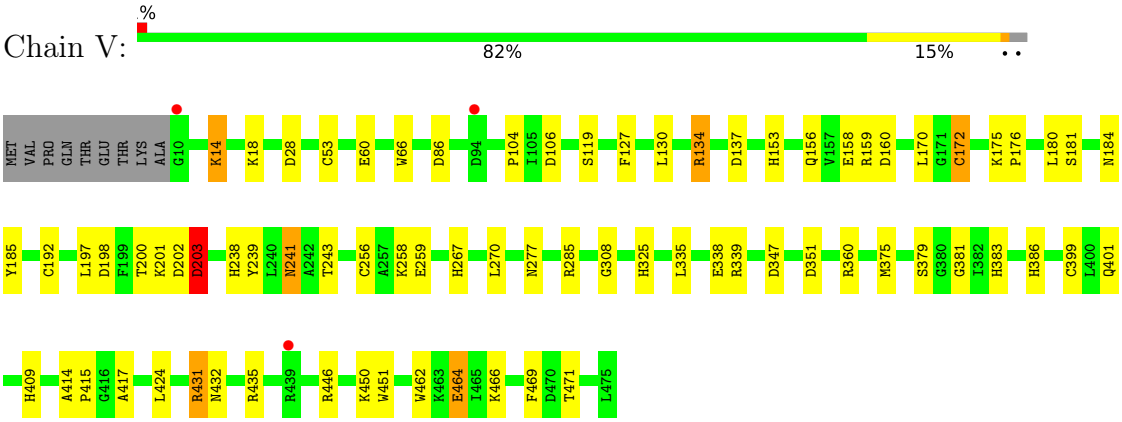
• Molecule 1: Ribulose bisphosphate carboxylase large chain

Chain R:

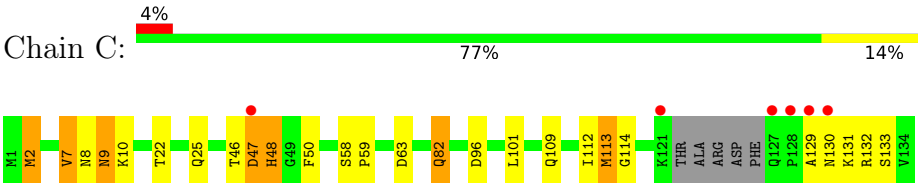




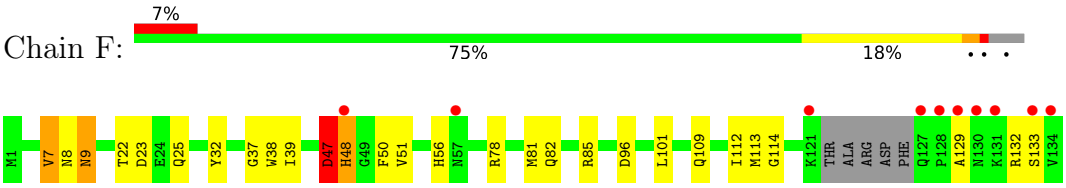
• Molecule 1: Ribulose bisphosphate carboxylase large chain



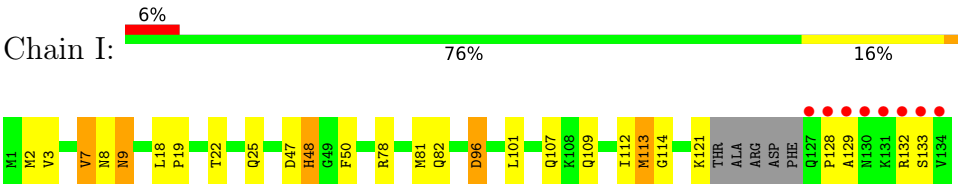
• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic



• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

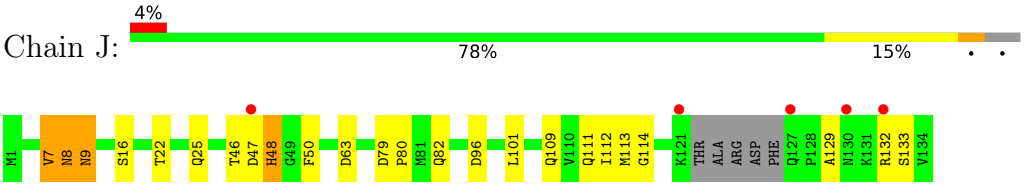


• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic



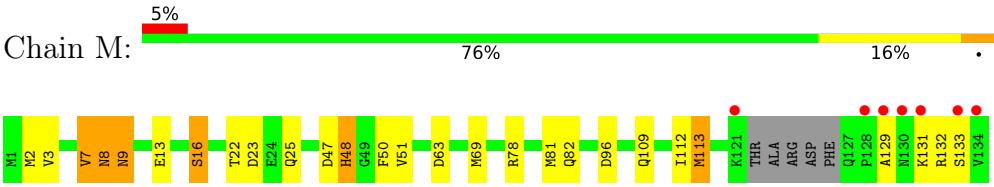
• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

Chain J:



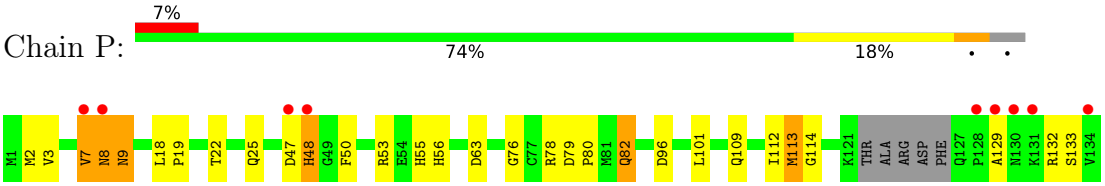
• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

Chain M:



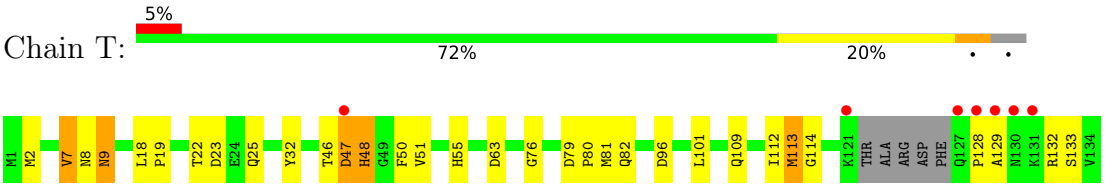
• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

Chain P:



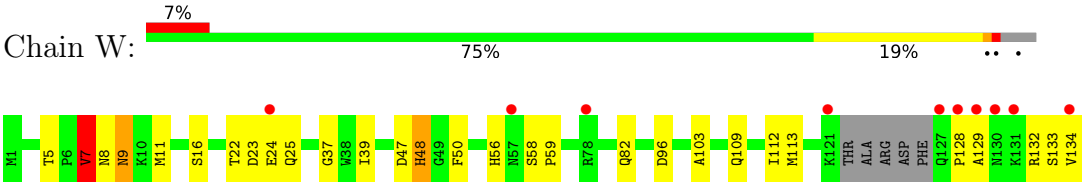
• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

Chain T:



• Molecule 2: Ribulose bisphosphate carboxylase small chain 1, chloroplastic,Ribulose bisphosphate carboxylase small chain 2, chloroplastic,Ribulose bisphosphate carboxylase small chain 1, chloroplastic

Chain W:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	220.01Å 224.08Å 111.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 49.81 – 2.38	Depositor EDS
% Data completeness (in resolution range)	93.3 (50.00-2.40) 92.0 (49.81-2.38)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.39Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.188 , 0.230 0.190 , 0.229	Depositor DCC
R_{free} test set	10149 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.0	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 31.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.037 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	40055	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: EDO, HYP, KCX, SMC, MG, CAP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.66	0/3686	0.80	6/4981 (0.1%)
1	B	0.67	0/3684	0.80	11/4979 (0.2%)
1	E	0.66	0/3695	0.80	6/4993 (0.1%)
1	H	0.67	0/3700	0.81	6/5000 (0.1%)
1	K	0.68	0/3728	0.79	5/5037 (0.1%)
1	O	0.66	0/3711	0.81	8/5014 (0.2%)
1	R	0.67	0/3686	0.80	9/4981 (0.2%)
1	V	0.66	0/3690	0.81	7/4986 (0.1%)
2	C	0.66	0/1109	0.81	4/1506 (0.3%)
2	F	0.68	0/1138	0.78	2/1545 (0.1%)
2	I	0.65	0/1117	0.75	1/1517 (0.1%)
2	J	0.70	0/1117	0.77	3/1516 (0.2%)
2	M	0.65	0/1109	0.80	4/1506 (0.3%)
2	P	0.67	0/1109	0.76	4/1506 (0.3%)
2	T	0.66	0/1122	0.78	4/1524 (0.3%)
2	W	0.68	0/1123	0.77	3/1524 (0.2%)
All	All	0.67	0/38524	0.80	83/52115 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	F	0	1
2	I	0	1
2	J	0	1
2	M	0	1
2	P	0	1
2	T	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	W	0	1
All	All	0	8

There are no bond length outliers.

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	86	ASP	CB-CG-OD2	7.02	124.61	118.30
1	E	351	ASP	CB-CG-OD2	6.94	124.54	118.30
1	O	160	ASP	CB-CG-OD2	6.75	124.38	118.30
1	R	286	ASP	CB-CG-OD2	6.44	124.09	118.30
1	R	160	ASP	CB-CG-OD2	6.36	124.02	118.30
1	H	286	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	351	ASP	CB-CG-OD2	6.28	123.95	118.30
2	T	8	ASN	N-CA-C	-6.25	94.14	111.00
1	E	33	ASP	CB-CG-OD2	6.23	123.91	118.30
2	M	47	ASP	CB-CG-OD2	6.21	123.89	118.30
2	M	8	ASN	N-CA-C	-6.18	94.32	111.00
2	C	8	ASN	N-CA-C	-6.09	94.56	111.00
1	R	86	ASP	CB-CG-OD2	6.07	123.77	118.30
1	E	160	ASP	CB-CG-OD2	6.07	123.76	118.30
2	C	63	ASP	CB-CG-OD2	6.05	123.75	118.30
1	R	202	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	324	ASP	CB-CG-OD2	6.01	123.71	118.30
2	P	63	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	160	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	86	ASP	CB-CG-OD2	5.97	123.68	118.30
2	T	23	ASP	CB-CG-OD2	5.97	123.67	118.30
1	O	324	ASP	CB-CG-OD2	5.87	123.58	118.30
2	M	7	VAL	CB-CA-C	-5.80	100.39	111.40
2	W	8	ASN	N-CA-C	-5.79	95.35	111.00
1	A	286	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	352	ASP	CB-CG-OD2	5.76	123.49	118.30
1	K	160	ASP	CB-CG-OD2	5.76	123.48	118.30
1	K	351	ASP	CB-CG-OD2	5.74	123.46	118.30
1	R	324	ASP	CB-CG-OD2	5.72	123.45	118.30
2	J	8	ASN	N-CA-C	-5.72	95.57	111.00
2	C	7	VAL	CB-CA-C	-5.71	100.56	111.40
1	V	351	ASP	CB-CG-OD2	5.68	123.41	118.30
2	J	7	VAL	CB-CA-C	-5.66	100.65	111.40
1	K	203	ASP	CB-CG-OD2	5.65	123.38	118.30
2	C	47	ASP	CB-CG-OD2	5.63	123.37	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	T	7	VAL	CB-CA-C	-5.63	100.70	111.40
1	K	324	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	33	ASP	CB-CG-OD2	5.60	123.34	118.30
1	H	28	ASP	CB-CG-OD2	5.59	123.33	118.30
1	V	137	ASP	CB-CG-OD2	5.58	123.32	118.30
2	P	8	ASN	N-CA-C	-5.56	95.98	111.00
1	V	203	ASP	CB-CG-OD2	5.55	123.29	118.30
2	M	23	ASP	CB-CG-OD2	5.54	123.29	118.30
1	V	198	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	202	ASP	CB-CG-OD2	5.54	123.29	118.30
1	B	203	ASP	CB-CG-OD2	5.53	123.28	118.30
1	O	33	ASP	CB-CG-OD2	5.53	123.28	118.30
2	F	23	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	94	ASP	CB-CG-OD2	5.49	123.24	118.30
1	O	94	ASP	CB-CG-OD2	5.48	123.23	118.30
1	H	203	ASP	CB-CG-OD2	5.46	123.21	118.30
2	I	96	ASP	CB-CG-OD2	5.46	123.21	118.30
1	O	352	ASP	CB-CG-OD2	5.46	123.21	118.30
1	V	106	ASP	CB-CG-OD2	5.43	123.19	118.30
2	W	7	VAL	CB-CA-C	-5.41	101.12	111.40
1	K	33	ASP	CB-CG-OD2	5.37	123.13	118.30
1	O	203	ASP	CB-CG-OD2	5.35	123.12	118.30
1	H	324	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	86	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	94	ASP	CB-CG-OD2	5.26	123.03	118.30
2	P	47	ASP	CB-CG-OD2	5.26	123.03	118.30
1	O	28	ASP	CB-CG-OD2	5.25	123.03	118.30
2	W	23	ASP	CB-CG-OD2	5.24	123.02	118.30
1	R	351	ASP	CB-CG-OD2	5.24	123.02	118.30
1	R	203	ASP	CB-CG-OD2	5.23	123.01	118.30
1	E	198	ASP	CB-CG-OD2	5.23	123.01	118.30
1	H	215	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	J	63	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	324	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	286	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	351	ASP	CB-CG-OD2	5.15	122.93	118.30
2	F	47	ASP	CB-CG-OD2	5.14	122.92	118.30
1	R	94	ASP	CB-CG-OD2	5.13	122.92	118.30
1	O	78	ASP	CB-CG-OD2	5.13	122.92	118.30
1	E	94	ASP	CB-CG-OD2	5.12	122.90	118.30
1	E	436	ASP	CB-CG-OD2	5.07	122.87	118.30
2	P	7	VAL	CB-CA-C	-5.07	101.77	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	215	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	35	ASP	CB-CG-OD2	5.06	122.86	118.30
2	T	63	ASP	CB-CG-OD2	5.05	122.85	118.30
1	V	160	ASP	CB-CG-OD2	5.05	122.85	118.30
1	R	436	ASP	CB-CG-OD2	5.04	122.83	118.30
1	B	436	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	7	VAL	Peptide
2	F	7	VAL	Peptide
2	I	7	VAL	Peptide
2	J	7	VAL	Peptide
2	M	7	VAL	Peptide
2	P	7	VAL	Peptide
2	T	7	VAL	Peptide
2	W	7	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3637	0	3546	41	0
1	B	3641	0	3549	52	0
1	E	3640	0	3544	56	0
1	H	3657	0	3569	50	0
1	K	3669	0	3583	43	0
1	O	3661	0	3570	49	0
1	R	3637	0	3546	54	0
1	V	3641	0	3549	57	0
2	C	1070	0	1035	25	0
2	F	1083	0	1043	27	0
2	I	1073	0	1037	31	0
2	J	1072	0	1036	17	0
2	M	1070	0	1035	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	1070	0	1035	26	0
2	T	1078	0	1040	27	0
2	W	1073	0	1037	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	H	1	0	0	0	0
3	K	1	0	0	0	0
3	O	1	0	0	0	0
3	R	1	0	0	0	0
3	V	1	0	0	0	0
4	A	21	0	7	0	0
4	B	21	0	8	0	0
4	E	21	0	8	0	0
4	H	21	0	8	1	0
4	K	21	0	7	0	0
4	O	21	0	7	0	0
4	R	21	0	7	0	0
4	V	21	0	9	0	0
5	A	24	0	36	0	0
5	B	20	0	30	2	0
5	C	8	0	12	0	0
5	E	20	0	30	2	0
5	F	4	0	6	3	0
5	H	16	0	24	2	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	20	0	30	2	0
5	M	4	0	6	0	0
5	O	24	0	36	6	0
5	P	4	0	6	1	0
5	R	28	0	42	4	0
5	T	8	0	12	5	0
5	V	24	0	36	3	0
5	W	4	0	6	2	0
6	A	178	0	0	9	0
6	B	201	0	0	11	0
6	C	55	0	0	8	0
6	E	186	0	0	13	0
6	F	52	0	0	8	0
6	H	166	0	0	12	0
6	I	68	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	31	0	0	1	0
6	K	192	0	0	11	0
6	M	47	0	0	5	0
6	O	188	0	0	15	0
6	P	51	0	0	7	0
6	R	183	0	0	19	0
6	T	48	0	0	6	0
6	V	195	0	0	21	0
6	W	50	0	0	13	0
All	All	40055	0	37139	558	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 8.

