Full wwPDB X-ray Structure Validation Report (i)

May 17, 2020 – 11:37 am BST

PDB ID	:	1RBL
Title	:	STRUCTURE DETERMINATION AND REFINEMENT OF RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE(SLASH)OXYGENASE FROM SYNECHOCOCCUS PCC6301
Authors	:	Newman, J.; Gutteridge, S.; Branden, C.-I.; Jones, T.A.
Deposited on	:	1993-05-12
Resolution	:	2.20 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 following versions of software and data (see references (i)) were used in the production of this report:

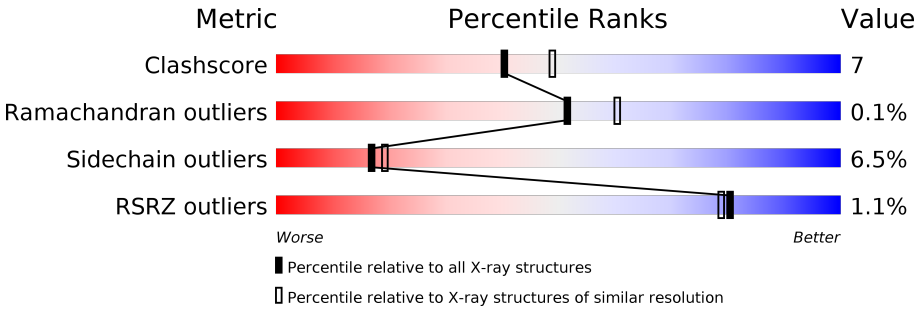
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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 on 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	467	% 81% 15% • •
1	B	467	81% 15% • •
1	C	467	82% 14% • •
1	D	467	82% 14% • •
1	E	467	81% 15% • •
1	F	467	% 81% 15% • •
1	G	467	% 81% 15% • •

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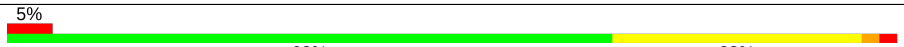
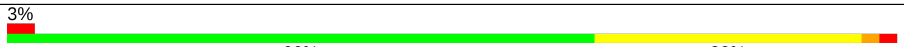
Mol	Chain	Length	Quality of chain
1	H	467	
2	I	109	
2	J	109	
2	K	109	
2	L	109	
2	M	109	
2	N	109	
2	O	109	
2	P	109	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36988 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 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	B	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	C	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	D	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	E	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	F	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	G	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			
1	H	467	Total	C	N	O	S	16	0	0
			3653	2324	638	673	18			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ARG	PRO	CONFLICT	UNP P00880
A	42	PHE	VAL	CONFLICT	UNP P00880
A	91	ALA	GLN	CONFLICT	UNP P00880
A	356	ALA	ARG	CONFLICT	UNP P00880
B	41	ARG	PRO	CONFLICT	UNP P00880
B	42	PHE	VAL	CONFLICT	UNP P00880
B	91	ALA	GLN	CONFLICT	UNP P00880
B	356	ALA	ARG	CONFLICT	UNP P00880
C	41	ARG	PRO	CONFLICT	UNP P00880
C	42	PHE	VAL	CONFLICT	UNP P00880
C	91	ALA	GLN	CONFLICT	UNP P00880
C	356	ALA	ARG	CONFLICT	UNP P00880

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Chain	Residue	Modelled	Actual	Comment	Reference
D	41	ARG	PRO	CONFLICT	UNP P00880
D	42	PHE	VAL	CONFLICT	UNP P00880
D	91	ALA	GLN	CONFLICT	UNP P00880
D	356	ALA	ARG	CONFLICT	UNP P00880
E	41	ARG	PRO	CONFLICT	UNP P00880
E	42	PHE	VAL	CONFLICT	UNP P00880
E	91	ALA	GLN	CONFLICT	UNP P00880
E	356	ALA	ARG	CONFLICT	UNP P00880
F	41	ARG	PRO	CONFLICT	UNP P00880
F	42	PHE	VAL	CONFLICT	UNP P00880
F	91	ALA	GLN	CONFLICT	UNP P00880
F	356	ALA	ARG	CONFLICT	UNP P00880
G	41	ARG	PRO	CONFLICT	UNP P00880
G	42	PHE	VAL	CONFLICT	UNP P00880
G	91	ALA	GLN	CONFLICT	UNP P00880
G	356	ALA	ARG	CONFLICT	UNP P00880
H	41	ARG	PRO	CONFLICT	UNP P00880
H	42	PHE	VAL	CONFLICT	UNP P00880
H	91	ALA	GLN	CONFLICT	UNP P00880
H	356	ALA	ARG	CONFLICT	UNP P00880

- Molecule 2 is a protein called RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	I	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	N	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	J	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	O	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	K	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	P	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			
2	L	109	Total	C	N	O	S	12	0	0
			909	581	154	167	7			