All (558) 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)
2:I:107:GLN:HG3	6:I:2053:HOH:O	1.45	1.13
1:R:169:LEU:HB3	6:R:2077:HOH:O	1.51	1.10
2:P:8:ASN:HB2	6:P:2005:HOH:O	1.49	1.09
1:K:460:GLU:HB3	6:K:2174:HOH:O	1.56	1.04
1:K:267:HIS:CD2	1:K:277:ASN:HD22	1.76	1.03
1:A:267:HIS:CD2	1:A:277:ASN:HD22	1.79	1.01
1:O:431:ARG:HH21	1:O:432:ASN:HD21	1.10	1.00
1:V:267:HIS:HD2	1:V:277:ASN:HD22	0.99	0.98
1:K:92:GLY:HA3	6:K:2041:HOH:O	1.62	0.98
1:E:267:HIS:CD2	1:E:277:ASN:HD22	1.80	0.97
1:R:12:GLY:HA3	6:R:2002:HOH:O	1.62	0.96
1:H:184:ASN:HD22	2:W:109:GLN:HE21	1.12	0.96
1:B:267:HIS:CD2	1:B:277:ASN:HD22	1.84	0.95
1:R:460:GLU:HG3	6:R:2168:HOH:O	1.67	0.95
1:R:267:HIS:CD2	1:R:277:ASN:HD22	1.84	0.94
1:O:267:HIS:CD2	1:O:277:ASN:HD22	1.83	0.94
1:E:184:ASN:HD22	2:J:109:GLN:HE21	1.16	0.94
1:B:439:ARG:HG2	6:B:2177:HOH:O	1.66	0.94
1:V:267:HIS:CD2	1:V:277:ASN:HD22	1.84	0.94
1:K:267:HIS:HD2	1:K:277:ASN:ND2	1.68	0.92
1:R:431:ARG:HH21	1:R:432:ASN:HD21	1.15	0.92
1:H:267:HIS:CD2	1:H:277:ASN:HD22	1.87	0.92
1:B:184:ASN:HD22	2:F:109:GLN:HE21	1.16	0.89
1:E:21:ARG:CZ	1:E:51[B]:GLU:HG3	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:ARG:HH21	1:E:432:ASN:HD21	1.18	0.88
2:P:109:GLN:HE21	1:R:184:ASN:HD22	1.17	0.88
1:V:375:MET:HG2	6:V:2135:HOH:O	1.73	0.88
2:C:109:GLN:HE21	1:V:184:ASN:HD22	1.18	0.88
1:R:267:HIS:HD2	1:R:277:ASN:HD22	0.92	0.88
2:I:109:GLN:HE21	1:K:184:ASN:HD22	1.18	0.87
1:A:267:HIS:HD2	1:A:277:ASN:HD22	0.88	0.87
1:O:267:HIS:HD2	1:O:277:ASN:HD22	0.91	0.87
1:B:267:HIS:HD2	1:B:277:ASN:HD22	0.92	0.87
1:H:431:ARG:HH21	1:H:432:ASN:HD21	1.21	0.86
1:O:91:PRO:HA	6:O:2036:HOH:O	1.75	0.86
1:E:267:HIS:HD2	1:E:277:ASN:ND2	1.73	0.86
1:H:267:HIS:HD2	1:H:277:ASN:HD22	0.94	0.86
1:V:431:ARG:HH21	1:V:432:ASN:HD21	1.22	0.86
2:M:109:GLN:HE21	1:O:184:ASN:HD22	1.23	0.86
1:A:431:ARG:HH21	1:A:432:ASN:HD21	1.19	0.85
1:A:184:ASN:HD22	2:T:109:GLN:HE21	1.21	0.85
1:E:383:HIS:H	1:E:386:HIS:HD2	1.26	0.84
1:E:267:HIS:HD2	1:E:277:ASN:HD22	0.88	0.84
1:K:431:ARG:HH21	1:K:432:ASN:HD21	1.21	0.84
1:A:267:HIS:HD2	1:A:277:ASN:ND2	1.73	0.82
2:I:81:MET:HE3	6:I:2046:HOH:O	1.78	0.81
1:B:431:ARG:HH21	1:B:432:ASN:HD21	1.26	0.81
1:R:466:LYS:HD2	6:R:2069:HOH:O	1.79	0.80
1:R:267:HIS:HD2	1:R:277:ASN:ND2	1.77	0.80
1:E:451:TRP:HZ2	2:F:129:ALA:HB1	1.46	0.79
2:M:129:ALA:HB1	1:R:451:TRP:HZ2	1.46	0.79
2:P:56:HIS:HE1	6:P:2021:HOH:O	1.66	0.78
2:W:134:VAL:HG22	6:W:2002:HOH:O	1.83	0.78
1:O:267:HIS:HD2	1:O:277:ASN:ND2	1.76	0.76
1:V:270:LEU:O	5:V:1478:EDO:H12	1.85	0.76
1:V:399:CYS:HB2	6:V:2135:HOH:O	1.84	0.76
2:T:128:PRO:HB3	6:T:2046:HOH:O	1.84	0.76
1:E:258:LYS:HE2	6:E:2106:HOH:O	1.84	0.76
1:A:383:HIS:H	1:A:386:HIS:HD2	1.33	0.76
1:E:21:ARG:NH2	1:E:51[A]:GLU:OE2	2.19	0.75
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.70	0.75
1:O:439:ARG:HG2	6:O:2167:HOH:O	1.86	0.75
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.70	0.74
1:V:202:ASP:OD1	1:V:238:HIS:HE1	1.71	0.74
1:A:450:LYS:HB2	6:A:2158:HOH:O	1.86	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ARG:NH1	1:E:51[B]:GLU:HG3	2.01	0.74
1:H:267:HIS:HD2	1:H:277:ASN:ND2	1.78	0.74
1:H:383:HIS:H	1:H:386:HIS:HD2	1.36	0.73
1:O:32:ARG:HD2	6:O:2037:HOH:O	1.89	0.73
1:B:267:HIS:HD2	1:B:277:ASN:ND2	1.77	0.73
2:I:2:MET:SD	6:I:2068:HOH:O	2.46	0.73
2:I:78:ARG:HD2	6:I:2039:HOH:O	1.88	0.72
2:I:78:ARG:CD	6:I:2039:HOH:O	2.36	0.72
1:K:383:HIS:H	1:K:386:HIS:HD2	1.36	0.72
1:B:451:TRP:HZ2	2:C:129:ALA:HB1	1.55	0.71
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.72	0.71
1:V:203:ASP:HB2	6:V:2081:HOH:O	1.89	0.71
1:B:339:ARG:HD3	6:B:2139:HOH:O	1.90	0.71
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.73	0.71
1:A:451:TRP:HZ2	2:I:129:ALA:HB1	1.56	0.71
1:R:11:ALA:N	6:R:2001:HOH:O	2.24	0.71
1:R:89:PRO:HD2	6:R:2034:HOH:O	1.91	0.70
1:B:449:CYS:HG	1:B:459:CYS:HG	1.38	0.70
1:R:227:LYS:N	5:R:1482:EDO:H21	2.08	0.69
2:W:5:THR:HB	6:W:2002:HOH:O	1.92	0.69
1:R:202:ASP:OD1	1:R:238:HIS:HE1	1.76	0.69
2:F:47:ASP:HB2	6:F:2024:HOH:O	1.94	0.68
5:E:1480:EDO:H21	6:E:2015:HOH:O	1.93	0.68
1:B:474:LYS:HE2	6:B:2192:HOH:O	1.93	0.68
1:R:383:HIS:H	1:R:386:HIS:HD2	1.40	0.68
1:B:11:ALA:HB3	6:B:2001:HOH:O	1.92	0.68
1:V:451:TRP:HZ2	2:W:129:ALA:HB1	1.57	0.68
1:B:383:HIS:H	1:B:386:HIS:HD2	1.42	0.68
1:K:451:TRP:HZ2	2:P:129:ALA:HB1	1.58	0.68
1:E:439:ARG:HG2	6:E:2076:HOH:O	1.92	0.67
1:K:255:VAL:O	1:K:259[B]:GLU:HG2	1.95	0.67
4:H:1477:CAP:O2P	6:H:2162:HOH:O	2.13	0.66
2:W:48[B]:HIS:HD2	2:W:50:PHE:O	1.78	0.66
1:E:93:GLU:HA	6:E:2046:HOH:O	1.95	0.66
2:T:47:ASP:HB2	6:T:2016:HOH:O	1.94	0.66
1:A:450:LYS:CB	6:A:2158:HOH:O	2.43	0.66
1:O:431:ARG:HH21	1:O:432:ASN:ND2	1.90	0.66
2:T:22:THR:H	2:T:25:GLN:HE21	1.43	0.66
1:V:383:HIS:H	1:V:386:HIS:HD2	1.41	0.66
1:V:14:LYS:HE3	6:V:2003:HOH:O	1.95	0.66
1:E:297:MET:SD	6:E:2110:HOH:O	2.54	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:W:22:THR:H	2:W:25:GLN:HE21	1.43	0.66
2:M:22:THR:H	2:M:25:GLN:HE21	1.43	0.65
1:E:449:CYS:HG	1:E:459:CYS:HG	1.41	0.65
1:O:383:HIS:H	1:O:386:HIS:HD2	1.44	0.65
1:E:21:ARG:NE	6:E:2017:HOH:O	2.30	0.65
2:C:131:LYS:HG2	6:C:2050:HOH:O	1.96	0.64
2:M:63:ASP:OD1	5:O:1483:EDO:H22	1.96	0.64
2:F:22:THR:H	2:F:25:GLN:HE21	1.42	0.64
1:H:21:ARG:HD2	6:H:2009:HOH:O	1.97	0.64
6:K:2096:HOH:O	2:P:53:ARG:HD2	1.97	0.64
1:O:451:TRP:HZ2	2:T:129:ALA:HB1	1.60	0.64
1:A:181:SER:H	2:T:109:GLN:NE2	1.95	0.64
1:O:161:LYS:CD	6:O:2071:HOH:O	2.44	0.64
1:O:161:LYS:HD2	6:O:2071:HOH:O	1.96	0.64
2:C:109:GLN:NE2	1:V:181:SER:H	1.96	0.64
1:K:267:HIS:HD2	1:K:277:ASN:HD22	0.84	0.64
1:V:258:LYS:HD3	6:V:2108:HOH:O	1.98	0.64
1:R:431:ARG:HH21	1:R:432:ASN:ND2	1.94	0.63
6:B:2105:HOH:O	2:C:59:PRO:HD2	1.97	0.63
2:C:47:ASP:HB2	6:C:2016:HOH:O	1.97	0.63
2:I:48[B]:HIS:HD2	2:I:50:PHE:O	1.82	0.63
1:E:181:SER:H	2:J:109:GLN:NE2	1.95	0.63
1:H:304:GLN:NE2	6:H:2111:HOH:O	2.32	0.63
1:E:379:SER:HB2	1:E:401:GLN:HB2	1.81	0.63
1:R:435:ARG:HD3	6:R:2153:HOH:O	1.99	0.63
2:M:48[B]:HIS:HD2	2:M:50:PHE:O	1.82	0.62
1:O:34:THR:HG23	6:O:2015:HOH:O	2.00	0.62
2:I:22:THR:H	2:I:25:GLN:HE21	1.45	0.62
2:J:48[B]:HIS:HD2	2:J:50:PHE:O	1.83	0.62
2:C:22:THR:H	2:C:25:GLN:HE21	1.46	0.61
1:E:466:LYS:HE3	6:E:2178:HOH:O	1.98	0.61
1:V:464:GLU:HB2	6:V:2183:HOH:O	2.01	0.61
1:O:202:ASP:OD1	1:O:238:HIS:HE1	1.84	0.61
2:C:48[B]:HIS:HD2	2:C:50:PHE:O	1.83	0.61
2:P:22:THR:H	2:P:25:GLN:HE21	1.48	0.61
1:K:202:ASP:OD1	1:K:238:HIS:HE1	1.84	0.61
2:M:63:ASP:HB3	5:O:1483:EDO:H22	1.81	0.61
1:R:464:GLU:HG3	6:R:2171:HOH:O	1.99	0.61
2:P:48[B]:HIS:HD2	2:P:50:PHE:O	1.84	0.61
1:V:156[B]:GLN:CD	6:V:2069:HOH:O	2.38	0.61
2:W:24:GLU:HB2	6:W:2013:HOH:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LYS:HG3	6:A:2158:HOH:O	2.02	0.60
1:V:469:PHE:CE2	5:V:1482:EDO:H21	2.36	0.60
1:A:450:LYS:CG	6:A:2158:HOH:O	2.49	0.60
2:J:22:THR:H	2:J:25:GLN:HE21	1.49	0.59
1:R:460:GLU:CG	6:R:2168:HOH:O	2.37	0.59
2:F:37:GLY:O	5:F:1135:EDO:H12	2.03	0.59
2:P:55:HIS:HE1	5:R:1482:EDO:O1	1.86	0.59
1:V:192:CYS:HB3	1:V:197:LEU:HD12	1.84	0.59
1:V:347:ASP:OD2	1:V:360[B]:ARG:NH1	2.25	0.59
1:E:435:ARG:HD3	6:E:2169:HOH:O	2.02	0.59
2:F:48[B]:HIS:HD2	2:F:50:PHE:O	1.86	0.59
2:M:129:ALA:HB1	1:R:451:TRP:CZ2	2.33	0.59
1:O:414:ALA:HB3	1:O:415:PRO:HD3	1.85	0.59
1:V:466:LYS:HD2	6:V:2187:HOH:O	2.04	0.58
1:V:267:HIS:HD2	1:V:277:ASN:ND2	1.84	0.58
1:E:431:ARG:HH21	1:E:432:ASN:ND2	1.96	0.58
1:K:379:SER:HB2	1:K:401:GLN:HB2	1.85	0.58
1:R:259:GLU:HG2	6:R:2098:HOH:O	2.03	0.57
1:H:21:ARG:CD	6:H:2009:HOH:O	2.50	0.57
1:H:360:ARG:HD3	6:H:2133:HOH:O	2.04	0.57
2:C:82:GLN:HG3	6:C:2031:HOH:O	2.05	0.57
1:H:181:SER:H	2:W:109:GLN:NE2	2.01	0.57
1:H:451:TRP:HZ2	2:J:129:ALA:HB1	1.69	0.57
1:V:159:ARG:NH2	6:V:2077:HOH:O	2.37	0.57
2:I:109:GLN:HE22	1:K:180:LEU:HA	1.70	0.57
2:T:76:GLY:H	5:T:1136:EDO:H21	1.69	0.57
1:E:297:MET:CE	6:E:2110:HOH:O	2.52	0.57
1:B:181:SER:H	2:F:109:GLN:NE2	2.01	0.57
1:B:192:CYS:HB3	1:B:197:LEU:HD12	1.87	0.56
1:E:451:TRP:CZ2	2:F:129:ALA:HB1	2.35	0.56
1:H:229:GLN:HE21	1:H:236:LYS:H	1.53	0.56
1:V:379:SER:HB2	1:V:401:GLN:HB2	1.87	0.56
1:O:153:HIS:HE1	6:O:2104:HOH:O	1.88	0.56
1:R:42:MET:SD	6:R:2020:HOH:O	2.58	0.56
1:K:439:ARG:HD2	6:K:2169:HOH:O	2.05	0.56
1:O:197:LEU:HG	1:O:417:ALA:HB1	1.87	0.56
1:R:32:ARG:HD2	6:R:2017:HOH:O	2.05	0.56
1:R:414:ALA:HB3	1:R:415:PRO:HD3	1.88	0.56
1:R:197:LEU:HG	1:R:417:ALA:HB1	1.88	0.56
2:F:81:MET:HE3	6:F:2038:HOH:O	2.06	0.56
2:F:47:ASP:CB	6:F:2024:HOH:O	2.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:383:HIS:H	1:E:386:HIS:CD2	2.15	0.55
1:V:462:TRP:HH2	6:V:2160:HOH:O	1.87	0.55
1:H:464:GLU:HB2	6:H:2157:HOH:O	2.06	0.55
2:P:109:GLN:NE2	1:R:181:SER:H	2.03	0.55
1:V:431:ARG:HD3	6:V:2167:HOH:O	2.06	0.55
2:T:76:GLY:N	5:T:1136:EDO:H21	2.22	0.55
1:E:297:MET:HE2	6:E:2110:HOH:O	2.06	0.55
2:P:9:ASN:HD21	2:P:132:ARG:HD3	1.72	0.55
2:W:9:ASN:HD21	2:W:132:ARG:HD3	1.72	0.55
1:H:431:ARG:HH21	1:H:432:ASN:ND2	1.99	0.55
2:M:109:GLN:NE2	1:O:181:SER:H	2.05	0.55
2:W:48[B]:HIS:CE1	6:W:2018:HOH:O	2.60	0.55
2:M:22:THR:H	2:M:25:GLN:NE2	2.05	0.55
1:A:474:LYS:HE3	6:A:2171:HOH:O	2.07	0.54
1:V:153:HIS:HE1	6:V:2115:HOH:O	1.89	0.54
1:A:253:ARG:HD3	6:A:2088:HOH:O	2.07	0.54
2:M:63:ASP:OD1	5:O:1483:EDO:C2	2.55	0.54
2:W:128:PRO:HB3	6:W:2048:HOH:O	2.07	0.54
1:A:449:CYS:HG	1:A:459:CYS:HG	1.46	0.54
1:O:177:LYS:HG2	1:O:203:ASP:OD2	2.07	0.54
2:P:82:GLN:HG3	6:P:2030:HOH:O	2.06	0.54
2:T:47:ASP:CB	6:T:2016:HOH:O	2.52	0.54
1:B:439:ARG:CG	6:B:2177:HOH:O	2.39	0.54
2:M:63:ASP:CG	5:O:1483:EDO:H22	2.28	0.54
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.91	0.53
1:A:383:HIS:H	1:A:386:HIS:CD2	2.21	0.53
1:V:28:ASP:HB2	6:V:2016:HOH:O	2.08	0.53
2:W:56:HIS:HE1	6:W:2024:HOH:O	1.91	0.53
1:A:379:SER:HB2	1:A:401:GLN:HB2	1.89	0.53
1:E:197:LEU:HG	1:E:417:ALA:HB1	1.90	0.53
2:W:22:THR:H	2:W:25:GLN:NE2	2.05	0.53
1:H:60:GLU:HG3	1:H:127:PHE:CZ	2.44	0.53
1:K:460:GLU:CG	6:K:2174:HOH:O	2.57	0.53
2:P:56:HIS:CE1	6:P:2021:HOH:O	2.52	0.53
1:B:379:SER:HB2	1:B:401:GLN:HB2	1.90	0.53
1:K:463:LYS:HD2	6:K:2175:HOH:O	2.08	0.53
2:M:63:ASP:CB	5:O:1483:EDO:H22	2.38	0.53
1:V:172:CYS:HB3	1:V:197:LEU:HD13	1.90	0.53
1:H:172:CYS:HB3	1:H:197:LEU:HD13	1.90	0.53
1:H:255:VAL:O	1:H:259:GLU:HG3	2.08	0.53
2:T:55:HIS:HE1	5:T:1135:EDO:O2	1.92	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:H	2:T:109:GLN:HE22	1.57	0.52
2:C:47:ASP:HB2	6:C:2015:HOH:O	2.09	0.52
2:F:48[A]:HIS:HD2	6:F:2023:HOH:O	1.91	0.52
1:K:172:CYS:HB3	1:K:197:LEU:HD13	1.91	0.52
2:T:128:PRO:HG2	6:T:2047:HOH:O	2.08	0.52
2:W:48[B]:HIS:HE1	6:W:2018:HOH:O	1.91	0.52
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.91	0.52
1:K:414:ALA:HB3	1:K:415:PRO:HD3	1.91	0.52
2:M:81:MET:HE3	6:M:2026:HOH:O	2.10	0.52
2:I:109:GLN:NE2	1:K:181:SER:H	2.07	0.52
1:R:304:GLN:NE2	6:R:2113:HOH:O	2.43	0.52
1:O:200:THR:OG1	1:O:238:HIS:HD2	1.92	0.52
2:F:39:ILE:HG12	5:F:1135:EDO:H22	1.92	0.52
1:H:259:GLU:HG2	6:H:2100:HOH:O	2.08	0.52
1:R:200:THR:OG1	1:R:238:HIS:HD2	1.92	0.52
1:R:172:CYS:HB3	1:R:197:LEU:HD13	1.90	0.52
1:E:172:CYS:HB3	1:E:197:LEU:HD13	1.91	0.52
1:A:451:TRP:CZ2	2:I:129:ALA:HB1	2.42	0.52
1:E:439:ARG:NH1	6:E:2168:HOH:O	2.43	0.52
1:V:156[B]:GLN:HG3	6:V:2069:HOH:O	2.09	0.52
2:W:37:GLY:O	5:W:1135:EDO:H11	2.10	0.52
2:C:109:GLN:HE22	1:V:180:LEU:HA	1.75	0.51
1:H:91:PRO:HA	6:H:2039:HOH:O	2.10	0.51
1:K:192:CYS:HB3	1:K:197:LEU:HD12	1.92	0.51
2:T:48[B]:HIS:HD2	2:T:50:PHE:O	1.93	0.51
1:E:181:SER:H	2:J:109:GLN:HE22	1.57	0.51
1:H:258:LYS:HD3	6:H:2100:HOH:O	2.10	0.51
2:F:78:ARG:HD2	6:F:2037:HOH:O	2.10	0.51
2:I:78:ARG:HD3	6:I:2039:HOH:O	2.06	0.51
1:B:241:ASN:ND2	1:B:243:THR:H	2.09	0.51
6:B:2097:HOH:O	2:C:10:LYS:HE3	2.10	0.51
1:B:197:LEU:HG	1:B:417:ALA:HB1	1.93	0.51
2:F:22:THR:H	2:F:25:GLN:NE2	2.07	0.51
2:M:78:ARG:CD	6:M:2025:HOH:O	2.58	0.51
2:C:9:ASN:HD21	2:C:132:ARG:HD3	1.76	0.51
1:H:379:SER:HB2	1:H:401:GLN:HB2	1.93	0.51
1:O:379:SER:HB2	1:O:401:GLN:HB2	1.93	0.51
1:E:383:HIS:N	1:E:386:HIS:HD2	2.03	0.51
1:V:200:THR:OG1	1:V:238:HIS:HD2	1.93	0.51
2:F:9:ASN:HD21	2:F:132:ARG:HD3	1.76	0.50
1:B:172:CYS:HB3	1:B:197:LEU:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:ARG:HD3	6:P:2026:HOH:O	2.11	0.50
1:H:273:GLY:HA2	5:R:1483:EDO:H22	1.92	0.50
2:J:22:THR:H	2:J:25:GLN:NE2	2.08	0.50
2:T:22:THR:H	2:T:25:GLN:NE2	2.08	0.50
1:A:197:LEU:HG	1:A:417:ALA:HB1	1.93	0.50
1:K:463:LYS:HD3	6:K:2178:HOH:O	2.11	0.50
1:K:241:ASN:ND2	1:K:243:THR:H	2.10	0.50
2:W:134:VAL:CG2	6:W:2002:HOH:O	2.53	0.50
2:C:22:THR:H	2:C:25:GLN:NE2	2.08	0.50
2:M:78:ARG:HD2	6:M:2025:HOH:O	2.12	0.50
1:R:54:GLY:HA2	6:R:2020:HOH:O	2.11	0.50
1:V:339:ARG:HD2	6:V:2139:HOH:O	2.11	0.50
2:P:2:MET:HB3	2:P:133:SER:HB2	1.92	0.50
2:I:48[B]:HIS:CE1	6:I:2027:HOH:O	2.65	0.50
1:V:134:ARG:HA	1:V:308:GLY:O	2.12	0.50
1:A:172:CYS:HB3	1:A:197:LEU:HD13	1.92	0.49
1:A:267:HIS:HE1	6:B:2112:HOH:O	1.95	0.49
2:P:22:THR:H	2:P:25:GLN:NE2	2.10	0.49
1:B:414:ALA:HB3	1:B:415:PRO:HD3	1.92	0.49
2:T:32[A]:TYR:HD2	2:T:113:MET:CE	2.24	0.49
1:V:451:TRP:CZ2	2:W:129:ALA:HB1	2.44	0.49
2:I:128:PRO:HD3	6:I:2064:HOH:O	2.12	0.49
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.48	0.49
1:E:192:CYS:HB3	1:E:197:LEU:HD12	1.95	0.49
1:O:172:CYS:HB3	1:O:197:LEU:HD13	1.94	0.49
1:H:386:HIS:HE1	6:H:2122:HOH:O	1.95	0.49
1:K:431:ARG:HH21	1:K:432:ASN:ND2	2.00	0.49
6:A:2093:HOH:O	1:B:267:HIS:HE1	1.95	0.49
1:H:181:SER:H	2:W:109:GLN:HE22	1.59	0.49
2:P:3:VAL:O	2:P:133:SER:HA	2.13	0.49
1:R:267:HIS:HE1	6:R:2094:HOH:O	1.96	0.49
1:V:175:LYS:HA	1:V:176:PRO:C	2.33	0.49
1:B:383:HIS:H	1:B:386:HIS:CD2	2.25	0.49
1:B:473:ASP:HB3	6:B:2191:HOH:O	2.13	0.48
2:F:39:ILE:CG1	5:F:1135:EDO:H22	2.44	0.48
2:I:9:ASN:HD21	2:I:132:ARG:HD3	1.77	0.48
1:A:200:THR:O	1:A:238:HIS:HA	2.13	0.48
2:C:113:MET:HB2	6:C:2043:HOH:O	2.14	0.48
2:T:81:MET:HE3	6:T:2031:HOH:O	2.13	0.48
1:B:229:GLN:HE21	1:B:236:LYS:H	1.61	0.48
1:H:134:ARG:HA	1:H:308:GLY:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:7:VAL:CG2	2:T:46:THR:HG21	2.42	0.48
2:M:109:GLN:HE22	1:O:180:LEU:HA	1.78	0.48
1:B:336:GLU:O	5:B:1482:EDO:H22	2.13	0.48
1:H:241:ASN:ND2	1:H:243:THR:H	2.11	0.48
2:W:48[B]:HIS:CD2	2:W:50:PHE:O	2.63	0.48
1:K:33:ASP:HB2	6:K:2015:HOH:O	2.13	0.48
1:K:18:LYS:HG2	5:K:1479:EDO:H21	1.96	0.48
2:M:9:ASN:HD21	2:M:132:ARG:HD3	1.79	0.48
2:M:131:LYS:HG3	6:M:2046:HOH:O	2.14	0.48
1:B:190:TYR:CZ	1:B:227:LYS:HE3	2.49	0.48
2:I:128:PRO:HD2	6:I:2063:HOH:O	2.14	0.48
1:K:197:LEU:HG	1:K:417:ALA:HB1	1.96	0.48
2:M:69:MET:HE3	6:O:2068:HOH:O	2.13	0.48
1:E:21:ARG:NH1	1:E:51[B]:GLU:CG	2.75	0.47
1:R:383:HIS:H	1:R:386:HIS:CD2	2.28	0.47
2:F:56:HIS:HD2	6:F:2026:HOH:O	1.97	0.47
1:A:414:ALA:HB3	1:A:415:PRO:HD3	1.95	0.47
1:B:180:LEU:HA	2:F:109:GLN:HE22	1.80	0.47
1:R:379:SER:HB2	1:R:401:GLN:HB2	1.94	0.47
1:B:202:ASP:OD1	1:B:238:HIS:CE1	2.60	0.47
1:V:60:GLU:HG3	1:V:127:PHE:CZ	2.49	0.47
1:O:382:ILE:HA	1:O:386:HIS:CD2	2.50	0.47
1:E:175:LYS:HA	1:E:176:PRO:C	2.35	0.47
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.49	0.47
1:H:383:HIS:H	1:H:386:HIS:CD2	2.23	0.47
2:I:22:THR:H	2:I:25:GLN:NE2	2.11	0.47
1:K:200:THR:OG1	1:K:238:HIS:HD2	1.96	0.47
1:O:192:CYS:HB3	1:O:197:LEU:HD12	1.96	0.47
1:V:197:LEU:HG	1:V:417:ALA:HB1	1.95	0.47
1:A:180:LEU:HA	2:T:109:GLN:HE22	1.80	0.47
1:A:431:ARG:HH21	1:A:432:ASN:ND2	2.00	0.47
1:K:229:GLN:HE21	1:K:236:LYS:H	1.63	0.47
1:H:383:HIS:N	1:H:386:HIS:HD2	2.07	0.47
1:K:431:ARG:HD3	6:K:2157:HOH:O	2.15	0.47
1:O:473:ASP:HB3	6:O:2123:HOH:O	2.15	0.47
1:B:212:MET:SD	1:B:217:ARG:HD3	2.55	0.47
1:K:175:LYS:HA	1:K:176:PRO:C	2.35	0.47
1:R:435:ARG:HG3	6:R:2154:HOH:O	2.15	0.47
2:T:9:ASN:HD21	2:T:132:ARG:HD3	1.79	0.47
1:V:383:HIS:H	1:V:386:HIS:CD2	2.28	0.47
1:V:431:ARG:HH21	1:V:432:ASN:ND2	2.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:175:LYS:HA	1:H:176:PRO:C	2.36	0.46
1:K:451:TRP:CZ2	2:P:129:ALA:HB1	2.46	0.46
2:W:16[B]:SER:HB2	6:W:2044:HOH:O	2.14	0.46
2:I:2:MET:HB3	2:I:133:SER:HB2	1.98	0.46
1:E:203:ASP:HB2	6:E:2080:HOH:O	2.15	0.46
1:H:66:TRP:CD1	1:R:381:GLY:HA2	2.50	0.46
1:B:302:ASP:HA	6:B:2122:HOH:O	2.16	0.46
1:O:191:GLU:HG3	6:O:2068:HOH:O	2.15	0.46
2:I:48[B]:HIS:CE1	6:I:2026:HOH:O	2.69	0.46
1:R:133:LEU:O	1:R:307:HIS:HA	2.15	0.46
1:V:241:ASN:ND2	1:V:243:THR:H	2.13	0.46
1:A:383:HIS:N	1:A:386:HIS:HD2	2.09	0.46
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.97	0.46
2:T:76:GLY:H	5:T:1136:EDO:C2	2.29	0.46
1:K:383:HIS:H	1:K:386:HIS:CD2	2.24	0.46
2:J:101:LEU:O	2:J:114:GLY:HA2	2.16	0.46
1:E:25:TYR:CZ	1:E:51[A]:GLU:HG2	2.51	0.46
2:F:7:VAL:CG2	2:J:46:THR:HG21	2.46	0.46
1:K:60:GLU:HG3	1:K:127:PHE:CZ	2.50	0.46
1:O:277:ASN:HD21	1:O:293:ILE:HD12	1.81	0.46
1:R:383:HIS:N	1:R:386:HIS:HD2	2.10	0.46
2:T:113:MET:HB2	6:T:2042:HOH:O	2.16	0.46
1:K:382:ILE:HA	1:K:386:HIS:CD2	2.51	0.45
1:O:241:ASN:ND2	1:O:243:THR:H	2.14	0.45
1:O:383:HIS:H	1:O:386:HIS:CD2	2.29	0.45
1:R:229:GLN:HE21	1:R:236:LYS:H	1.62	0.45
1:B:431:ARG:HH21	1:B:432:ASN:ND2	2.04	0.45
1:V:156[B]:GLN:NE2	6:V:2070:HOH:O	2.50	0.45
1:V:409:HIS:N	6:V:2160:HOH:O	2.48	0.45
2:C:48[B]:HIS:CD2	2:C:50:PHE:O	2.68	0.45
2:C:109:GLN:HE22	1:V:181:SER:H	1.62	0.45
1:O:175:LYS:HA	1:O:176:PRO:C	2.36	0.45
2:W:58:SER:HB2	2:W:59:PRO:HD2	1.97	0.45
2:F:85:ARG:HG3	6:F:2038:HOH:O	2.16	0.45
5:H:1480:EDO:H21	6:H:2024:HOH:O	2.17	0.45
2:F:133:SER:HB3	6:F:2002:HOH:O	2.17	0.45
2:M:2:MET:HB3	2:M:133:SER:HB2	1.99	0.45
1:O:451:TRP:CZ2	2:T:129:ALA:HB1	2.47	0.45
1:O:239:TYR:HB3	1:O:266:MET:HB3	1.98	0.44
1:B:239:TYR:HB3	1:B:266:MET:HB3	2.00	0.44
1:B:411:TRP:CZ3	2:C:2:MET:HG3	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:128:PRO:HA	6:I:2065:HOH:O	2.17	0.44
1:K:158:GLU:CD	1:K:325:HIS:HE2	2.20	0.44
1:O:158:GLU:CD	1:O:325:HIS:HE2	2.18	0.44
1:V:156[B]:GLN:CG	6:V:2069:HOH:O	2.65	0.44
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.52	0.44
2:I:128:PRO:HG2	6:I:2063:HOH:O	2.18	0.44
1:B:451:TRP:CZ2	2:C:129:ALA:HB1	2.43	0.44
1:H:200:THR:OG1	1:H:238:HIS:HD2	2.01	0.44
1:O:259:GLU:HG3	6:O:2096:HOH:O	2.17	0.44
1:R:158:GLU:CD	1:R:325:HIS:HE2	2.21	0.44
1:R:200:THR:O	1:R:238:HIS:HA	2.16	0.44
1:A:175:LYS:HA	1:A:176:PRO:C	2.38	0.44
1:E:273:GLY:HA3	1:K:273:GLY:HA3	1.99	0.44
1:H:170:LEU:HD11	1:H:421:ARG:HA	1.99	0.44
2:I:47:ASP:HB2	6:I:2025:HOH:O	2.16	0.44
2:J:9:ASN:HD21	2:J:132:ARG:HD3	1.81	0.44
1:R:198:ASP:HB2	6:R:2077:HOH:O	2.16	0.44
1:E:151:HYP:HA	1:E:152:PRO:HD3	1.92	0.44
2:T:101:LEU:O	2:T:114:GLY:HA2	2.18	0.44
1:H:77:LEU:HD21	5:H:1478:EDO:H12	2.00	0.44
2:M:3:VAL:O	2:M:133:SER:HA	2.18	0.44
1:V:18:LYS:O	5:V:1480:EDO:H22	2.18	0.44
2:F:32[A]:TYR:CE2	2:F:38:TRP:HZ3	2.36	0.44
1:H:239:TYR:HB3	1:H:266:MET:HB3	2.00	0.44
2:I:113:MET:HB2	6:I:2057:HOH:O	2.18	0.44
1:H:296:ALA:O	1:H:297:MET:CB	2.65	0.44
1:H:414:ALA:HB3	1:H:415:PRO:HD3	1.98	0.44
1:E:229:GLN:HE21	1:E:236:LYS:H	1.65	0.43
2:C:47:ASP:CB	6:C:2016:HOH:O	2.62	0.43
1:E:180:LEU:HA	2:J:109:GLN:HE22	1.82	0.43
1:H:156[B]:GLN:CD	6:H:2066:HOH:O	2.55	0.43
2:I:48[B]:HIS:CD2	2:I:50:PHE:O	2.66	0.43
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.66	0.43
1:A:446:ARG:HD3	6:A:2157:HOH:O	2.17	0.43
1:E:295:ARG:HG3	1:E:298:HIS:CD2	2.53	0.43
1:R:153:HIS:HE1	6:R:2108:HOH:O	2.00	0.43
1:B:175:LYS:HA	1:B:176:PRO:C	2.39	0.43
1:O:227:LYS:HB2	5:O:1483:EDO:H12	2.00	0.43
2:M:48[B]:HIS:CD2	2:M:50:PHE:O	2.68	0.43
1:B:435:ARG:HD2	1:B:440:GLU:OE1	2.19	0.43
2:J:48[B]:HIS:CD2	2:J:50:PHE:O	2.69	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:383:HIS:CE1	1:K:385:TRP:HB2	2.54	0.43
2:M:78:ARG:HD3	6:M:2025:HOH:O	2.19	0.43
2:C:46:THR:HG21	2:W:7:VAL:CG2	2.48	0.43
2:P:109:GLN:HE22	1:R:181:SER:H	1.66	0.43
1:B:436:ASP:OD2	1:B:439:ARG:HD3	2.19	0.43
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.52	0.43
1:H:192:CYS:HB3	1:H:197:LEU:HD12	2.01	0.43
1:K:239:TYR:HE2	1:K:401:GLN:HE22	1.65	0.43
5:E:1480:EDO:H11	6:E:2186:HOH:O	2.19	0.43
2:T:55:HIS:HE1	5:T:1135:EDO:H12	1.83	0.43
1:O:336:GLU:HG2	6:O:2123:HOH:O	2.18	0.43
1:O:381:GLY:HA2	1:V:66:TRP:CD1	2.54	0.43
1:E:60:GLU:HG3	1:E:127:PHE:CZ	2.54	0.42
1:O:66:TRP:CD1	1:V:381:GLY:HA2	2.54	0.42
1:R:241:ASN:ND2	1:R:243:THR:H	2.17	0.42
1:O:344:GLY:HA2	1:O:360[B]:ARG:NH1	2.34	0.42
1:V:285:ARG:NH2	6:V:2118:HOH:O	2.52	0.42
1:E:77:LEU:HD12	1:E:77:LEU:HA	1.93	0.42
1:E:381:GLY:HA2	1:K:66:TRP:CD1	2.54	0.42
1:R:318:LEU:HD13	1:R:318:LEU:C	2.39	0.42
1:V:414:ALA:HB3	1:V:415:PRO:HD3	2.00	0.42
1:B:200:THR:OG1	1:B:238:HIS:CD2	2.71	0.42
2:P:113:MET:HB2	6:P:2040:HOH:O	2.18	0.42
2:T:2:MET:HB3	2:T:133:SER:HB2	2.01	0.42
1:B:18:LYS:O	5:B:1479:EDO:H12	2.19	0.42
1:A:32:ARG:HD2	6:A:2034:HOH:O	2.20	0.42
1:A:241:ASN:ND2	1:A:243:THR:H	2.17	0.42
2:I:121:LYS:CE	6:I:2062:HOH:O	2.67	0.42
2:M:113:MET:HB2	6:R:2063:HOH:O	2.19	0.42
1:O:229:GLN:NE2	6:O:2089:HOH:O	2.43	0.42
2:P:101:LEU:O	2:P:114:GLY:HA2	2.20	0.42
1:V:200:THR:O	1:V:238:HIS:HA	2.19	0.42
1:V:446:ARG:HD3	6:V:2175:HOH:O	2.19	0.42
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.20	0.42
1:A:295:ARG:HG3	1:A:298:HIS:CD2	2.55	0.42
6:B:2183:HOH:O	2:C:133:SER:HB3	2.19	0.42
1:O:166:GLY:N	6:O:2073:HOH:O	2.38	0.42
1:O:229:GLN:HE21	1:O:236:LYS:H	1.66	0.42
1:R:239:TYR:HE2	1:R:401:GLN:HE22	1.68	0.42
1:E:110:GLU:HB3	1:E:147:THR:HB	2.02	0.42
1:H:165:TYR:CD1	2:J:111:GLN:HB3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:55:HIS:CE1	5:R:1482:EDO:O1	2.68	0.42
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.55	0.42
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.67	0.42
1:A:239:TYR:HB3	1:A:266:MET:HB3	2.02	0.42
1:E:214:TRP:CE3	1:E:253:ARG:HG2	2.55	0.42
1:H:229:GLN:HG3	1:H:234:GLU:O	2.19	0.42
1:H:302:ASP:OD1	1:H:302:ASP:C	2.58	0.42
1:O:151:HYP:HA	1:O:152:PRO:HD3	1.91	0.42
1:V:156[B]:GLN:CD	6:V:2070:HOH:O	2.57	0.42
1:V:170:LEU:HG	1:V:424:LEU:HD22	2.02	0.42
5:W:1135:EDO:H22	6:W:2034:HOH:O	2.20	0.42
2:C:130:ASN:HA	6:C:2049:HOH:O	2.20	0.41
1:E:267:HIS:HE1	6:K:2115:HOH:O	2.03	0.41
2:J:133:SER:HB3	6:J:2002:HOH:O	2.19	0.41
1:V:338:GLU:HB2	1:V:471:THR:HG21	2.01	0.41
2:F:48[B]:HIS:CD2	2:F:50:PHE:O	2.71	0.41
2:P:79:ASP:HA	2:P:80:PRO:HD2	1.89	0.41
2:W:11:MET:HE1	2:W:132:ARG:HD3	2.01	0.41
1:A:273:GLY:HA3	1:B:273:GLY:HA3	2.01	0.41
1:E:21:ARG:NH2	1:E:51[B]:GLU:HG3	2.31	0.41
1:H:171:GLY:HA2	1:H:199:PHE:O	2.21	0.41
2:I:18:LEU:HB3	2:I:19:PRO:HD2	2.01	0.41
1:B:133:LEU:O	1:B:307:HIS:HA	2.20	0.41
1:E:133:LEU:O	1:E:307:HIS:HA	2.20	0.41
1:H:381:GLY:HA2	1:R:66:TRP:CD1	2.55	0.41
1:V:383:HIS:N	1:V:386:HIS:HD2	2.13	0.41
2:I:3:VAL:O	2:I:133:SER:HA	2.20	0.41
1:O:156[A]:GLN:NE2	6:O:2066:HOH:O	2.53	0.41
1:R:347:ASP:OD2	1:R:360[B]:ARG:NH2	2.45	0.41
1:B:181:SER:H	2:F:109:GLN:HE22	1.66	0.41
2:F:101:LEU:O	2:F:114:GLY:HA2	2.21	0.41
1:R:190:TYR:CZ	1:R:227:LYS:HE3	2.56	0.41
2:W:24:GLU:CB	6:W:2013:HOH:O	2.62	0.41
2:W:39:ILE:O	2:W:103:ALA:HA	2.21	0.41
1:B:296:ALA:O	1:B:297:MET:CB	2.69	0.41
1:E:158:GLU:CD	1:E:325:HIS:HE2	2.21	0.41
1:H:292:HIS:HA	1:H:325:HIS:HB2	2.02	0.41
2:P:109:GLN:HE22	1:R:180:LEU:HA	1.85	0.41
1:R:77:LEU:HD12	1:R:77:LEU:HA	1.96	0.41
1:A:229:GLN:HG3	1:A:234:GLU:O	2.21	0.41
2:C:58:SER:HB3	6:C:2021:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:197:LEU:HG	1:H:417:ALA:HB1	2.01	0.41
1:K:18:LYS:H	5:K:1479:EDO:H21	1.85	0.41
1:V:158:GLU:CD	1:V:325:HIS:HE2	2.21	0.41
1:B:382:ILE:HA	1:B:386:HIS:HD2	1.85	0.41
1:E:200:THR:O	1:E:238:HIS:HA	2.21	0.41
1:E:414:ALA:HB3	1:E:415:PRO:HD3	2.03	0.41
2:I:101:LEU:O	2:I:114:GLY:HA2	2.21	0.41
1:K:329:GLY:HA2	6:K:2185:HOH:O	2.20	0.41
1:R:60:GLU:HG3	1:R:127:PHE:CZ	2.56	0.41
1:V:464:GLU:HA	1:V:464:GLU:OE1	2.21	0.41
1:R:218:PHE:CD1	1:R:240:LEU:HD22	2.56	0.41
2:W:132:ARG:NH1	6:W:2050:HOH:O	2.53	0.41
1:B:383:HIS:N	1:B:386:HIS:HD2	2.14	0.40
1:K:77:LEU:HD12	1:K:77:LEU:HA	1.91	0.40
1:O:60:GLU:HG3	1:O:127:PHE:CZ	2.56	0.40
2:P:48[B]:HIS:CD2	2:P:50:PHE:O	2.70	0.40
1:B:158:GLU:HG3	1:B:290:LEU:HD22	2.03	0.40
1:E:296:ALA:O	1:E:297:MET:CB	2.69	0.40
1:O:7:THR:N	1:O:8:LYS:HE3	2.35	0.40
1:R:212:MET:SD	1:R:217:ARG:HD3	2.61	0.40
1:B:134:ARG:HA	1:B:308:GLY:O	2.21	0.40
2:C:101:LEU:O	2:C:114:GLY:HA2	2.21	0.40
1:E:295:ARG:O	1:E:296:ALA:C	2.60	0.40
2:J:79:ASP:HA	2:J:80:PRO:HD2	1.92	0.40
2:P:18:LEU:HB3	2:P:19:PRO:HD2	2.02	0.40
2:T:18:LEU:HB3	2:T:19:PRO:HD2	2.03	0.40
2:T:79:ASP:HA	2:T:80:PRO:HD2	1.88	0.40
1:A:66:TRP:CD1	1:B:381:GLY:HA2	2.56	0.40
1:K:219[A]:LEU:HD12	1:K:260:LEU:HD21	2.04	0.40
1:O:24:TYR:CD2	1:O:59:ALA:HB2	2.56	0.40
2:P:76:GLY:HA2	5:P:1135:EDO:H22	2.03	0.40
1:H:295:ARG:HG3	1:H:298:HIS:CD2	2.56	0.40
2:M:13:GLU:O	2:M:16:SER:OG	2.36	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	460/475 (97%)	448 (97%)	12 (3%)	0	100	100
1	B	461/475 (97%)	446 (97%)	15 (3%)	0	100	100
1	E	461/475 (97%)	448 (97%)	13 (3%)	0	100	100
1	H	463/475 (98%)	450 (97%)	13 (3%)	0	100	100
1	K	466/475 (98%)	453 (97%)	13 (3%)	0	100	100
1	O	464/475 (98%)	449 (97%)	15 (3%)	0	100	100
1	R	460/475 (97%)	446 (97%)	14 (3%)	0	100	100
1	V	461/475 (97%)	449 (97%)	12 (3%)	0	100	100
2	C	126/134 (94%)	118 (94%)	8 (6%)	0	100	100
2	F	129/134 (96%)	120 (93%)	7 (5%)	2 (2%)	9	13
2	I	127/134 (95%)	118 (93%)	7 (6%)	2 (2%)	9	13
2	J	127/134 (95%)	121 (95%)	6 (5%)	0	100	100
2	M	126/134 (94%)	120 (95%)	6 (5%)	0	100	100
2	P	126/134 (94%)	118 (94%)	8 (6%)	0	100	100
2	T	127/134 (95%)	121 (95%)	6 (5%)	0	100	100
2	W	128/134 (96%)	121 (94%)	7 (6%)	0	100	100
All	All	4712/4872 (97%)	4546 (96%)	162 (3%)	4 (0%)	100	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	8[A]	ASN
2	F	8[B]	ASN
2	I	8[A]	ASN
2	I	8[B]	ASN

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	370/376 (98%)	357 (96%)	13 (4%)	36	55
1	B	369/376 (98%)	355 (96%)	14 (4%)	33	51
1	E	371/376 (99%)	358 (96%)	13 (4%)	36	55
1	H	371/376 (99%)	355 (96%)	16 (4%)	29	46
1	K	374/376 (100%)	363 (97%)	11 (3%)	42	62
1	O	372/376 (99%)	360 (97%)	12 (3%)	39	59
1	R	370/376 (98%)	357 (96%)	13 (4%)	36	55
1	V	370/376 (98%)	354 (96%)	16 (4%)	29	46
2	C	115/118 (98%)	107 (93%)	8 (7%)	15	24
2	F	118/118 (100%)	109 (92%)	9 (8%)	13	20
2	I	116/118 (98%)	109 (94%)	7 (6%)	19	31
2	J	116/118 (98%)	107 (92%)	9 (8%)	12	19
2	M	115/118 (98%)	105 (91%)	10 (9%)	10	15
2	P	115/118 (98%)	108 (94%)	7 (6%)	18	30
2	T	116/118 (98%)	107 (92%)	9 (8%)	12	19
2	W	117/118 (99%)	110 (94%)	7 (6%)	19	31
All	All	3895/3952 (99%)	3721 (96%)	174 (4%)	29	44