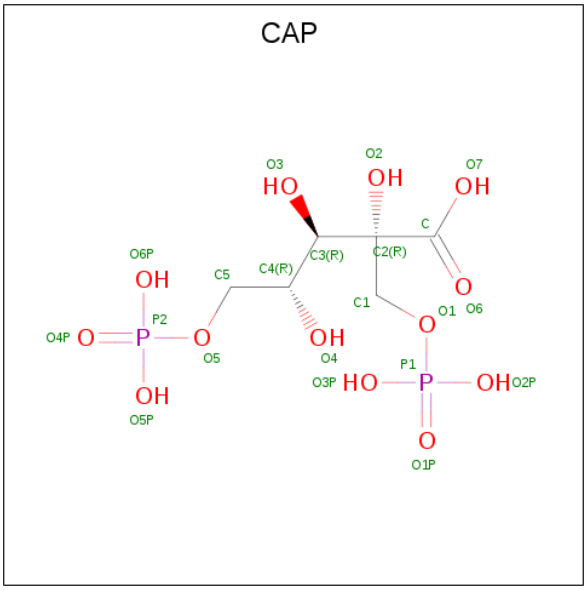
There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	76	ALA	ASP	CONFLICT	UNP P04716
M	78	ALA	LYS	CONFLICT	UNP P04716
M	79	ALA	SER	CONFLICT	UNP P04716
M	109	GLU	GLN	CONFLICT	UNP P04716
M	113	SER	VAL	CONFLICT	UNP P04716
I	76	ALA	ASP	CONFLICT	UNP P04716
I	78	ALA	LYS	CONFLICT	UNP P04716
I	79	ALA	SER	CONFLICT	UNP P04716
I	109	GLU	GLN	CONFLICT	UNP P04716
I	113	SER	VAL	CONFLICT	UNP P04716
N	76	ALA	ASP	CONFLICT	UNP P04716
N	78	ALA	LYS	CONFLICT	UNP P04716
N	79	ALA	SER	CONFLICT	UNP P04716
N	109	GLU	GLN	CONFLICT	UNP P04716
N	113	SER	VAL	CONFLICT	UNP P04716
J	76	ALA	ASP	CONFLICT	UNP P04716
J	78	ALA	LYS	CONFLICT	UNP P04716
J	79	ALA	SER	CONFLICT	UNP P04716
J	109	GLU	GLN	CONFLICT	UNP P04716
J	113	SER	VAL	CONFLICT	UNP P04716
O	76	ALA	ASP	CONFLICT	UNP P04716
O	78	ALA	LYS	CONFLICT	UNP P04716
O	79	ALA	SER	CONFLICT	UNP P04716
O	109	GLU	GLN	CONFLICT	UNP P04716
O	113	SER	VAL	CONFLICT	UNP P04716
K	76	ALA	ASP	CONFLICT	UNP P04716
K	78	ALA	LYS	CONFLICT	UNP P04716
K	79	ALA	SER	CONFLICT	UNP P04716
K	109	GLU	GLN	CONFLICT	UNP P04716
K	113	SER	VAL	CONFLICT	UNP P04716
P	76	ALA	ASP	CONFLICT	UNP P04716
P	78	ALA	LYS	CONFLICT	UNP P04716
P	79	ALA	SER	CONFLICT	UNP P04716
P	109	GLU	GLN	CONFLICT	UNP P04716
P	113	SER	VAL	CONFLICT	UNP P04716
L	76	ALA	ASP	CONFLICT	UNP P04716
L	78	ALA	LYS	CONFLICT	UNP P04716
L	79	ALA	SER	CONFLICT	UNP P04716
L	109	GLU	GLN	CONFLICT	UNP P04716
L	113	SER	VAL	CONFLICT	UNP P04716

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

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

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

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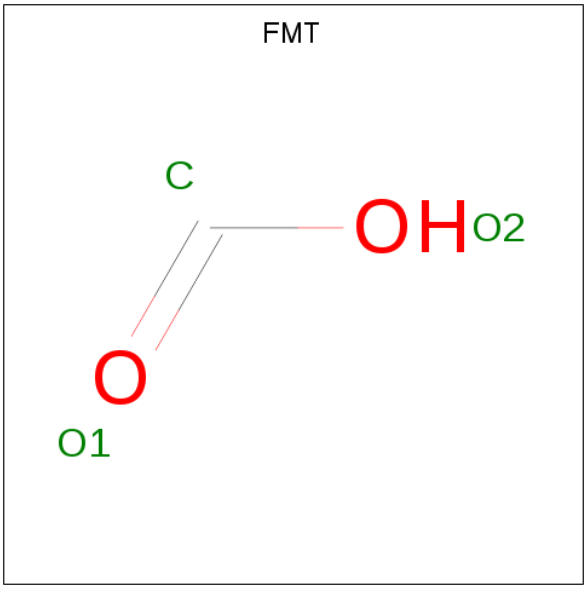
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C O P 21 6 13 2	0	0
4	E	1	Total C O P 21 6 13 2	0	0
4	F	1	Total C O P 21 6 13 2	0	0
4	G	1	Total C O P 21 6 13 2	0	0
4	H	1	Total C O P 21 6 13 2	0	0

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 3 1 2	0	0
5	B	1	Total C O 3 1 2	0	0
5	C	1	Total C O 3 1 2	0	0
5	D	1	Total C O 3 1 2	0	0
5	E	1	Total C O 3 1 2	0	0
5	F	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total C O 3 1 2	0	0
5	H	1	Total C O 3 1 2	0	0

- Molecule 6 is water.

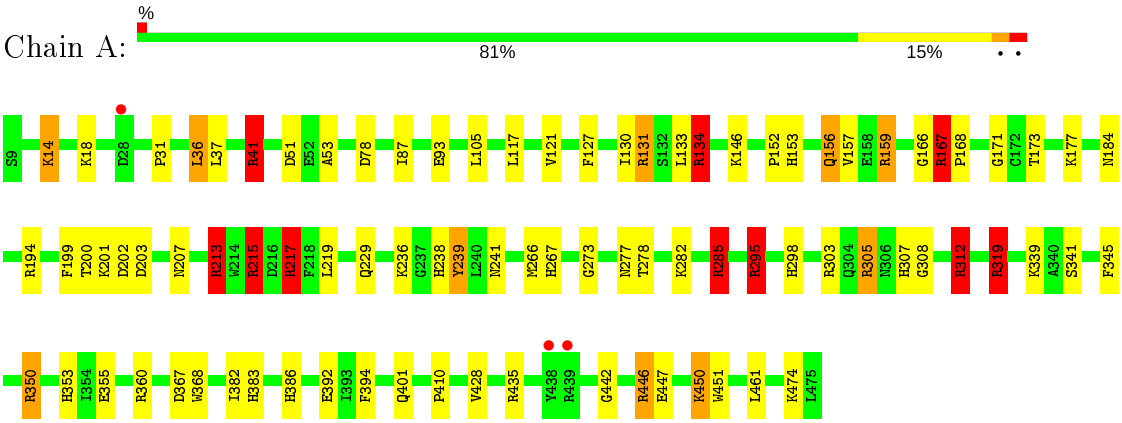
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	214	Total O 214 214	0	0
6	M	53	Total O 53 53	0	0
6	B	4	Total O 4 4	0	0
6	C	9	Total O 9 9	0	0
6	N	5	Total O 5 5	0	0
6	D	3	Total O 3 3	0	0
6	G	2	Total O 2 2	0	0
6	P	2	Total O 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