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	53	CYS
1	A	127	PHE
1	A	130	LEU
1	A	134	ARG
1	A	172	CYS
1	A	239	TYR
1	A	241	ASN

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Mol	Chain	Res	Type
1	A	335	LEU
1	A	431	ARG
1	A	435	ARG
1	A	450	LYS
1	A	464	GLU
1	B	14	LYS
1	B	50	PRO
1	B	53	CYS
1	B	130	LEU
1	B	134	ARG
1	B	172	CYS
1	B	203	ASP
1	B	239	TYR
1	B	241	ASN
1	B	335	LEU
1	B	431	ARG
1	B	435	ARG
1	B	450	LYS
1	B	464	GLU
2	C	2	MET
2	C	9	ASN
2	C	48[A]	HIS
2	C	48[B]	HIS
2	C	82	GLN
2	C	96	ASP
2	C	112	ILE
2	C	113	MET
1	E	14	LYS
1	E	53	CYS
1	E	89	PRO
1	E	127	PHE
1	E	130	LEU
1	E	134	ARG
1	E	172	CYS
1	E	203	ASP
1	E	239	TYR
1	E	241	ASN
1	E	431	ARG
1	E	450	LYS
1	E	464	GLU
2	F	9	ASN
2	F	47	ASP

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Mol	Chain	Res	Type
2	F	48[A]	HIS
2	F	48[B]	HIS
2	F	51	VAL
2	F	82	GLN
2	F	96	ASP
2	F	112	ILE
2	F	113	MET
1	H	8	LYS
1	H	14	LYS
1	H	53	CYS
1	H	119	SER
1	H	127	PHE
1	H	130	LEU
1	H	134	ARG
1	H	172	CYS
1	H	185	TYR
1	H	203	ASP
1	H	239	TYR
1	H	241	ASN
1	H	431	ARG
1	H	435	ARG
1	H	450	LYS
1	H	464	GLU
2	I	9	ASN
2	I	48[A]	HIS
2	I	48[B]	HIS
2	I	82	GLN
2	I	96	ASP
2	I	112	ILE
2	I	113	MET
2	J	8	ASN
2	J	9	ASN
2	J	16	SER
2	J	48[A]	HIS
2	J	48[B]	HIS
2	J	82	GLN
2	J	96	ASP
2	J	112	ILE
2	J	113	MET
1	K	7	THR
1	K	14	LYS
1	K	89	PRO

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Mol	Chain	Res	Type
1	K	130	LEU
1	K	134	ARG
1	K	172	CYS
1	K	241	ASN
1	K	335	LEU
1	K	431	ARG
1	K	450	LYS
1	K	464	GLU
2	M	8	ASN
2	M	9	ASN
2	M	16	SER
2	M	48[A]	HIS
2	M	48[B]	HIS
2	M	51	VAL
2	M	82	GLN
2	M	96	ASP
2	M	112	ILE
2	M	113	MET
1	O	8	LYS
1	O	14	LYS
1	O	127	PHE
1	O	134	ARG
1	O	172	CYS
1	O	185	TYR
1	O	239	TYR
1	O	241	ASN
1	O	335	LEU
1	O	431	ARG
1	O	450	LYS
1	O	464	GLU
2	P	9	ASN
2	P	48[A]	HIS
2	P	48[B]	HIS
2	P	82	GLN
2	P	96	ASP
2	P	112	ILE
2	P	113	MET
1	R	14	LYS
1	R	53	CYS
1	R	89	PRO
1	R	119	SER
1	R	130	LEU

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Mol	Chain	Res	Type
1	R	134	ARG
1	R	172	CYS
1	R	241	ASN
1	R	259	GLU
1	R	335	LEU
1	R	431	ARG
1	R	450	LYS
1	R	464	GLU
2	T	9	ASN
2	T	47	ASP
2	T	48[A]	HIS
2	T	48[B]	HIS
2	T	51	VAL
2	T	82	GLN
2	T	96	ASP
2	T	112	ILE
2	T	113	MET
1	V	14	LYS
1	V	53	CYS
1	V	119	SER
1	V	130	LEU
1	V	134	ARG
1	V	172	CYS
1	V	185	TYR
1	V	203	ASP
1	V	239	TYR
1	V	241	ASN
1	V	259	GLU
1	V	335	LEU
1	V	431	ARG
1	V	435	ARG
1	V	450	LYS
1	V	464	GLU
2	W	9	ASN
2	W	48[A]	HIS
2	W	48[B]	HIS
2	W	82	GLN
2	W	96	ASP
2	W	112	ILE
2	W	113	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	163	ASN
1	A	229	GLN
1	A	238	HIS
1	A	241	ASN
1	A	267	HIS
1	A	277	ASN
1	A	304	GLN
1	A	386	HIS
1	A	401	GLN
1	A	432	ASN
1	B	153	HIS
1	B	229	GLN
1	B	238	HIS
1	B	241	ASN
1	B	267	HIS
1	B	277	ASN
1	B	304	GLN
1	B	386	HIS
1	B	432	ASN
2	C	9	ASN
2	C	25	GLN
2	C	29	GLN
2	C	109	GLN
2	C	127	GLN
1	E	153	HIS
1	E	229	GLN
1	E	238	HIS
1	E	241	ASN
1	E	267	HIS
1	E	277	ASN
1	E	304	GLN
1	E	386	HIS
1	E	432	ASN
2	F	9	ASN
2	F	25	GLN
2	F	29	GLN
2	F	56	HIS
2	F	109	GLN
2	F	127	GLN
1	H	153	HIS
1	H	163	ASN
1	H	229	GLN

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Mol	Chain	Res	Type
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	386	HIS
1	H	432	ASN
2	I	9	ASN
2	I	25	GLN
2	I	29	GLN
2	I	109	GLN
2	I	127	GLN
2	J	8	ASN
2	J	9	ASN
2	J	25	GLN
2	J	29	GLN
2	J	55	HIS
2	J	109	GLN
2	J	127	GLN
1	K	153	HIS
1	K	229	GLN
1	K	238	HIS
1	K	241	ASN
1	K	267	HIS
1	K	277	ASN
1	K	304	GLN
1	K	386	HIS
1	K	432	ASN
2	M	9	ASN
2	M	25	GLN
2	M	29	GLN
2	M	55	HIS
2	M	109	GLN
2	M	127	GLN
1	O	153	HIS
1	O	229	GLN
1	O	238	HIS
1	O	241	ASN
1	O	267	HIS
1	O	277	ASN
1	O	304	GLN
1	O	386	HIS

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Mol	Chain	Res	Type
1	O	432	ASN
2	P	9	ASN
2	P	25	GLN
2	P	29	GLN
2	P	55	HIS
2	P	56	HIS
2	P	109	GLN
2	P	127	GLN
1	R	153	HIS
1	R	229	GLN
1	R	238	HIS
1	R	241	ASN
1	R	267	HIS
1	R	277	ASN
1	R	304	GLN
1	R	386	HIS
1	R	420	ASN
1	R	432	ASN
2	T	9	ASN
2	T	25	GLN
2	T	29	GLN
2	T	55	HIS
2	T	109	GLN
2	T	127	GLN
1	V	153	HIS
1	V	229	GLN
1	V	238	HIS
1	V	241	ASN
1	V	267	HIS
1	V	277	ASN
1	V	304	GLN
1	V	386	HIS
1	V	432	ASN
2	W	9	ASN
2	W	25	GLN
2	W	29	GLN
2	W	109	GLN
2	W	127	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

40 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	H	201	1,3	9,11,12	1.02	0	5,12,14	0.97	0
1	HYP	R	151	1	6,8,9	0.59	0	5,10,12	1.58	2 (40%)
1	KCX	K	201	1,3	9,11,12	1.00	0	5,12,14	0.77	0
1	SMC	V	369	1	5,6,7	0.91	0	2,6,8	0.62	0
1	HYP	B	104	1	6,8,9	0.71	0	5,10,12	1.07	0
1	HYP	K	104	1	6,8,9	0.65	0	5,10,12	1.53	0
1	HYP	A	151	1	6,8,9	0.88	0	5,10,12	1.65	2 (40%)
1	HYP	K	151	1	6,8,9	0.55	0	5,10,12	1.69	2 (40%)
1	SMC	A	369	1	5,6,7	0.78	0	2,6,8	1.26	0
1	HYP	A	104	1	6,8,9	0.76	0	5,10,12	1.21	0
1	SMC	B	256	1	5,6,7	1.05	0	2,6,8	1.29	0
1	SMC	K	256	1	5,6,7	0.67	0	2,6,8	1.29	0
1	KCX	R	201	1,3	9,11,12	0.82	0	5,12,14	0.86	0
1	SMC	A	256	1	5,6,7	1.06	0	2,6,8	2.18	1 (50%)
1	SMC	K	369	1	5,6,7	0.62	0	2,6,8	1.45	0
1	KCX	V	201	1,3	9,11,12	1.10	0	5,12,14	1.76	1 (20%)
1	SMC	H	369	1	5,6,7	1.31	1 (20%)	2,6,8	1.12	0
1	KCX	O	201	1,3	9,11,12	1.00	0	5,12,14	1.50	1 (20%)
1	HYP	R	104	1	6,8,9	0.58	0	5,10,12	1.50	0
1	HYP	H	104	1	6,8,9	0.55	0	5,10,12	1.64	2 (40%)
1	SMC	E	369	1	5,6,7	0.98	1 (20%)	2,6,8	0.98	0
1	HYP	H	151	1	6,8,9	0.82	0	5,10,12	1.18	0
1	SMC	E	256	1	5,6,7	0.72	0	2,6,8	0.95	0
1	KCX	A	201	1,3	9,11,12	0.72	0	5,12,14	1.04	0
1	HYP	E	151	1	6,8,9	0.63	0	5,10,12	1.17	0
1	HYP	V	151	1	6,8,9	0.71	0	5,10,12	1.51	0
1	HYP	O	151	1	6,8,9	0.74	0	5,10,12	1.24	0
1	HYP	O	104	1	6,8,9	0.58	0	5,10,12	1.58	1 (20%)
1	KCX	B	201	1,3	9,11,12	1.01	0	5,12,14	0.65	0
1	HYP	V	104	1	6,8,9	0.67	0	5,10,12	1.39	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	SMC	R	256	1	5,6,7	0.86	0	2,6,8	1.42	0
1	SMC	V	256	1	5,6,7	1.46	1 (20%)	2,6,8	0.67	0
1	SMC	O	256	1	5,6,7	0.82	0	2,6,8	0.55	0
1	HYP	B	151	1	6,8,9	0.64	0	5,10,12	1.13	0
1	KCX	E	201	1,3	9,11,12	0.97	0	5,12,14	0.97	1 (20%)
1	SMC	H	256	1	5,6,7	0.76	0	2,6,8	1.92	1 (50%)
1	SMC	R	369	1	5,6,7	0.95	0	2,6,8	0.97	0
1	HYP	E	104	1	6,8,9	0.95	0	5,10,12	1.16	0
1	SMC	B	369	1	5,6,7	1.35	1 (20%)	2,6,8	0.22	0
1	SMC	O	369	1	5,6,7	0.47	0	2,6,8	1.49	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	H	201	1,3	-	1/9/10/12	-
1	HYP	R	151	1	-	0/0/11/13	0/1/1/1
1	KCX	K	201	1,3	-	0/9/10/12	-
1	SMC	V	369	1	-	1/3/5/7	-
1	HYP	B	104	1	-	0/0/11/13	0/1/1/1
1	HYP	K	104	1	-	0/0/11/13	0/1/1/1
1	HYP	A	151	1	-	0/0/11/13	0/1/1/1
1	HYP	K	151	1	-	0/0/11/13	0/1/1/1
1	SMC	A	369	1	-	1/3/5/7	-
1	HYP	A	104	1	-	0/0/11/13	0/1/1/1
1	SMC	B	256	1	-	0/3/5/7	-
1	SMC	K	256	1	-	0/3/5/7	-
1	KCX	R	201	1,3	-	0/9/10/12	-
1	SMC	A	256	1	-	0/3/5/7	-
1	SMC	K	369	1	-	1/3/5/7	-
1	KCX	V	201	1,3	-	0/9/10/12	-
1	SMC	H	369	1	-	1/3/5/7	-
1	KCX	O	201	1,3	-	0/9/10/12	-
1	HYP	R	104	1	-	0/0/11/13	0/1/1/1
1	HYP	H	104	1	-	0/0/11/13	0/1/1/1
1	SMC	E	369	1	-	1/3/5/7	-
1	HYP	H	151	1	-	0/0/11/13	0/1/1/1
1	SMC	E	256	1	-	0/3/5/7	-
1	KCX	A	201	1,3	-	0/9/10/12	-
1	HYP	E	151	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	V	151	1	-	0/0/11/13	0/1/1/1
1	HYP	O	151	1	-	0/0/11/13	0/1/1/1
1	HYP	O	104	1	-	0/0/11/13	0/1/1/1
1	KCX	B	201	1,3	-	0/9/10/12	-
1	HYP	V	104	1	-	0/0/11/13	0/1/1/1
1	SMC	R	256	1	-	0/3/5/7	-
1	SMC	V	256	1	-	0/3/5/7	-
1	SMC	O	256	1	-	0/3/5/7	-
1	HYP	B	151	1	-	0/0/11/13	0/1/1/1
1	KCX	E	201	1,3	-	0/9/10/12	-
1	SMC	H	256	1	-	0/3/5/7	-
1	SMC	R	369	1	-	1/3/5/7	-
1	HYP	E	104	1	-	0/0/11/13	0/1/1/1
1	SMC	B	369	1	-	1/3/5/7	-
1	SMC	O	369	1	-	1/3/5/7	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	V	256	SMC	CB-SG	3.03	1.85	1.80
1	B	369	SMC	CB-SG	2.78	1.84	1.80
1	H	369	SMC	CB-SG	2.65	1.84	1.80
1	E	369	SMC	CB-SG	2.00	1.83	1.80

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	V	201	KCX	OQ1-CX-NZ	-3.74	119.15	124.96
1	O	201	KCX	OQ1-CX-NZ	-2.96	120.37	124.96
1	A	256	SMC	CA-CB-SG	-2.82	109.49	114.04
1	H	104	HYP	OD1-CG-CB	-2.41	104.08	110.03
1	R	151	HYP	CB-CG-CD	-2.35	100.39	103.27
1	A	151	HYP	CB-CG-CD	-2.33	100.40	103.27
1	H	256	SMC	CS-SG-CB	-2.28	97.12	101.30
1	R	151	HYP	O-C-CA	-2.25	118.87	124.78
1	K	151	HYP	CG-CB-CA	-2.22	101.16	103.96
1	K	151	HYP	O-C-CA	-2.18	119.08	124.78
1	E	201	KCX	OQ1-CX-NZ	-2.13	121.66	124.96
1	A	151	HYP	O-C-CA	-2.12	119.22	124.78
1	O	104	HYP	OD1-CG-CB	-2.09	104.86	110.03
1	H	104	HYP	CB-CG-CD	2.05	105.78	103.27
1	V	104	HYP	OD1-CG-CB	-2.04	104.98	110.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	369	SMC	N-CA-CB-SG
1	E	369	SMC	N-CA-CB-SG
1	H	369	SMC	N-CA-CB-SG
1	O	369	SMC	N-CA-CB-SG
1	V	369	SMC	N-CA-CB-SG
1	H	201	KCX	CE-CD-CG-CB
1	A	369	SMC	N-CA-CB-SG
1	K	369	SMC	N-CA-CB-SG
1	R	369	SMC	N-CA-CB-SG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	151	HYP	1	0
1	O	151	HYP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 70 ligands modelled in this entry, 8 are monoatomic - leaving 62 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	$\#\|Z\| > 2$
5	EDO	V	1478	-	3,3,3	0.53	0	2,2,2	0.53	0
4	CAP	H	1477	3	17,20,20	1.67	2 (11%)	22,31,31	0.91	1 (4%)
4	CAP	K	1477	3	17,20,20	1.65	1 (5%)	22,31,31	1.42	2 (9%)
5	EDO	K	1481	-	3,3,3	0.36	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	A	1483	-	3,3,3	0.47	0	2,2,2	0.17	0
5	EDO	O	1478	-	3,3,3	0.51	0	2,2,2	0.32	0
5	EDO	V	1482	-	3,3,3	0.28	0	2,2,2	0.33	0
5	EDO	E	1482	-	3,3,3	0.62	0	2,2,2	0.69	0
5	EDO	A	1479	-	3,3,3	0.31	0	2,2,2	0.26	0
5	EDO	R	1478	-	3,3,3	0.35	0	2,2,2	0.22	0
5	EDO	T	1136	-	3,3,3	0.34	0	2,2,2	0.13	0
5	EDO	A	1482	-	3,3,3	0.37	0	2,2,2	0.28	0
5	EDO	R	1481	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	V	1483	-	3,3,3	0.44	0	2,2,2	0.23	0
5	EDO	W	1135	-	3,3,3	0.32	0	2,2,2	0.18	0
4	CAP	R	1477	3	17,20,20	1.68	2 (11%)	22,31,31	1.11	1 (4%)
5	EDO	O	1481	-	3,3,3	0.46	0	2,2,2	0.24	0
5	EDO	O	1480	-	3,3,3	0.36	0	2,2,2	0.18	0
5	EDO	A	1478	-	3,3,3	0.23	0	2,2,2	0.40	0
5	EDO	E	1479	-	3,3,3	0.37	0	2,2,2	0.41	0
5	EDO	V	1480	-	3,3,3	0.33	0	2,2,2	0.24	0
5	EDO	B	1482	-	3,3,3	0.41	0	2,2,2	0.45	0
5	EDO	A	1480	-	3,3,3	0.35	0	2,2,2	0.41	0
5	EDO	H	1478	-	3,3,3	0.48	0	2,2,2	0.08	0
5	EDO	K	1482	-	3,3,3	0.34	0	2,2,2	0.20	0
5	EDO	A	1481	-	3,3,3	0.31	0	2,2,2	0.46	0
5	EDO	J	1135	-	3,3,3	0.23	0	2,2,2	0.44	0
5	EDO	K	1480	-	3,3,3	0.38	0	2,2,2	0.11	0
5	EDO	B	1479	-	3,3,3	0.28	0	2,2,2	0.91	0
5	EDO	B	1480	-	3,3,3	0.32	0	2,2,2	0.17	0
5	EDO	I	1135	-	3,3,3	0.26	0	2,2,2	0.52	0
5	EDO	K	1479	-	3,3,3	0.36	0	2,2,2	0.69	0
4	CAP	B	1477	3	17,20,20	1.71	2 (11%)	22,31,31	1.14	3 (13%)
5	EDO	B	1481	-	3,3,3	0.32	0	2,2,2	0.35	0
5	EDO	P	1135	-	3,3,3	0.26	0	2,2,2	0.44	0
4	CAP	A	1477	3	17,20,20	1.60	1 (5%)	22,31,31	0.96	1 (4%)
5	EDO	R	1482	-	3,3,3	0.34	0	2,2,2	0.13	0
5	EDO	O	1482	-	3,3,3	0.23	0	2,2,2	0.37	0
5	EDO	M	1135	-	3,3,3	0.31	0	2,2,2	0.13	0
5	EDO	E	1478	-	3,3,3	0.39	0	2,2,2	0.13	0
5	EDO	R	1480	-	3,3,3	0.34	0	2,2,2	0.33	0
5	EDO	H	1479	-	3,3,3	0.38	0	2,2,2	0.58	0
5	EDO	R	1484	-	3,3,3	0.34	0	2,2,2	0.19	0
5	EDO	E	1480	-	3,3,3	0.27	0	2,2,2	0.36	0
5	EDO	F	1135	-	3,3,3	0.31	0	2,2,2	0.27	0
5	EDO	H	1481	-	3,3,3	0.25	0	2,2,2	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAP	E	1477	3	17,20,20	1.67	1 (5%)	22,31,31	1.44	5 (22%)
4	CAP	V	1477	3	17,20,20	1.76	2 (11%)	22,31,31	1.10	1 (4%)
5	EDO	E	1481	-	3,3,3	0.32	0	2,2,2	0.11	0
5	EDO	V	1479	-	3,3,3	0.39	0	2,2,2	0.14	0
5	EDO	V	1481	-	3,3,3	0.30	0	2,2,2	0.54	0
4	CAP	O	1477	3	17,20,20	1.64	2 (11%)	22,31,31	1.64	6 (27%)
5	EDO	B	1478	-	3,3,3	0.41	0	2,2,2	0.33	0
5	EDO	O	1479	-	3,3,3	0.33	0	2,2,2	0.55	0
5	EDO	K	1478	-	3,3,3	0.26	0	2,2,2	0.19	0
5	EDO	C	1135	-	3,3,3	0.30	0	2,2,2	0.39	0
5	EDO	R	1479	-	3,3,3	0.39	0	2,2,2	0.23	0
5	EDO	R	1483	-	3,3,3	0.53	0	2,2,2	0.58	0
5	EDO	O	1483	-	3,3,3	0.42	0	2,2,2	0.41	0
5	EDO	H	1480	-	3,3,3	0.29	0	2,2,2	0.24	0
5	EDO	C	1136	-	3,3,3	0.31	0	2,2,2	0.20	0
5	EDO	T	1135	-	3,3,3	0.37	0	2,2,2	0.12	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	V	1478	-	-	1/1/1/1	-
4	CAP	H	1477	3	-	10/29/29/29	-
4	CAP	K	1477	3	-	8/29/29/29	-
5	EDO	K	1481	-	-	0/1/1/1	-
5	EDO	A	1483	-	-	0/1/1/1	-
5	EDO	O	1478	-	-	0/1/1/1	-
5	EDO	V	1482	-	-	0/1/1/1	-
5	EDO	E	1482	-	-	0/1/1/1	-
5	EDO	A	1479	-	-	0/1/1/1	-
5	EDO	R	1478	-	-	0/1/1/1	-
5	EDO	T	1136	-	-	0/1/1/1	-
5	EDO	A	1482	-	-	1/1/1/1	-
5	EDO	R	1481	-	-	0/1/1/1	-
5	EDO	V	1483	-	-	1/1/1/1	-
5	EDO	W	1135	-	-	1/1/1/1	-
4	CAP	R	1477	3	-	7/29/29/29	-
5	EDO	O	1481	-	-	0/1/1/1	-
5	EDO	O	1480	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	A	1478	-	-	0/1/1/1	-
5	EDO	E	1479	-	-	1/1/1/1	-
5	EDO	V	1480	-	-	1/1/1/1	-
5	EDO	B	1482	-	-	1/1/1/1	-
5	EDO	A	1480	-	-	1/1/1/1	-
5	EDO	H	1478	-	-	0/1/1/1	-
5	EDO	K	1482	-	-	1/1/1/1	-
5	EDO	A	1481	-	-	0/1/1/1	-
5	EDO	J	1135	-	-	0/1/1/1	-
5	EDO	K	1480	-	-	1/1/1/1	-
5	EDO	B	1479	-	-	1/1/1/1	-
5	EDO	B	1480	-	-	0/1/1/1	-
5	EDO	I	1135	-	-	1/1/1/1	-
5	EDO	K	1479	-	-	1/1/1/1	-
4	CAP	B	1477	3	-	9/29/29/29	-
5	EDO	B	1481	-	-	1/1/1/1	-
5	EDO	P	1135	-	-	1/1/1/1	-
4	CAP	A	1477	3	-	6/29/29/29	-
5	EDO	R	1482	-	-	0/1/1/1	-
5	EDO	O	1482	-	-	1/1/1/1	-
5	EDO	M	1135	-	-	0/1/1/1	-
5	EDO	E	1478	-	-	0/1/1/1	-
5	EDO	R	1480	-	-	1/1/1/1	-
5	EDO	H	1479	-	-	0/1/1/1	-
5	EDO	R	1484	-	-	0/1/1/1	-
5	EDO	E	1480	-	-	0/1/1/1	-
5	EDO	F	1135	-	-	1/1/1/1	-
5	EDO	H	1481	-	-	1/1/1/1	-
4	CAP	E	1477	3	-	8/29/29/29	-
4	CAP	V	1477	3	-	7/29/29/29	-
5	EDO	E	1481	-	-	1/1/1/1	-
5	EDO	V	1479	-	-	0/1/1/1	-
5	EDO	V	1481	-	-	0/1/1/1	-
4	CAP	O	1477	3	-	9/29/29/29	-
5	EDO	B	1478	-	-	0/1/1/1	-
5	EDO	O	1479	-	-	0/1/1/1	-
5	EDO	K	1478	-	-	0/1/1/1	-
5	EDO	C	1135	-	-	1/1/1/1	-
5	EDO	R	1479	-	-	1/1/1/1	-
5	EDO	R	1483	-	-	0/1/1/1	-
5	EDO	O	1483	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	H	1480	-	-	1/1/1/1	-
5	EDO	C	1136	-	-	1/1/1/1	-
5	EDO	T	1135	-	-	1/1/1/1	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1477	CAP	O6-C	6.26	1.42	1.22
4	R	1477	CAP	O6-C	6.04	1.41	1.22
4	E	1477	CAP	O6-C	6.02	1.41	1.22
4	K	1477	CAP	O6-C	5.87	1.41	1.22
4	O	1477	CAP	O6-C	5.85	1.41	1.22
4	H	1477	CAP	O6-C	5.85	1.41	1.22
4	A	1477	CAP	O6-C	5.81	1.40	1.22
4	B	1477	CAP	O6-C	5.59	1.40	1.22
4	B	1477	CAP	O2-C2	3.07	1.49	1.42
4	H	1477	CAP	O2-C2	2.31	1.47	1.42
4	R	1477	CAP	O2-C2	2.29	1.47	1.42
4	O	1477	CAP	O4-C4	-2.16	1.38	1.43
4	V	1477	CAP	C4-C3	-2.05	1.52	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	K	1477	CAP	O2-C2-C	-4.39	100.94	108.97
4	O	1477	CAP	O2-C2-C	-3.12	103.28	108.97
4	E	1477	CAP	O4-C4-C5	-2.99	103.19	109.92
4	O	1477	CAP	O4-C4-C5	-2.98	103.21	109.92
4	O	1477	CAP	O4-C4-C3	-2.78	103.22	108.78
4	V	1477	CAP	O2-C2-C	-2.66	104.12	108.97
4	E	1477	CAP	O2-C2-C	-2.63	104.17	108.97
4	R	1477	CAP	O3P-P1-O1	2.48	113.33	106.73
4	O	1477	CAP	O2P-P1-O1	2.43	113.19	106.73
4	B	1477	CAP	O4-C4-C5	-2.36	104.62	109.92
4	B	1477	CAP	O4-C4-C3	-2.31	104.16	108.78
4	B	1477	CAP	O2P-P1-O1	2.30	112.85	106.73
4	O	1477	CAP	O3-C3-C4	2.28	114.02	109.13
4	E	1477	CAP	O1-P1-O1P	2.26	112.82	106.47
4	K	1477	CAP	O4-C4-C5	-2.25	104.86	109.92
4	O	1477	CAP	C5-C4-C3	2.23	116.50	111.94
4	E	1477	CAP	O5P-P2-O5	2.21	112.62	106.73
4	E	1477	CAP	P2-O5-C5	2.03	123.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1477	CAP	O1-P1-O1P	2.03	112.17	106.47
4	H	1477	CAP	O4-C4-C5	-2.02	105.39	109.92

There are no chirality outliers.

All (91) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1477	CAP	O2-C2-C3-C4
4	A	1477	CAP	O6-C-C2-C1
4	A	1477	CAP	O7-C-C2-C1
4	A	1477	CAP	O6-C-C2-O2
4	A	1477	CAP	O7-C-C2-O2
4	B	1477	CAP	O7-C-C2-C1
4	B	1477	CAP	O6-C-C2-O2
4	B	1477	CAP	O7-C-C2-O2
4	B	1477	CAP	O3-C3-C4-O4
4	E	1477	CAP	O2-C2-C3-C4
4	E	1477	CAP	O6-C-C2-C3
4	E	1477	CAP	O6-C-C2-O2
4	E	1477	CAP	O3-C3-C4-O4
4	H	1477	CAP	O1-C1-C2-O2
4	H	1477	CAP	O6-C-C2-O2
4	H	1477	CAP	O7-C-C2-O2
4	H	1477	CAP	C2-C3-C4-O4
4	H	1477	CAP	O3-C3-C4-O4
4	K	1477	CAP	O6-C-C2-O2
4	K	1477	CAP	C2-C3-C4-O4
4	K	1477	CAP	O3-C3-C4-O4
4	O	1477	CAP	O2-C2-C3-C4
4	O	1477	CAP	O6-C-C2-O2
4	O	1477	CAP	C2-C3-C4-O4
4	O	1477	CAP	O3-C3-C4-O4
4	R	1477	CAP	O2-C2-C3-C4
4	R	1477	CAP	O6-C-C2-C1
4	R	1477	CAP	O7-C-C2-C1
4	R	1477	CAP	O6-C-C2-O2
4	R	1477	CAP	O7-C-C2-O2
4	R	1477	CAP	O3-C3-C4-O4
4	V	1477	CAP	O6-C-C2-O2
4	V	1477	CAP	O3-C3-C4-O4
5	C	1136	EDO	O1-C1-C2-O2
5	K	1480	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	1477	CAP	O6-C-C2-C1
4	H	1477	CAP	O7-C-C2-C1
4	K	1477	CAP	O7-C-C2-C1
4	V	1477	CAP	O7-C-C2-C1
5	A	1480	EDO	O1-C1-C2-O2
5	B	1482	EDO	O1-C1-C2-O2
5	H	1481	EDO	O1-C1-C2-O2
5	O	1483	EDO	O1-C1-C2-O2
5	R	1479	EDO	O1-C1-C2-O2
5	T	1135	EDO	O1-C1-C2-O2
5	V	1483	EDO	O1-C1-C2-O2
4	B	1477	CAP	O2-C2-C3-C4
4	H	1477	CAP	O2-C2-C3-C4
4	K	1477	CAP	O2-C2-C3-C4
4	V	1477	CAP	O2-C2-C3-C4
4	B	1477	CAP	C2-C3-C4-O4
4	K	1477	CAP	O7-C-C2-O2
4	V	1477	CAP	O7-C-C2-O2
5	K	1479	EDO	O1-C1-C2-O2
5	O	1480	EDO	O1-C1-C2-O2
4	H	1477	CAP	O6-C-C2-C1
4	V	1477	CAP	O6-C-C2-C1
5	C	1135	EDO	O1-C1-C2-O2
5	I	1135	EDO	O1-C1-C2-O2
5	O	1482	EDO	O1-C1-C2-O2
4	B	1477	CAP	O6-C-C2-C3
4	H	1477	CAP	O6-C-C2-C3
4	K	1477	CAP	O6-C-C2-C3
4	O	1477	CAP	O6-C-C2-C3
5	A	1482	EDO	O1-C1-C2-O2
5	H	1480	EDO	O1-C1-C2-O2
5	K	1482	EDO	O1-C1-C2-O2
4	E	1477	CAP	C2-C3-C4-O4
5	P	1135	EDO	O1-C1-C2-O2
5	V	1478	EDO	O1-C1-C2-O2
5	V	1480	EDO	O1-C1-C2-O2
5	W	1135	EDO	O1-C1-C2-O2
4	B	1477	CAP	O7-C-C2-C3
4	E	1477	CAP	O7-C-C2-C3
4	H	1477	CAP	O7-C-C2-C3
4	O	1477	CAP	O7-C-C2-C3
4	V	1477	CAP	O7-C-C2-C3

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Mol	Chain	Res	Type	Atoms
4	O	1477	CAP	O7-C-C2-C1
5	E	1481	EDO	O1-C1-C2-O2
4	A	1477	CAP	O3-C3-C4-O4
4	K	1477	CAP	O6-C-C2-C1
4	R	1477	CAP	O4-C4-C5-O5
4	E	1477	CAP	O7-C-C2-O2
4	O	1477	CAP	O7-C-C2-O2
5	B	1479	EDO	O1-C1-C2-O2
5	B	1481	EDO	O1-C1-C2-O2
5	E	1479	EDO	O1-C1-C2-O2
5	F	1135	EDO	O1-C1-C2-O2
5	R	1480	EDO	O1-C1-C2-O2
4	E	1477	CAP	O7-C-C2-C1
4	O	1477	CAP	O6-C-C2-C1

There are no ring outliers.