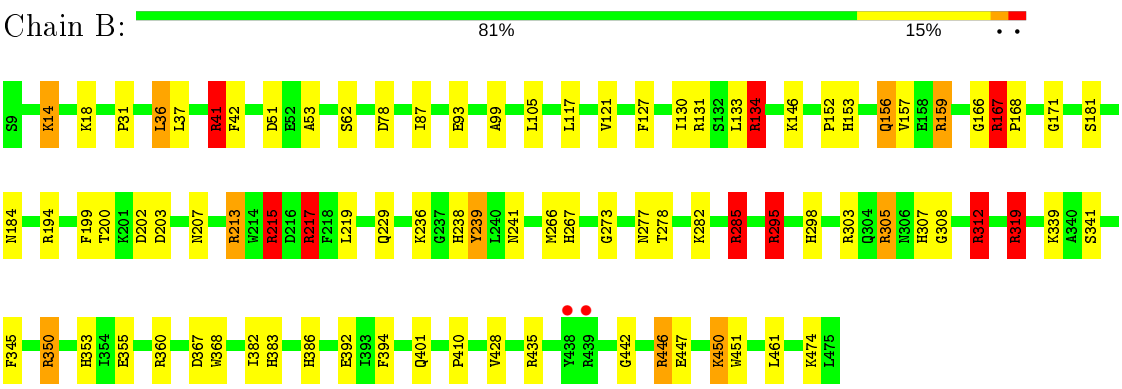
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain A:



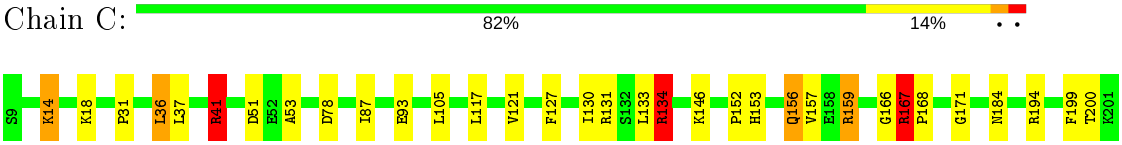
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

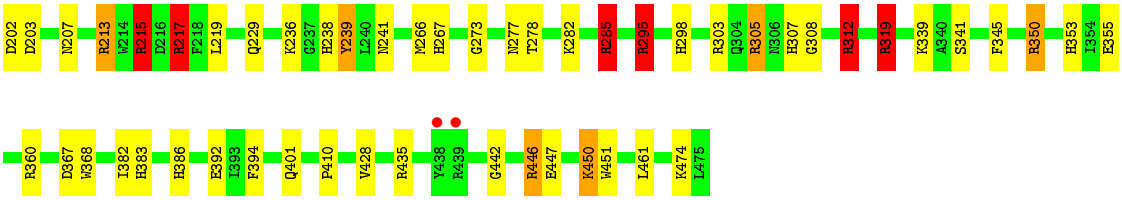
Chain B:



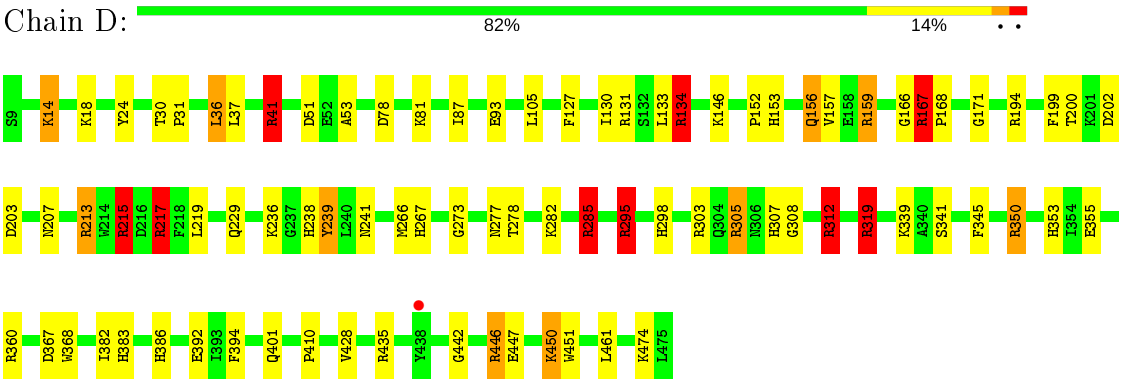
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain C:

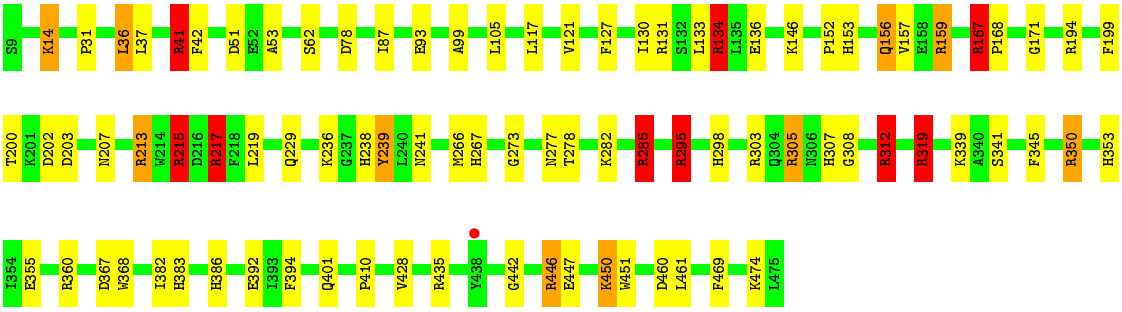




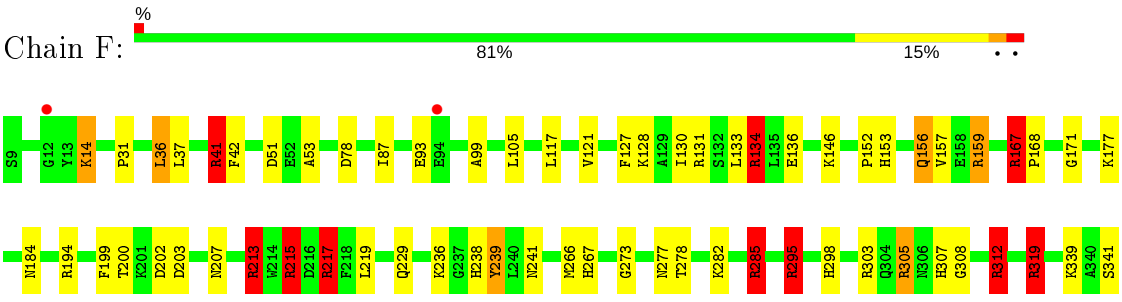
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

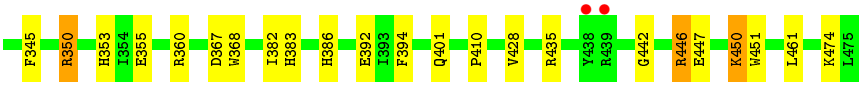


• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)



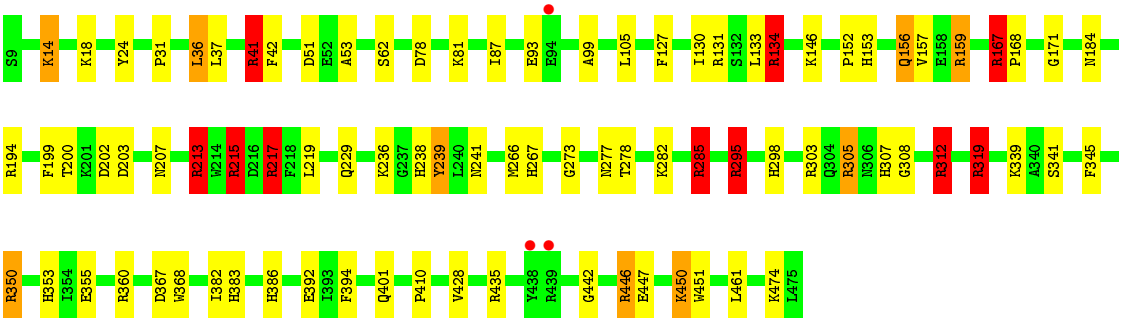
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)





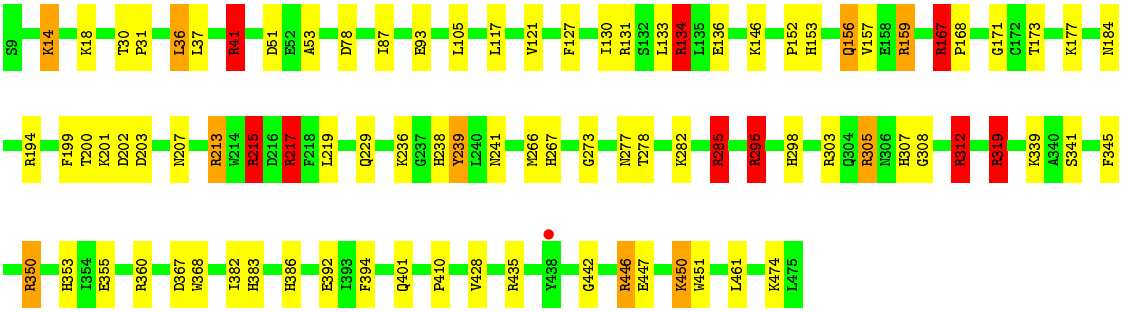
• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain G:



• Molecule 1: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (LARGE CHAIN)

Chain H:

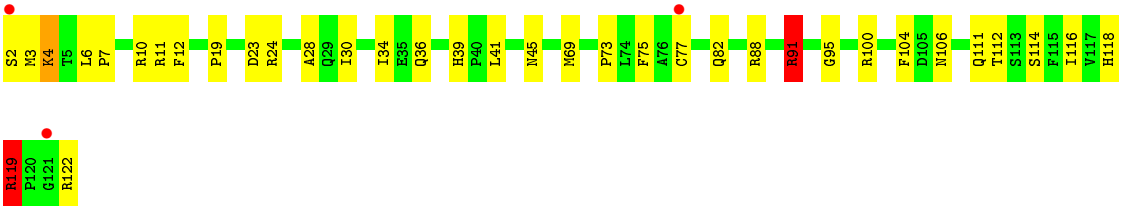


• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain M:

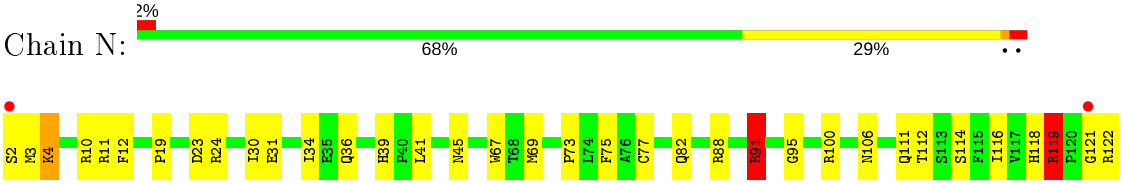
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain I:



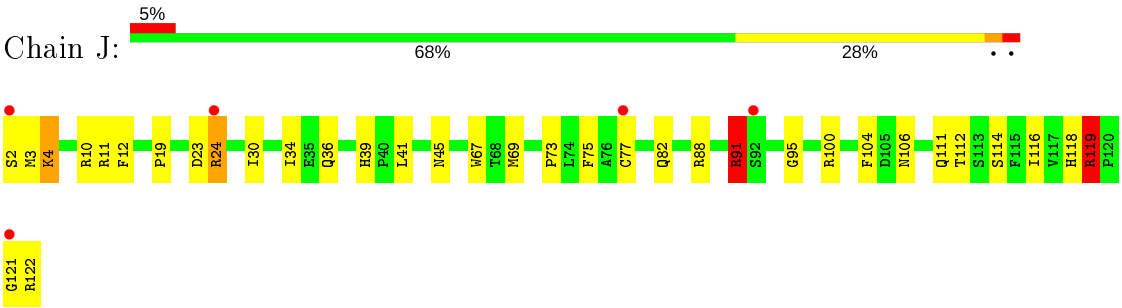
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain N:



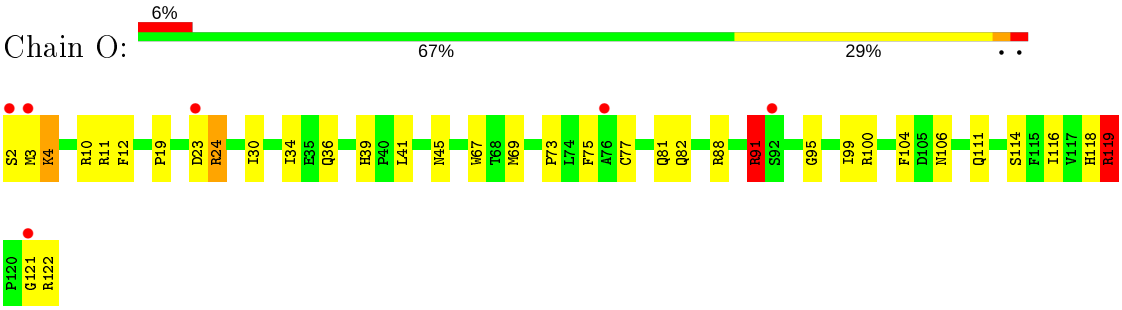
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain J:



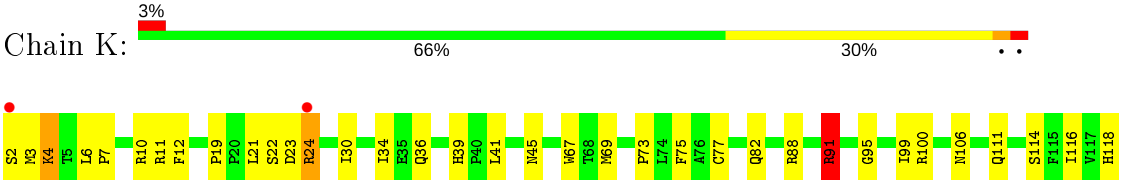
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain O:



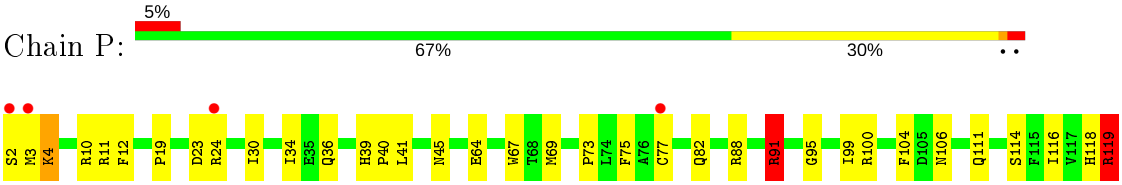
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain K:



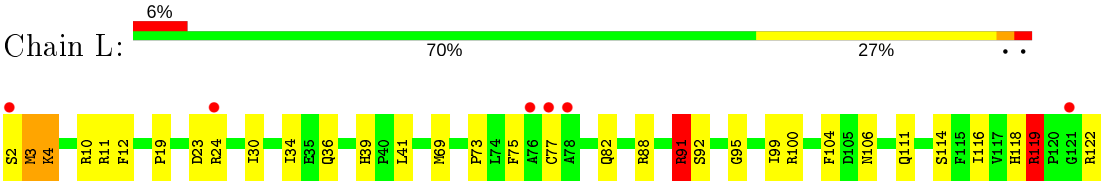
• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain P:



• Molecule 2: RIBULOSE 1,5 BISPHOSPHATE CARBOXYLASE/OXYGENASE (SMALL CHAIN)

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	223.90Å 111.90Å 199.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 19.99 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 39.6 (19.99-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.96 (at 2.19Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.200 , (Not available) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.632	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 22.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	36988	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.0290e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMT, CAP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/3745	0.63	8/5071 (0.2%)
1	B	0.34	0/3745	0.63	8/5071 (0.2%)
1	C	0.34	0/3745	0.63	8/5071 (0.2%)
1	D	0.34	0/3745	0.63	8/5071 (0.2%)
1	E	0.34	0/3745	0.63	8/5071 (0.2%)
1	F	0.34	0/3745	0.63	9/5071 (0.2%)
1	G	0.34	0/3745	0.63	9/5071 (0.2%)
1	H	0.34	0/3745	0.63	8/5071 (0.2%)
2	I	0.38	0/936	0.59	1/1265 (0.1%)
2	J	0.38	0/936	0.59	1/1265 (0.1%)
2	K	0.37	0/936	0.59	1/1265 (0.1%)
2	L	0.38	0/936	0.59	1/1265 (0.1%)
2	M	0.37	0/936	0.59	1/1265 (0.1%)
2	N	0.38	0/936	0.59	1/1265 (0.1%)
2	O	0.37	0/936	0.59	1/1265 (0.1%)
2	P	0.38	0/936	0.59	1/1265 (0.1%)
All	All	0.35	0/37448	0.62	74/50688 (0.1%)

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
1	A	0	17
1	B	0	17
1	C	0	17
1	D	0	17
1	E	0	17
1	F	0	17
1	G	0	17

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	17
2	I	0	5
2	J	0	5
2	K	0	5
2	L	0	5
2	M	0	5
2	N	0	5
2	O	0	5
2	P	0	5
All	All	0	176