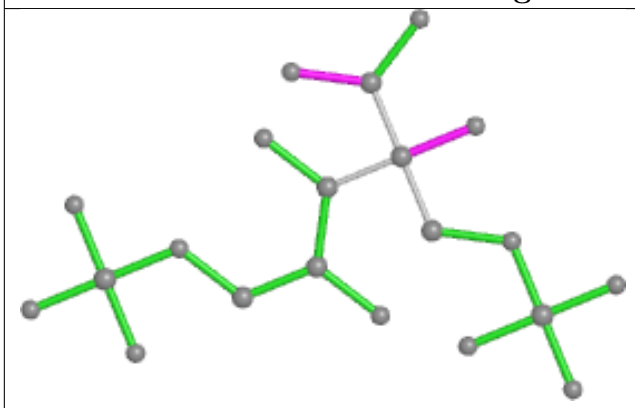
18 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	V	1478	EDO	1	0
4	H	1477	CAP	1	0
5	V	1482	EDO	1	0
5	T	1136	EDO	3	0
5	W	1135	EDO	2	0
5	V	1480	EDO	1	0
5	B	1482	EDO	1	0
5	H	1478	EDO	1	0
5	B	1479	EDO	1	0
5	K	1479	EDO	2	0
5	P	1135	EDO	1	0
5	R	1482	EDO	3	0
5	E	1480	EDO	2	0
5	F	1135	EDO	3	0
5	R	1483	EDO	1	0
5	O	1483	EDO	6	0
5	H	1480	EDO	1	0
5	T	1135	EDO	2	0

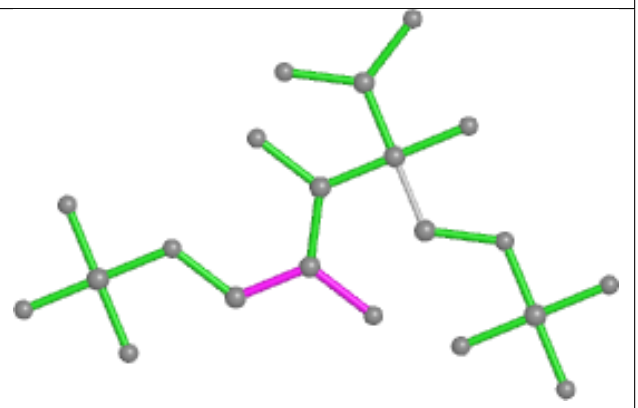
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

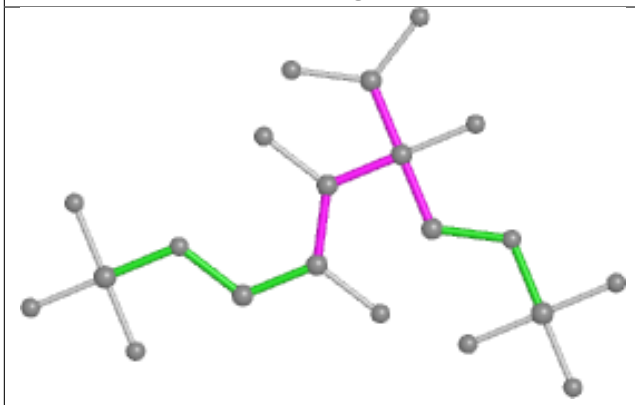
Ligand CAP H 1477



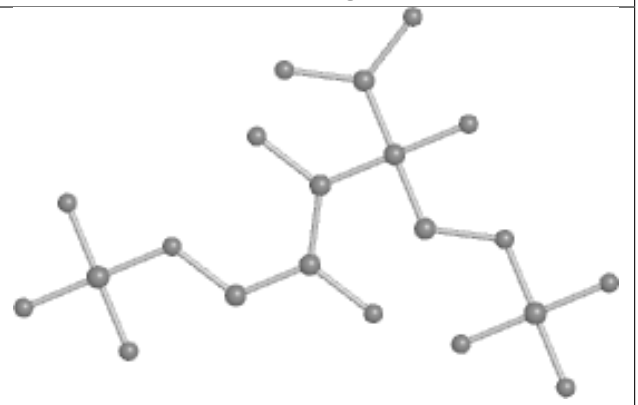
Bond lengths



Bond angles

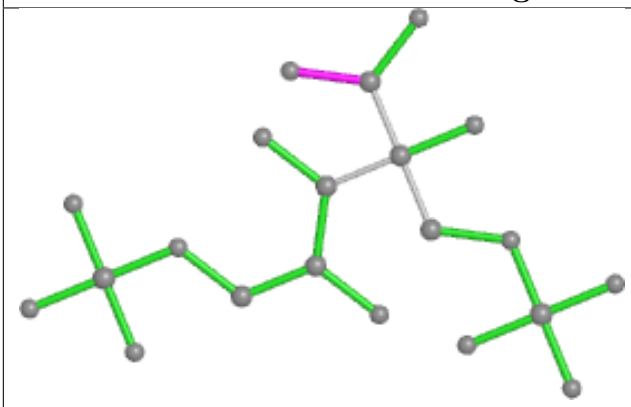


Torsions

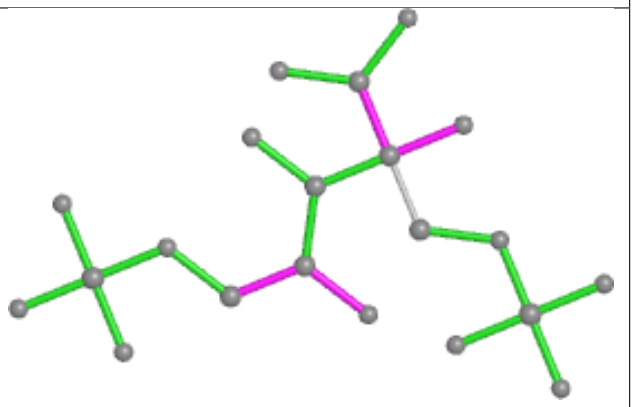


Rings

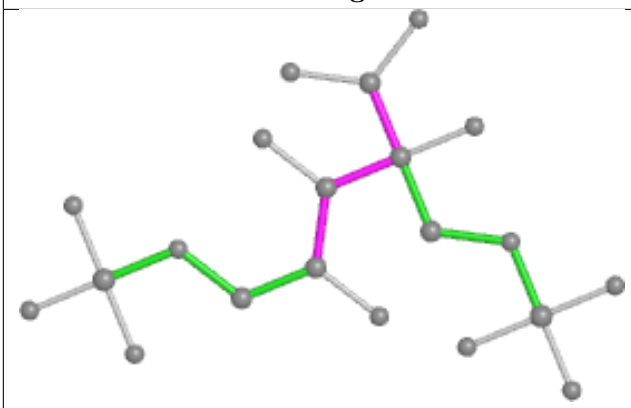
Ligand CAP K 1477



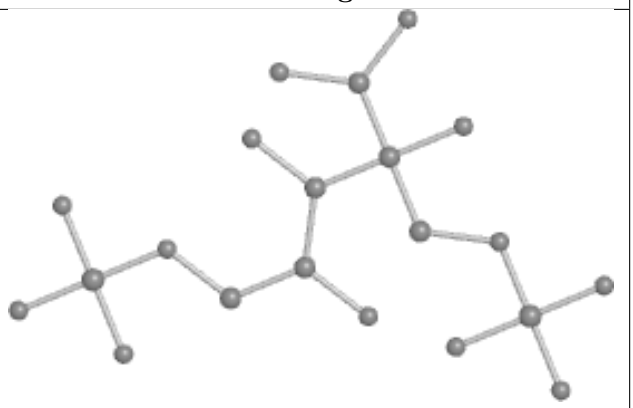
Bond lengths



Bond angles

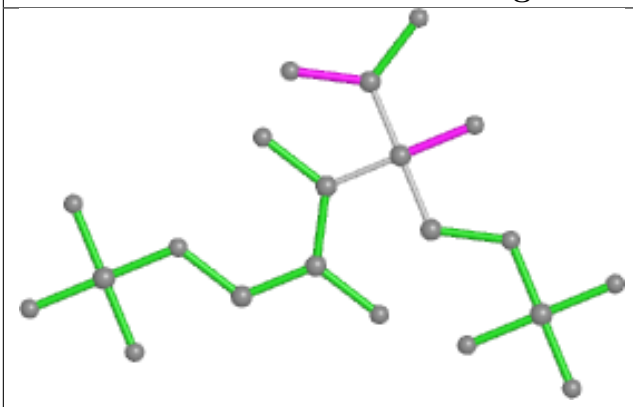


Torsions

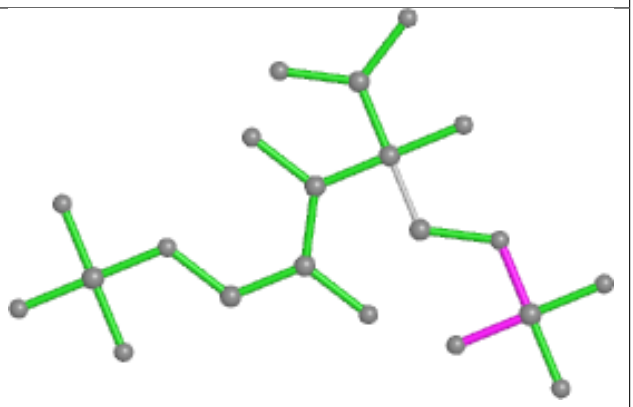


Rings

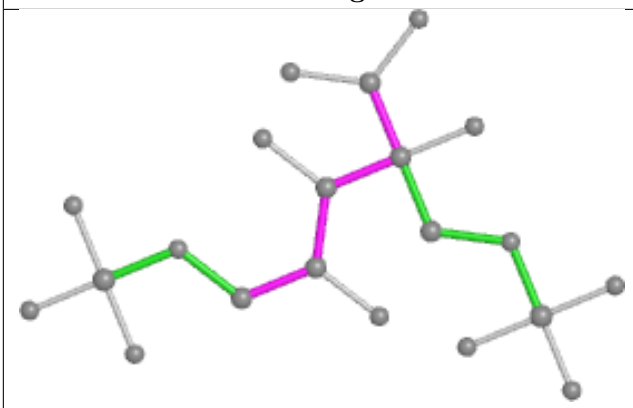
Ligand CAP R 1477



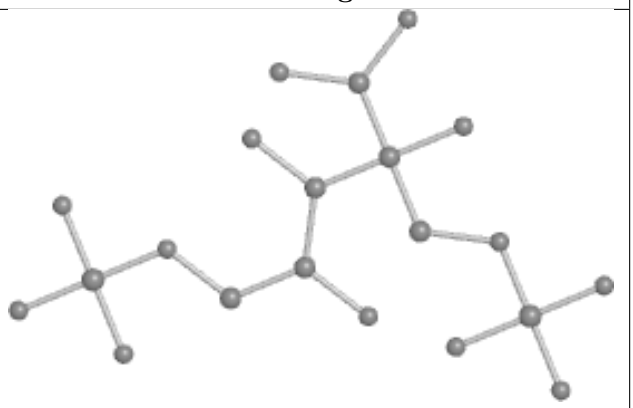
Bond lengths



Bond angles

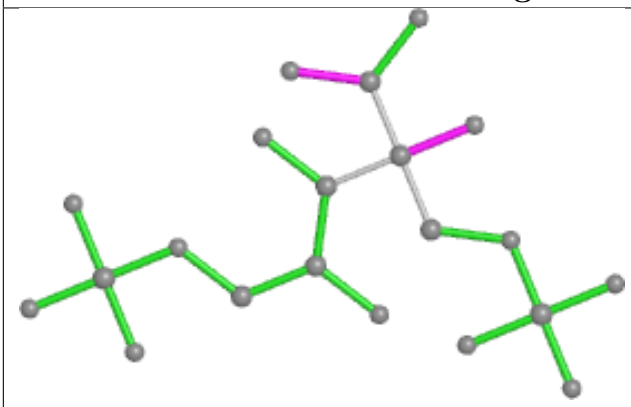


Torsions

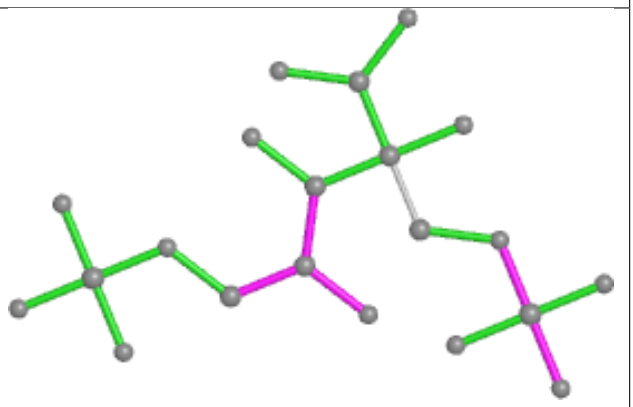


Rings

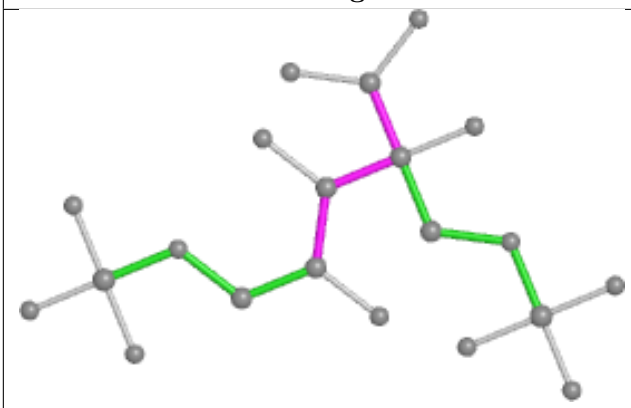
Ligand CAP B 1477



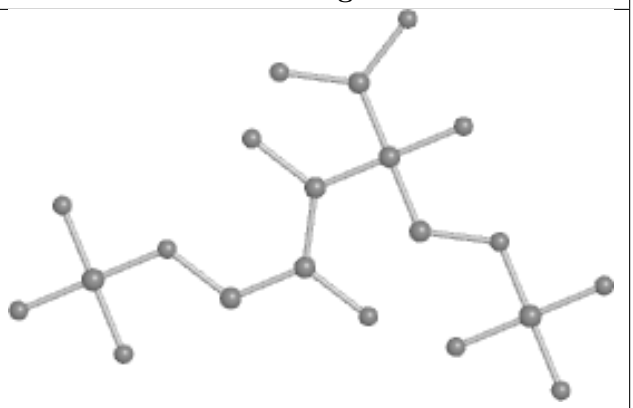
Bond lengths



Bond angles

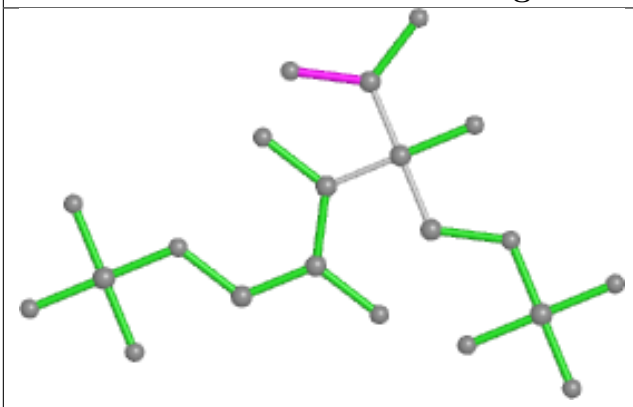


Torsions

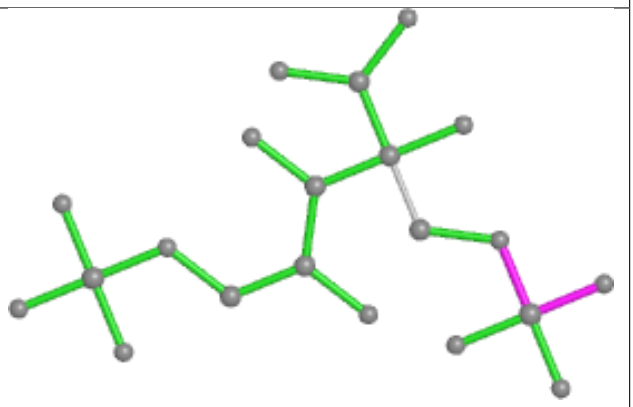


Rings

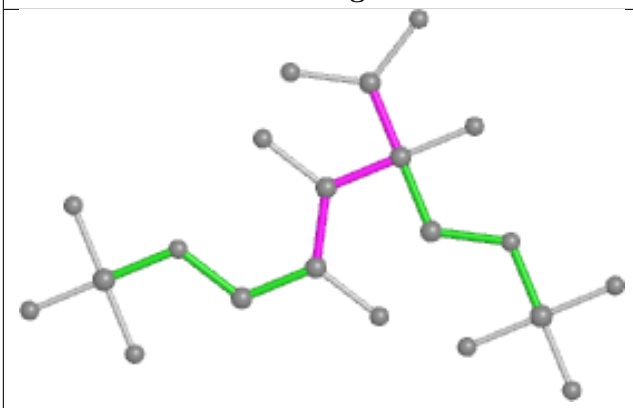
Ligand CAP A 1477



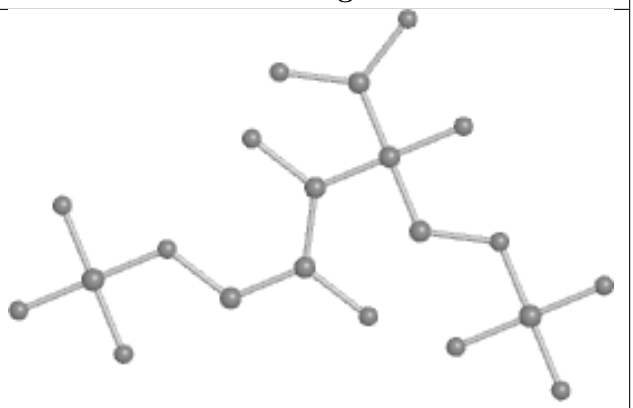
Bond lengths



Bond angles

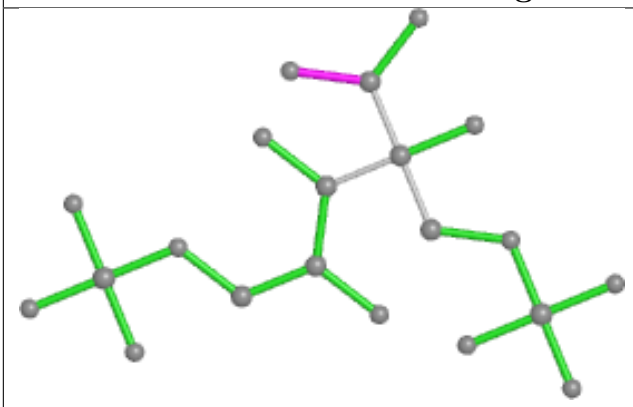


Torsions

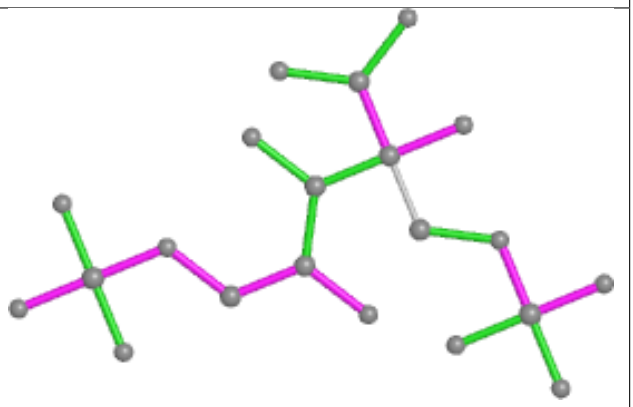


Rings

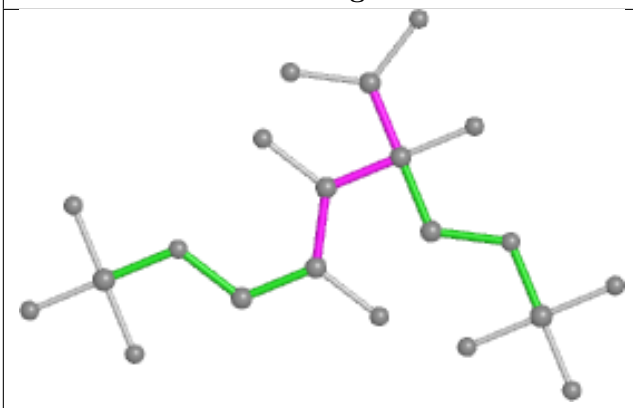
Ligand CAP E 1477



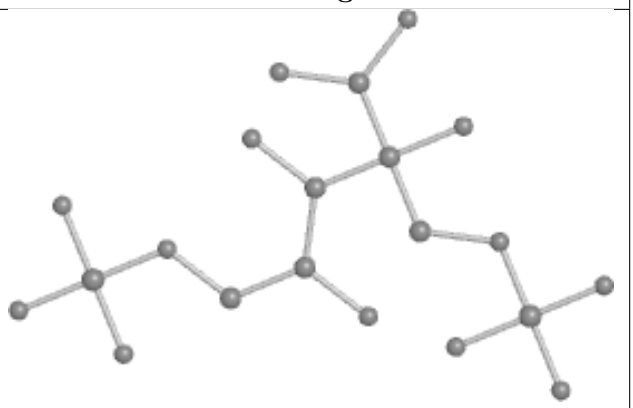
Bond lengths



Bond angles

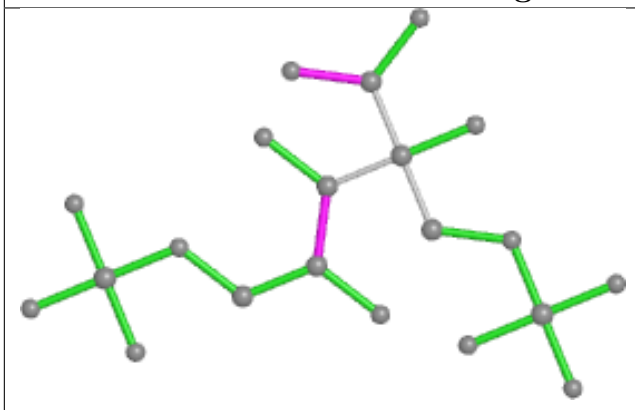


Torsions

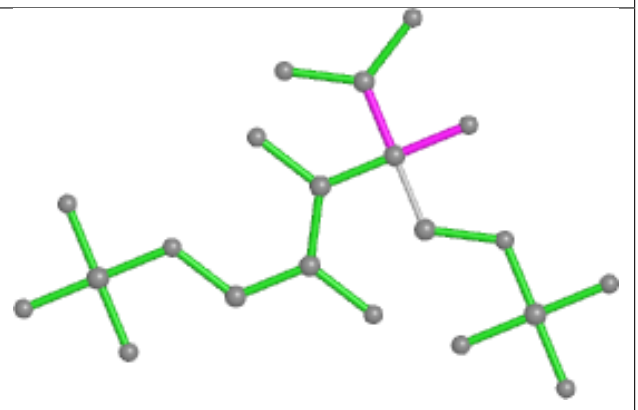


Rings

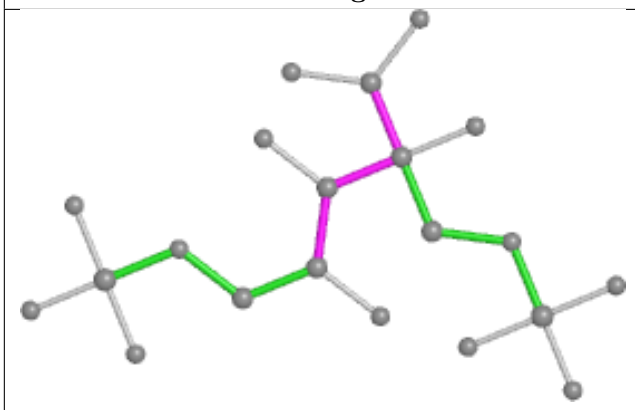
Ligand CAP V 1477



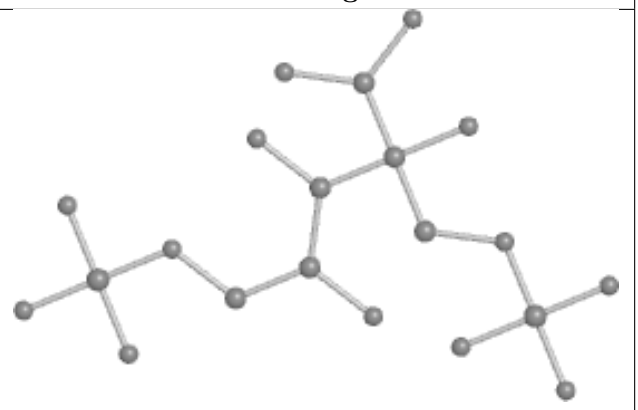
Bond lengths



Bond angles

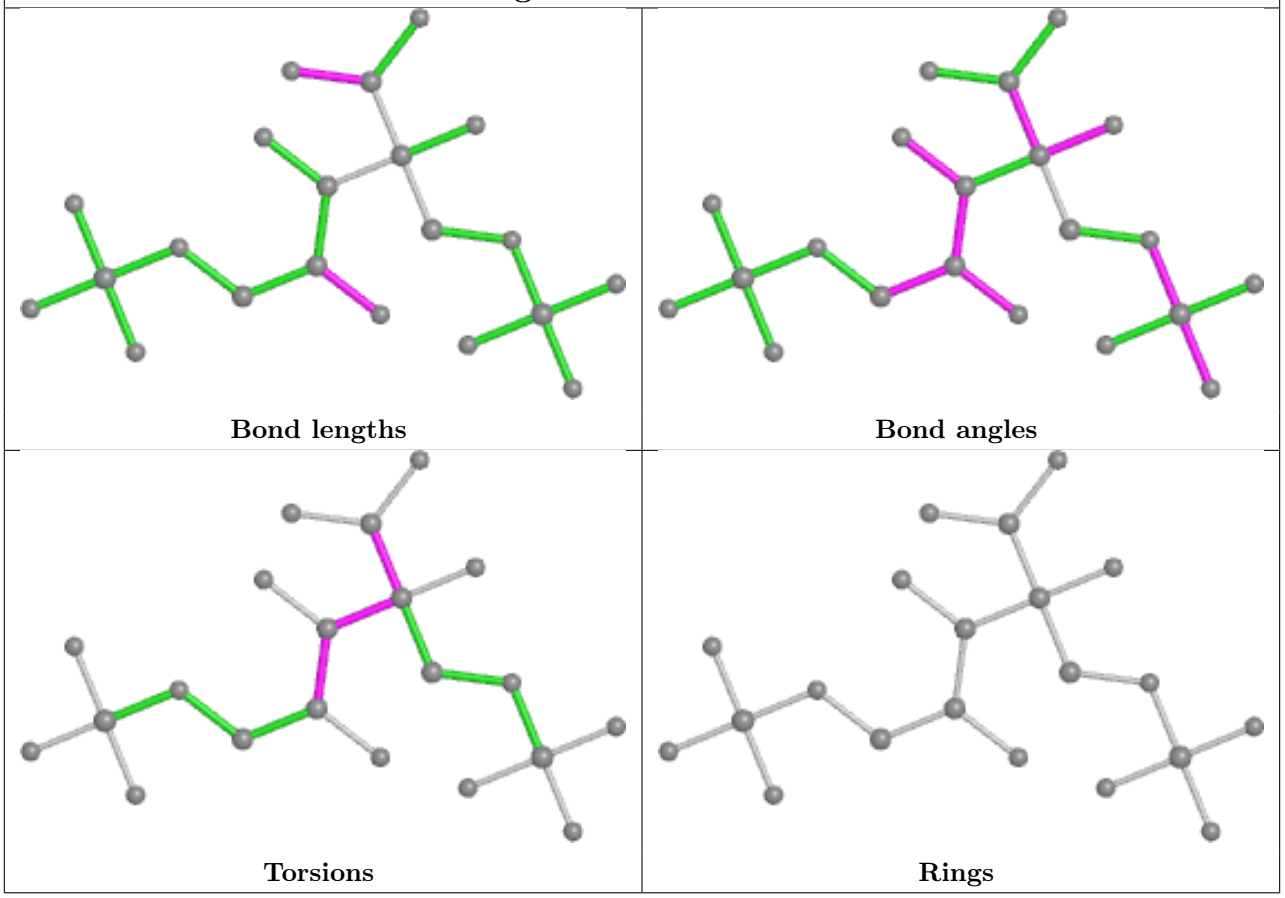


Torsions



Rings

Ligand CAP O 1477



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	460/475 (96%)	-0.61	3 (0%) 87 86	9, 16, 32, 49	0
1	B	462/475 (97%)	-0.62	5 (1%) 80 79	9, 16, 33, 55	0
1	E	460/475 (96%)	-0.71	0 100 100	9, 16, 32, 49	0
1	H	464/475 (97%)	-0.63	5 (1%) 80 79	9, 16, 34, 70	0
1	K	464/475 (97%)	-0.63	7 (1%) 73 72	9, 16, 34, 66	0
1	O	464/475 (97%)	-0.62	5 (1%) 80 79	9, 16, 34, 66	0
1	R	460/475 (96%)	-0.66	1 (0%) 95 94	9, 16, 32, 49	0
1	V	461/475 (97%)	-0.59	3 (0%) 87 86	9, 16, 32, 49	0
2	C	129/134 (96%)	-0.06	6 (4%) 31 30	14, 25, 50, 58	0
2	F	129/134 (96%)	-0.07	10 (7%) 13 11	14, 25, 50, 58	0
2	I	129/134 (96%)	-0.25	8 (6%) 20 19	14, 25, 50, 58	0
2	J	129/134 (96%)	-0.11	5 (3%) 39 38	14, 26, 50, 58	0
2	M	129/134 (96%)	-0.13	7 (5%) 25 24	15, 25, 50, 58	0
2	P	129/134 (96%)	-0.16	9 (6%) 16 15	14, 25, 50, 58	0
2	T	129/134 (96%)	-0.21	7 (5%) 25 24	14, 25, 50, 58	0
2	W	129/134 (96%)	0.00	10 (7%) 13 11	14, 25, 50, 58	0
All	All	4727/4872 (97%)	-0.52	91 (1%) 66 64	9, 18, 38, 70	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	W	129	ALA	6.0
2	F	130	ASN	5.9
2	W	128	PRO	5.8
1	B	9	ALA	5.6
2	W	130	ASN	5.6

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Mol	Chain	Res	Type	RSRZ
2	M	129	ALA	5.5
2	M	130	ASN	5.4
2	F	129	ALA	5.3
2	C	130	ASN	5.3
2	P	131	LYS	5.3
1	H	8	LYS	4.8
2	F	128	PRO	4.8
1	H	9	ALA	4.7
2	C	129	ALA	4.5
2	P	129	ALA	4.4
2	I	129	ALA	4.0
2	I	130	ASN	4.0
2	F	133	SER	4.0
2	M	128	PRO	3.9
2	F	127	GLN	3.9
1	O	9	ALA	3.9
2	M	134	VAL	3.9
1	H	7	THR	3.9
2	I	127	GLN	3.8
2	I	128	PRO	3.6
2	J	121	LYS	3.5
2	C	121	LYS	3.4
2	C	47	ASP	3.4
2	F	131	LYS	3.3
2	I	131	LYS	3.3
2	W	78	ARG	3.3
2	C	128	PRO	3.3
1	V	439	ARG	3.0
2	T	128	PRO	3.0
1	O	7	THR	2.9
1	H	10	GLY	2.9
1	V	10	GLY	2.9
2	C	127	GLN	2.9
1	K	91	PRO	2.9
2	M	121	LYS	2.8
2	P	48[A]	HIS	2.8
2	T	131	LYS	2.7
2	W	121	LYS	2.7
2	J	47	ASP	2.7
1	A	94	ASP	2.7
1	K	94	ASP	2.7
2	I	134	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	W	127	GLN	2.6
1	R	94	ASP	2.6
1	O	8	LYS	2.6
1	H	92	GLY	2.6
1	K	7	THR	2.6
2	P	130	ASN	2.6
2	T	130	ASN	2.6
2	M	131	LYS	2.5
1	A	475	LEU	2.5
2	J	130	ASN	2.5
2	P	47	ASP	2.5
2	M	133	SER	2.5
2	W	134	VAL	2.5
2	T	129	ALA	2.4
2	T	121	LYS	2.4
2	P	134	VAL	2.4
1	B	10	GLY	2.3
2	F	48[A]	HIS	2.3
2	J	132	ARG	2.3
1	B	92	GLY	2.3
1	K	8	LYS	2.3
2	T	127	GLN	2.3
2	J	127	GLN	2.2
1	O	94	ASP	2.2
2	W	131	LYS	2.2
2	F	121	LYS	2.2
1	A	92	GLY	2.2
1	B	94	ASP	2.2
2	W	57	ASN	2.2
2	I	133	SER	2.2
2	F	134	VAL	2.2
1	B	439	ARG	2.1
2	P	8	ASN	2.1
2	W	24	GLU	2.1
1	K	10	GLY	2.1
1	K	9	ALA	2.1
2	P	7	VAL	2.1
2	F	57	ASN	2.1
2	T	47	ASP	2.1
1	O	10	GLY	2.1
1	V	94	ASP	2.0
1	K	439	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	P	128	PRO	2.0
2	I	132	ARG	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	SMC	R	369	7/8	0.94	0.11	18,19,21,26	0
1	HYP	O	104	8/9	0.95	0.11	12,13,14,17	0
1	HYP	E	151	8/9	0.95	0.11	12,13,14,14	0
1	KCX	V	201	12/13	0.95	0.15	11,13,14,14	0
1	HYP	K	151	8/9	0.96	0.08	12,13,14,14	0
1	SMC	K	369	7/8	0.96	0.09	18,19,21,26	0
1	SMC	A	369	7/8	0.96	0.10	18,19,21,25	0
1	SMC	O	369	7/8	0.96	0.09	18,19,21,25	0
1	KCX	E	201	12/13	0.96	0.12	11,13,14,15	0
1	HYP	V	104	8/9	0.96	0.10	11,13,14,17	0
1	SMC	H	369	7/8	0.96	0.10	18,19,21,26	0
1	SMC	V	369	7/8	0.96	0.10	18,19,21,26	0
1	SMC	B	369	7/8	0.97	0.07	18,19,21,26	0
1	SMC	E	369	7/8	0.97	0.08	18,19,21,25	0
1	HYP	O	151	8/9	0.97	0.13	12,13,13,13	0
1	KCX	O	201	12/13	0.97	0.15	11,13,14,14	0
1	HYP	H	151	8/9	0.97	0.12	12,13,14,14	0
1	HYP	R	104	8/9	0.97	0.10	12,13,13,17	0
1	KCX	H	201	12/13	0.97	0.11	11,13,14,14	0
1	HYP	E	104	8/9	0.97	0.08	12,13,14,17	0
1	HYP	V	151	8/9	0.97	0.11	12,13,14,14	0
1	HYP	K	104	8/9	0.97	0.10	12,13,13,17	0
1	KCX	A	201	12/13	0.97	0.14	11,13,14,14	0
1	HYP	H	104	8/9	0.98	0.10	12,13,13,17	0
1	KCX	B	201	12/13	0.98	0.12	11,13,14,14	0
1	SMC	O	256	7/8	0.98	0.07	6,9,11,11	0
1	SMC	B	256	7/8	0.98	0.07	6,10,11,12	0
1	HYP	A	104	8/9	0.98	0.09	12,13,13,17	0
1	HYP	R	151	8/9	0.98	0.10	12,12,13,13	0
1	KCX	R	201	12/13	0.98	0.14	11,13,14,14	0
1	SMC	R	256	7/8	0.98	0.07	6,10,11,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	SMC	A	256	7/8	0.98	0.08	6,10,11,12	0
1	HYP	A	151	8/9	0.98	0.14	12,12,14,14	0
1	KCX	K	201	12/13	0.98	0.11	11,13,14,14	0
1	HYP	B	104	8/9	0.98	0.08	12,13,13,16	0
1	SMC	V	256	7/8	0.98	0.08	6,10,11,11	0
1	HYP	B	151	8/9	0.98	0.10	12,13,14,14	0
1	SMC	H	256	7/8	0.99	0.05	6,10,11,11	0
1	SMC	K	256	7/8	0.99	0.07	6,9,11,11	0
1	SMC	E	256	7/8	0.99	0.07	6,10,11,11	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
5	EDO	R	1484	4/4	0.42	0.49	84,86,87,88	0
5	EDO	K	1482	4/4	0.62	0.43	62,66,68,69	0
5	EDO	K	1480	4/4	0.72	0.26	42,45,49,51	0
5	EDO	T	1135	4/4	0.74	0.29	56,57,60,62	0
5	EDO	R	1482	4/4	0.76	0.29	49,54,55,56	0
5	EDO	W	1135	4/4	0.80	0.20	40,41,45,47	0
5	EDO	V	1483	4/4	0.81	0.23	42,42,42,43	0
5	EDO	E	1478	4/4	0.82	0.20	43,45,45,47	0
5	EDO	C	1135	4/4	0.83	0.28	61,61,64,65	0
5	EDO	H	1481	4/4	0.83	0.23	40,43,43,49	0
5	EDO	O	1480	4/4	0.83	0.14	40,42,45,45	0
5	EDO	J	1135	4/4	0.83	0.16	37,39,43,50	0
5	EDO	P	1135	4/4	0.84	0.27	57,59,61,61	0
5	EDO	V	1478	4/4	0.86	0.28	28,30,32,32	0
5	EDO	E	1482	4/4	0.86	0.26	23,25,28,33	0
5	EDO	A	1480	4/4	0.86	0.23	30,31,32,34	0
5	EDO	B	1482	4/4	0.88	0.20	34,36,40,44	0
5	EDO	R	1481	4/4	0.88	0.18	28,34,35,37	0
5	EDO	I	1135	4/4	0.88	0.26	37,41,43,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	O	1483	4/4	0.88	0.26	28,42,43,48	0
5	EDO	A	1482	4/4	0.89	0.19	39,41,44,45	0
5	EDO	O	1482	4/4	0.89	0.18	40,41,43,44	0
5	EDO	R	1483	4/4	0.89	0.22	31,32,34,36	0
5	EDO	R	1480	4/4	0.89	0.20	41,43,45,47	0
5	EDO	V	1481	4/4	0.90	0.31	39,41,42,44	0
5	EDO	O	1478	4/4	0.90	0.16	21,32,33,36	0
5	EDO	A	1483	4/4	0.90	0.20	25,29,35,36	0
5	EDO	T	1136	4/4	0.91	0.13	38,41,45,45	0
5	EDO	F	1135	4/4	0.92	0.20	29,32,33,36	0
5	EDO	H	1478	4/4	0.92	0.15	25,27,31,32	0
5	EDO	B	1480	4/4	0.92	0.21	30,43,46,48	0
5	EDO	M	1135	4/4	0.92	0.16	29,32,33,34	0
5	EDO	B	1481	4/4	0.92	0.14	38,39,40,41	0
5	EDO	C	1136	4/4	0.93	0.14	26,32,35,40	0
5	EDO	A	1478	4/4	0.93	0.13	31,31,32,34	0
5	EDO	E	1481	4/4	0.93	0.23	30,36,40,44	0
5	EDO	B	1478	4/4	0.93	0.13	22,29,30,33	0
5	EDO	E	1480	4/4	0.94	0.26	40,44,45,52	0
5	EDO	V	1479	4/4	0.94	0.13	20,25,28,32	0
5	EDO	K	1481	4/4	0.94	0.20	22,33,35,37	0
3	MG	E	1476	1/1	0.94	0.10	29,29,29,29	0
5	EDO	K	1479	4/4	0.94	0.14	25,32,33,33	0
3	MG	H	1476	1/1	0.95	0.07	24,24,24,24	0
3	MG	K	1476	1/1	0.95	0.08	18,18,18,18	0
5	EDO	R	1478	4/4	0.95	0.13	27,29,31,35	0
5	EDO	V	1482	4/4	0.95	0.15	25,26,27,33	0
5	EDO	H	1479	4/4	0.95	0.13	21,26,27,30	0
5	EDO	K	1478	4/4	0.95	0.17	26,27,29,33	0
3	MG	B	1476	1/1	0.96	0.10	24,24,24,24	0
5	EDO	A	1481	4/4	0.96	0.12	36,38,44,48	0
5	EDO	R	1479	4/4	0.96	0.10	17,18,22,23	0
5	EDO	V	1480	4/4	0.96	0.11	9,16,18,26	0
5	EDO	O	1481	4/4	0.97	0.13	31,31,35,35	0
5	EDO	H	1480	4/4	0.97	0.18	55,55,58,59	0
5	EDO	O	1479	4/4	0.97	0.12	21,24,24,25	0
5	EDO	B	1479	4/4	0.97	0.08	16,16,19,20	0
5	EDO	E	1479	4/4	0.98	0.11	13,19,20,21	0
3	MG	V	1476	1/1	0.98	0.07	17,17,17,17	0
4	CAP	H	1477	21/21	0.98	0.09	7,17,21,25	0
4	CAP	O	1477	21/21	0.98	0.09	7,14,19,23	0
3	MG	A	1476	1/1	0.98	0.09	11,11,11,11	0