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	159	ARG	NE-CZ-NH1	-8.23	116.19	120.30
1	E	159	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	C	159	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	A	159	ARG	NE-CZ-NH1	-8.19	116.21	120.30
1	H	159	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	D	159	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	G	159	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	F	285	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	D	285	ARG	NE-CZ-NH2	-8.13	116.24	120.30
1	B	285	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	H	285	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	B	159	ARG	NE-CZ-NH1	-8.08	116.26	120.30
1	A	285	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	C	285	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	E	285	ARG	NE-CZ-NH2	-8.03	116.28	120.30
1	G	285	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	F	312	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	C	312	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	G	312	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	312	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	E	312	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	A	312	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	B	312	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	H	312	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	D	217	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	F	217	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	G	217	ARG	NE-CZ-NH1	-7.71	116.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	217	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	E	217	ARG	NE-CZ-NH1	-7.69	116.45	120.30
1	A	217	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	H	217	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	C	217	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	F	36	LEU	CA-CB-CG	6.67	130.63	115.30
1	B	36	LEU	CA-CB-CG	6.66	130.62	115.30
1	D	36	LEU	CA-CB-CG	6.66	130.62	115.30
1	G	36	LEU	CA-CB-CG	6.66	130.62	115.30
1	A	36	LEU	CA-CB-CG	6.66	130.61	115.30
1	H	36	LEU	CA-CB-CG	6.65	130.60	115.30
1	C	36	LEU	CA-CB-CG	6.65	130.59	115.30
1	E	36	LEU	CA-CB-CG	6.64	130.57	115.30
1	H	215	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	D	215	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	A	215	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	G	215	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	134	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	B	215	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	E	215	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	H	134	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	F	134	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	C	215	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	134	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	134	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	E	134	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	F	215	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	G	134	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	C	134	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	H	41	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	D	41	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	K	91	ARG	NE-CZ-NH1	-5.15	117.72	120.30
2	I	91	ARG	NE-CZ-NH1	-5.15	117.72	120.30
2	O	91	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	41	ARG	NE-CZ-NH2	-5.12	117.74	120.30
2	L	91	ARG	NE-CZ-NH1	-5.09	117.75	120.30
2	M	91	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	F	41	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	A	41	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	G	41	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	F	213	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	J	91	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	91	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	G	213	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	41	ARG	NE-CZ-NH2	-5.03	117.79	120.30
2	N	91	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	E	41	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (176) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	131	ARG	Sidechain
1	A	134	ARG	Sidechain
1	A	159	ARG	Sidechain
1	A	167	ARG	Sidechain
1	A	194	ARG	Sidechain
1	A	213	ARG	Sidechain
1	A	215	ARG	Sidechain
1	A	217	ARG	Sidechain
1	A	285	ARG	Sidechain
1	A	295	ARG	Sidechain
1	A	305	ARG	Sidechain
1	A	312	ARG	Sidechain
1	A	319	ARG	Sidechain
1	A	350	ARG	Sidechain
1	A	360	ARG	Sidechain
1	A	41	ARG	Sidechain
1	A	446	ARG	Sidechain
1	B	131	ARG	Sidechain
1	B	134	ARG	Sidechain
1	B	159	ARG	Sidechain
1	B	167	ARG	Sidechain
1	B	194	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	215	ARG	Sidechain
1	B	217	ARG	Sidechain
1	B	285	ARG	Sidechain
1	B	295	ARG	Sidechain
1	B	305	ARG	Sidechain
1	B	312	ARG	Sidechain
1	B	319	ARG	Sidechain
1	B	350	ARG	Sidechain
1	B	360	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	41	ARG	Sidechain
1	B	446	ARG	Sidechain
1	C	131	ARG	Sidechain
1	C	134	ARG	Sidechain
1	C	159	ARG	Sidechain
1	C	167	ARG	Sidechain
1	C	194	ARG	Sidechain
1	C	213	ARG	Sidechain
1	C	215	ARG	Sidechain
1	C	217	ARG	Sidechain
1	C	285	ARG	Sidechain
1	C	295	ARG	Sidechain
1	C	305	ARG	Sidechain
1	C	312	ARG	Sidechain
1	C	319	ARG	Sidechain
1	C	350	ARG	Sidechain
1	C	360	ARG	Sidechain
1	C	41	ARG	Sidechain
1	C	446	ARG	Sidechain
1	D	131	ARG	Sidechain
1	D	134	ARG	Sidechain
1	D	159	ARG	Sidechain
1	D	167	ARG	Sidechain
1	D	194	ARG	Sidechain
1	D	213	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	217	ARG	Sidechain
1	D	285	ARG	Sidechain
1	D	295	ARG	Sidechain
1	D	305	ARG	Sidechain
1	D	312	ARG	Sidechain
1	D	319	ARG	Sidechain
1	D	350	ARG	Sidechain
1	D	360	ARG	Sidechain
1	D	41	ARG	Sidechain
1	D	446	ARG	Sidechain
1	E	131	ARG	Sidechain
1	E	134	ARG	Sidechain
1	E	159	ARG	Sidechain
1	E	167	ARG	Sidechain
1	E	194	ARG	Sidechain
1	E	213	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	215	ARG	Sidechain
1	E	217	ARG	Sidechain
1	E	285	ARG	Sidechain
1	E	295	ARG	Sidechain
1	E	305	ARG	Sidechain
1	E	312	ARG	Sidechain
1	E	319	ARG	Sidechain
1	E	350	ARG	Sidechain
1	E	360	ARG	Sidechain
1	E	41	ARG	Sidechain
1	E	446	ARG	Sidechain
1	F	131	ARG	Sidechain
1	F	134	ARG	Sidechain
1	F	159	ARG	Sidechain
1	F	167	ARG	Sidechain
1	F	194	ARG	Sidechain
1	F	213	ARG	Sidechain
1	F	215	ARG	Sidechain
1	F	217	ARG	Sidechain
1	F	285	ARG	Sidechain
1	F	295	ARG	Sidechain
1	F	305	ARG	Sidechain
1	F	312	ARG	Sidechain
1	F	319	ARG	Sidechain
1	F	350	ARG	Sidechain
1	F	360	ARG	Sidechain
1	F	41	ARG	Sidechain
1	F	446	ARG	Sidechain
1	G	131	ARG	Sidechain
1	G	134	ARG	Sidechain
1	G	159	ARG	Sidechain
1	G	167	ARG	Sidechain
1	G	194	ARG	Sidechain
1	G	213	ARG	Sidechain
1	G	215	ARG	Sidechain
1	G	217	ARG	Sidechain
1	G	285	ARG	Sidechain
1	G	295	ARG	Sidechain
1	G	305	ARG	Sidechain
1	G	312	ARG	Sidechain
1	G	319	ARG	Sidechain
1	G	350	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	G	360	ARG	Sidechain
1	G	41	ARG	Sidechain
1	G	446	ARG	Sidechain
1	H	131	ARG	Sidechain
1	H	134	ARG	Sidechain
1	H	159	ARG	Sidechain
1	H	167	ARG	Sidechain
1	H	194	ARG	Sidechain
1	H	213	ARG	Sidechain
1	H	215	ARG	Sidechain
1	H	217	ARG	Sidechain
1	H	285	ARG	Sidechain
1	H	295	ARG	Sidechain
1	H	305	ARG	Sidechain
1	H	312	ARG	Sidechain
1	H	319	ARG	Sidechain
1	H	350	ARG	Sidechain
1	H	360	ARG	Sidechain
1	H	41	ARG	Sidechain
1	H	446	ARG	Sidechain
2	I	10	ARG	Sidechain
2	I	11	ARG	Sidechain
2	I	119	ARG	Sidechain
2	I	88	ARG	Sidechain
2	I	91	ARG	Sidechain
2	J	10	ARG	Sidechain
2	J	11	ARG	Sidechain
2	J	119	ARG	Sidechain
2	J	88	ARG	Sidechain
2	J	91	ARG	Sidechain
2	K	10	ARG	Sidechain
2	K	11	ARG	Sidechain
2	K	119	ARG	Sidechain
2	K	88	ARG	Sidechain
2	K	91	ARG	Sidechain
2	L	10	ARG	Sidechain
2	L	11	ARG	Sidechain
2	L	119	ARG	Sidechain
2	L	88	ARG	Sidechain
2	L	91	ARG	Sidechain
2	M	10	ARG	Sidechain
2	M	11	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	M	119	ARG	Sidechain
2	M	88	ARG	Sidechain
2	M	91	ARG	Sidechain
2	N	10	ARG	Sidechain
2	N	11	ARG	Sidechain
2	N	119	ARG	Sidechain
2	N	88	ARG	Sidechain
2	N	91	ARG	Sidechain
2	O	10	ARG	Sidechain
2	O	11	ARG	Sidechain
2	O	119	ARG	Sidechain
2	O	88	ARG	Sidechain
2	O	91	ARG	Sidechain
2	P	10	ARG	Sidechain
2	P	11	ARG	Sidechain
2	P	119	ARG	Sidechain
2	P	88	ARG	Sidechain
2	P	91	ARG	Sidechain

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	3653	0	3568	54	0
1	B	3653	0	3568	54	0
1	C	3653	0	3568	48	0
1	D	3653	0	3568	49	0
1	E	3653	0	3568	50	4
1	F	3653	0	3568	49	0
1	G	3653	0	3568	48	0
1	H	3653	0	3568	52	0
2	I	909	0	865	20	2
2	J	909	0	865	18	2
2	K	909	0	865	20	28
2	L	909	0	865	18	4
2	M	909	0	865	22	1
2	N	909	0	865	18	1
2	O	909	0	865	19	28

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	909	0	865	20	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	21	0	9	1	0
4	B	21	0	9	1	0
4	C	21	0	9	1	0
4	D	21	0	9	1	0
4	E	21	0	9	1	0
4	F	21	0	9	1	0
4	G	21	0	9	1	0
4	H	21	0	9	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	3	0	0	0	0
5	G	3	0	0	0	0
5	H	3	0	0	0	0
6	A	214	0	0	5	0
6	B	4	0	0	0	0
6	C	9	0	0	0	0
6	D	3	0	0	0	0
6	G	2	0	0	0	0
6	M	53	0	0	3	0
6	N	5	0	0	0	0
6	P	2	0	0	0	0
All	All	36988	0	35536	518	35

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 7.