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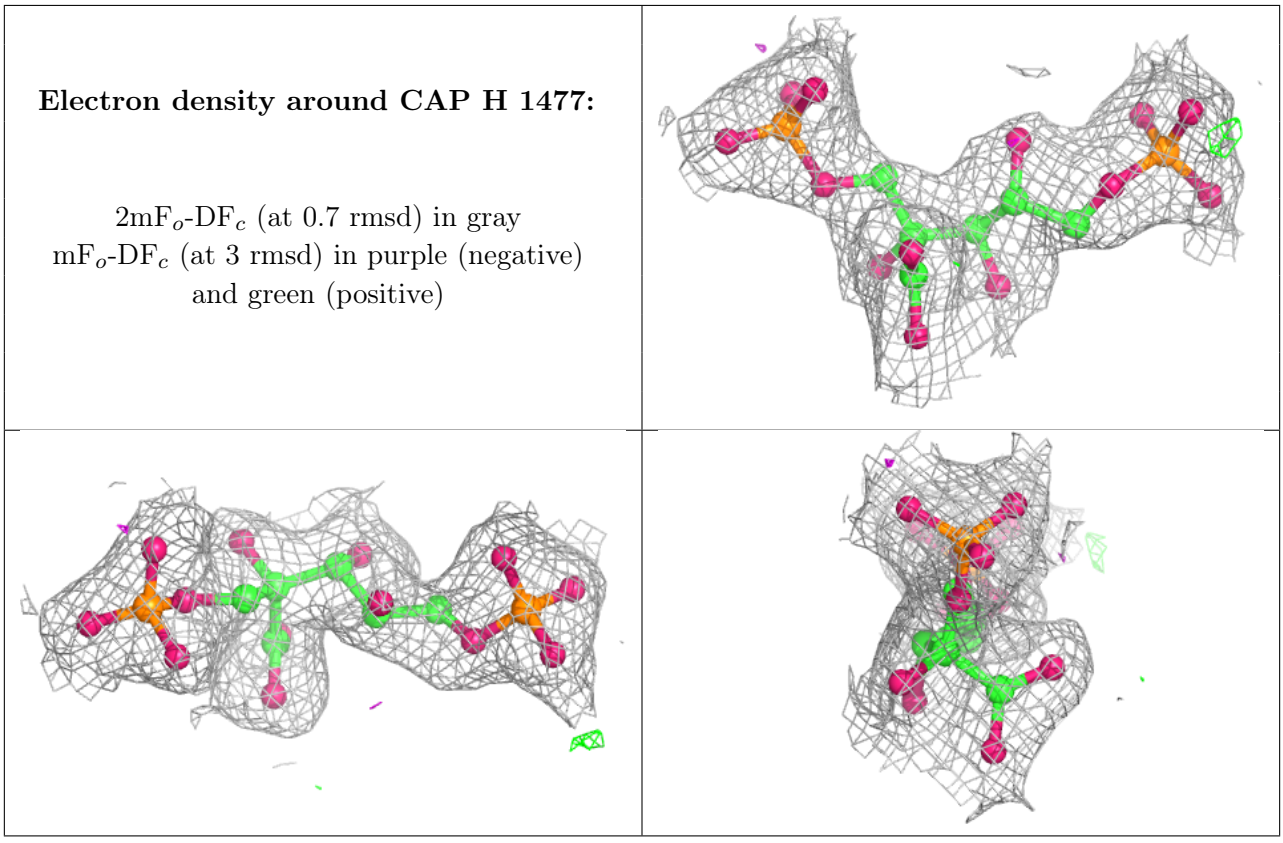
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CAP	A	1477	21/21	0.99	0.08	9,14,21,25	0
5	EDO	A	1479	4/4	0.99	0.07	7,8,10,12	0
4	CAP	B	1477	21/21	0.99	0.10	7,11,17,21	0
4	CAP	E	1477	21/21	0.99	0.09	12,17,20,22	0
3	MG	R	1476	1/1	0.99	0.12	12,12,12,12	0
4	CAP	K	1477	21/21	0.99	0.09	7,14,21,29	0
3	MG	O	1476	1/1	0.99	0.10	13,13,13,13	0
4	CAP	R	1477	21/21	0.99	0.12	7,15,21,21	0
4	CAP	V	1477	21/21	0.99	0.10	6,16,19,22	0

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

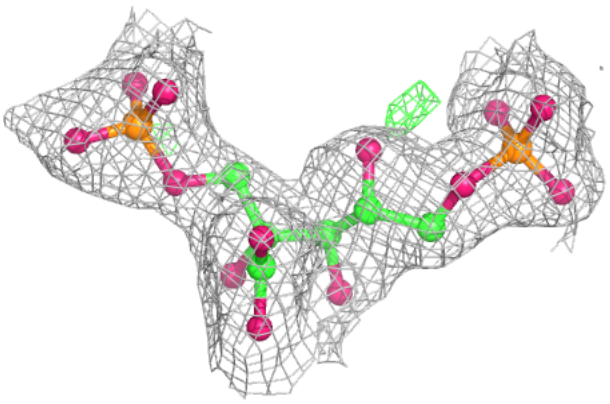
Electron density around CAP H 1477:

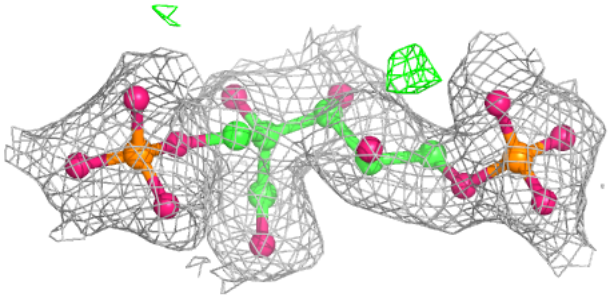
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

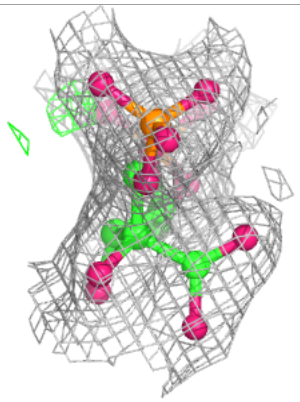


Electron density around CAP O 1477:

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

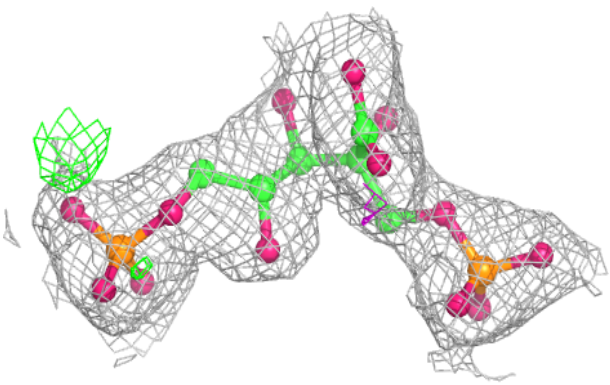


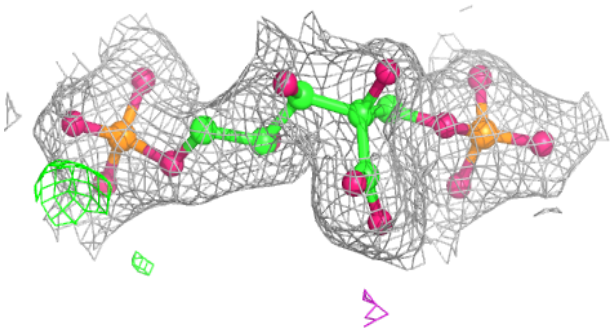


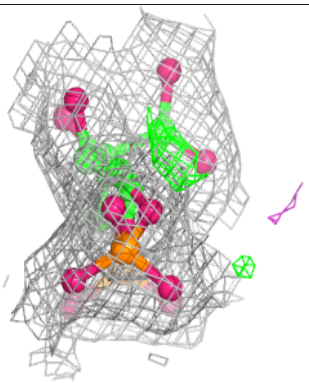


Electron density around CAP A 1477:

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

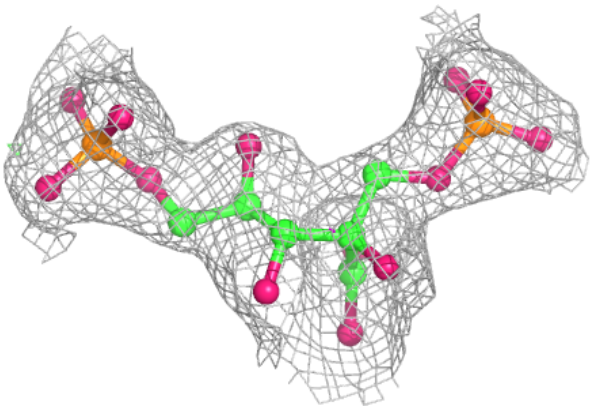


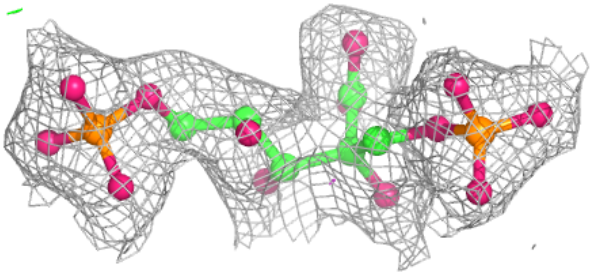


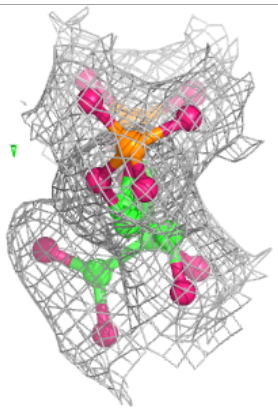


Electron density around CAP B 1477:

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

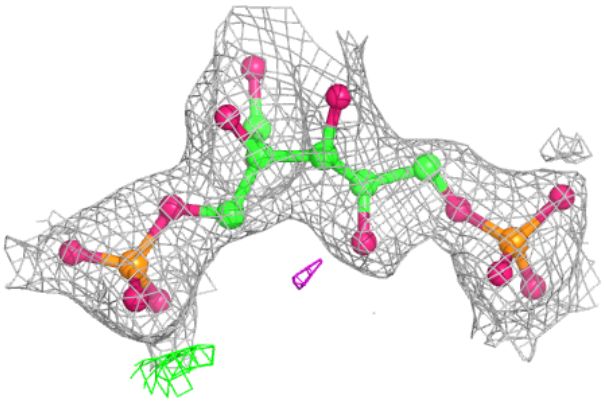


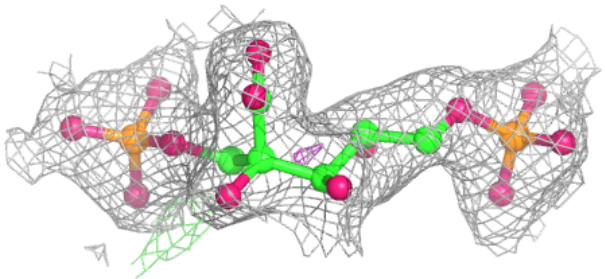


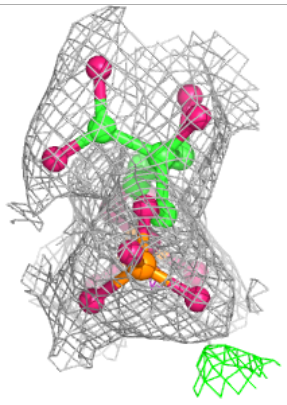


Electron density around CAP E 1477:

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

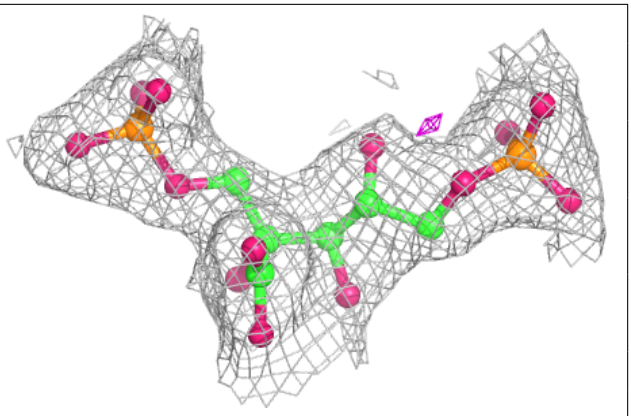


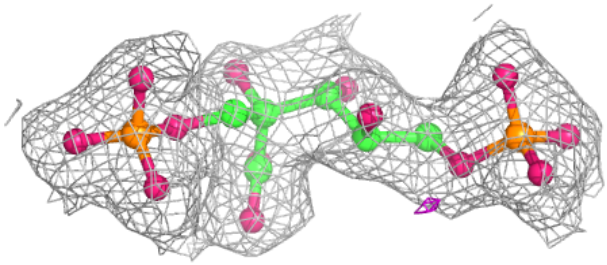


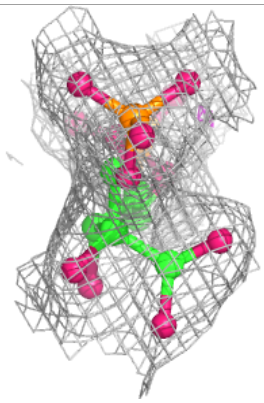


Electron density around CAP K 1477:

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

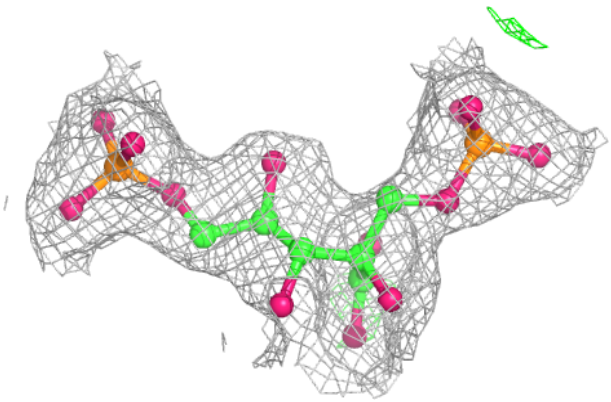


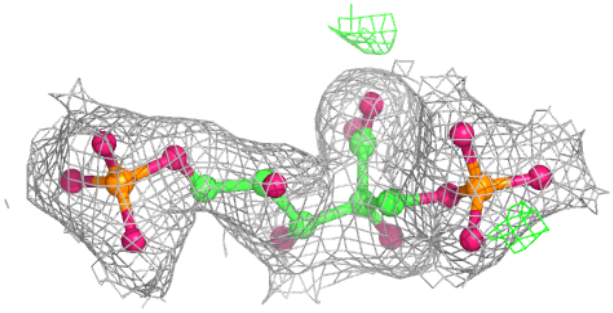


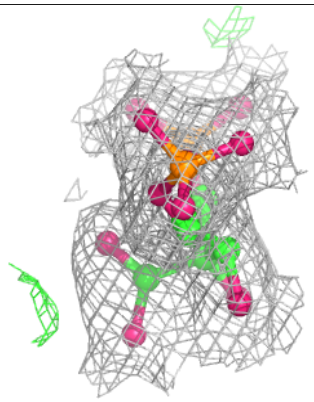


Electron density around CAP R 1477:

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

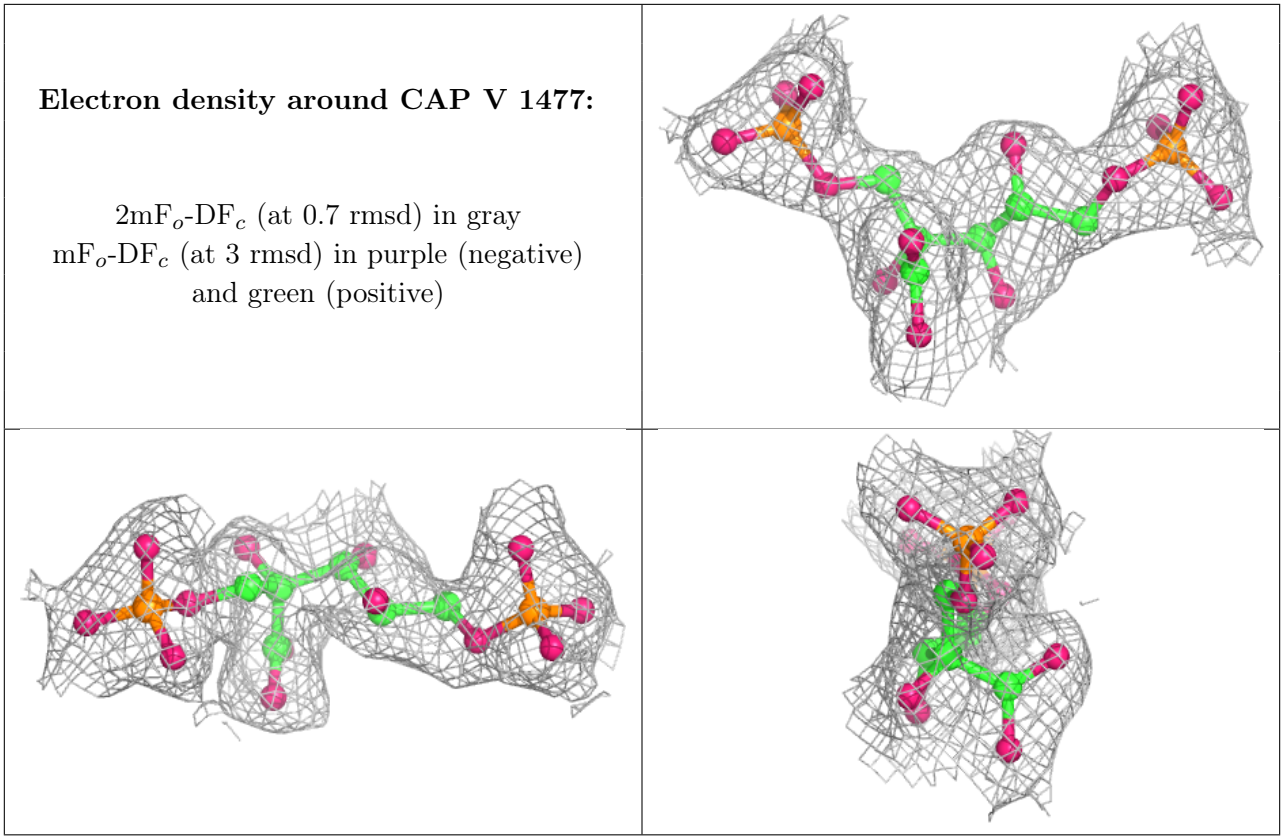






Electron density around CAP V 1477:

$2mF_o$-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.