All (518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:ARG:HD2	4:C:476:CAP:O5P	1.74	0.88
1:A:295:ARG:HD2	4:A:476:CAP:O5P	1.74	0.88
1:G:295:ARG:HD2	4:G:476:CAP:O5P	1.74	0.87
1:E:295:ARG:HD2	4:E:476:CAP:O5P	1.74	0.87
1:B:295:ARG:HD2	4:B:476:CAP:O5P	1.74	0.86
1:D:295:ARG:HD2	4:D:476:CAP:O5P	1.74	0.86
1:H:295:ARG:HD2	4:H:476:CAP:O5P	1.74	0.86
1:F:295:ARG:HD2	4:F:476:CAP:O5P	1.74	0.86
1:C:267:HIS:HD2	1:C:277:ASN:HD22	1.26	0.83
1:B:267:HIS:HD2	1:B:277:ASN:HD22	1.26	0.83
1:G:267:HIS:HD2	1:G:277:ASN:HD22	1.26	0.83
1:F:267:HIS:HD2	1:F:277:ASN:HD22	1.26	0.82
1:D:267:HIS:HD2	1:D:277:ASN:HD22	1.26	0.81
1:A:267:HIS:HD2	1:A:277:ASN:HD22	1.26	0.81
1:H:267:HIS:HD2	1:H:277:ASN:HD22	1.26	0.81
1:E:267:HIS:HD2	1:E:277:ASN:HD22	1.26	0.81
1:E:410:PRO:HD3	1:E:461:LEU:HD22	1.68	0.76
1:H:410:PRO:HD3	1:H:461:LEU:HD22	1.68	0.76
1:B:410:PRO:HD3	1:B:461:LEU:HD22	1.68	0.76
1:C:410:PRO:HD3	1:C:461:LEU:HD22	1.68	0.76
1:D:410:PRO:HD3	1:D:461:LEU:HD22	1.68	0.75
1:F:410:PRO:HD3	1:F:461:LEU:HD22	1.68	0.75
1:A:410:PRO:HD3	1:A:461:LEU:HD22	1.68	0.75
1:G:410:PRO:HD3	1:G:461:LEU:HD22	1.68	0.75
1:C:350:ARG:NH2	1:C:394:PHE:O	2.21	0.74
1:E:350:ARG:NH2	1:E:394:PHE:O	2.21	0.73
1:B:350:ARG:NH2	1:B:394:PHE:O	2.21	0.73
1:D:383:HIS:H	1:D:386:HIS:HD2	1.37	0.73
1:F:383:HIS:H	1:F:386:HIS:HD2	1.37	0.73
1:H:350:ARG:NH2	1:H:394:PHE:O	2.21	0.73
1:G:383:HIS:H	1:G:386:HIS:HD2	1.37	0.73
1:E:383:HIS:H	1:E:386:HIS:HD2	1.37	0.72
1:A:383:HIS:H	1:A:386:HIS:HD2	1.37	0.72
1:H:383:HIS:H	1:H:386:HIS:HD2	1.37	0.72
1:C:383:HIS:H	1:C:386:HIS:HD2	1.37	0.71
1:D:350:ARG:NH2	1:D:394:PHE:O	2.21	0.71
1:A:350:ARG:NH2	1:A:394:PHE:O	2.21	0.71
1:G:350:ARG:NH2	1:G:394:PHE:O	2.21	0.71
1:B:383:HIS:H	1:B:386:HIS:HD2	1.37	0.71
1:F:350:ARG:NH2	1:F:394:PHE:O	2.21	0.70
1:D:239:TYR:HE2	1:D:401:GLN:HE22	1.41	0.68
1:E:167:ARG:HB2	1:E:428:VAL:HG21	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HB2	1:B:428:VAL:HG21	1.76	0.68
1:C:167:ARG:HB2	1:C:428:VAL:HG21	1.75	0.68
1:D:167:ARG:HB2	1:D:428:VAL:HG21	1.75	0.68
1:F:295:ARG:HD3	1:F:298:HIS:CD2	2.29	0.68
1:E:295:ARG:HD3	1:E:298:HIS:CD2	2.29	0.68
1:F:239:TYR:HE2	1:F:401:GLN:HE22	1.41	0.68
1:B:295:ARG:HD3	1:B:298:HIS:CD2	2.29	0.67
1:H:167:ARG:HB2	1:H:428:VAL:HG21	1.75	0.67
1:D:295:ARG:HD3	1:D:298:HIS:CD2	2.29	0.67
1:H:295:ARG:HD3	1:H:298:HIS:CD2	2.29	0.67
1:A:295:ARG:HD3	1:A:298:HIS:CD2	2.29	0.67
1:G:167:ARG:HB2	1:G:428:VAL:HG21	1.76	0.67
1:C:239:TYR:HE2	1:C:401:GLN:HE22	1.41	0.67
1:F:167:ARG:HB2	1:F:428:VAL:HG21	1.75	0.67
1:G:295:ARG:HD3	1:G:298:HIS:CD2	2.29	0.67
1:A:239:TYR:HE2	1:A:401:GLN:HE22	1.41	0.67
1:C:295:ARG:HD3	1:C:298:HIS:CD2	2.29	0.67
1:E:239:TYR:HE2	1:E:401:GLN:HE22	1.41	0.66
1:B:239:TYR:HE2	1:B:401:GLN:HE22	1.41	0.66
1:H:239:TYR:HE2	1:H:401:GLN:HE22	1.41	0.66
1:A:167:ARG:HB2	1:A:428:VAL:HG21	1.75	0.66
1:G:239:TYR:HE2	1:G:401:GLN:HE22	1.41	0.66
1:B:14:LYS:HE3	1:B:14:LYS:O	1.98	0.64
1:G:14:LYS:HE3	1:G:14:LYS:O	1.98	0.64
1:F:14:LYS:HE3	1:F:14:LYS:O	1.98	0.64
1:E:14:LYS:HE3	1:E:14:LYS:O	1.98	0.64
1:C:14:LYS:O	1:C:14:LYS:HE3	1.98	0.64
1:D:14:LYS:O	1:D:14:LYS:HE3	1.98	0.63
1:H:14:LYS:O	1:H:14:LYS:HE3	1.98	0.63
1:A:14:LYS:HE3	1:A:14:LYS:O	1.98	0.63
1:E:278:THR:O	1:E:282:LYS:HG2	1.99	0.63
1:H:278:THR:O	1:H:282:LYS:HG2	1.99	0.63
1:F:278:THR:O	1:F:282:LYS:HG2	1.99	0.62
1:G:278:THR:O	1:G:282:LYS:HG2	1.99	0.62
1:A:278:THR:O	1:A:282:LYS:HG2	1.99	0.62
1:C:278:THR:O	1:C:282:LYS:HG2	1.99	0.62
1:D:278:THR:O	1:D:282:LYS:HG2	1.99	0.61
1:B:278:THR:O	1:B:282:LYS:HG2	1.99	0.61
1:A:213:ARG:HD3	6:A:554:HOH:O	2.01	0.60
1:A:53:ALA:HB1	1:A:130:ILE:HD11	1.85	0.59
1:E:53:ALA:HB1	1:E:130:ILE:HD11	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ALA:HB1	1:D:130:ILE:HD11	1.85	0.59
1:H:53:ALA:HB1	1:H:130:ILE:HD11	1.85	0.59
2:K:2:SER:O	2:K:3:MET:HG2	2.03	0.59
2:O:2:SER:O	2:O:3:MET:HG2	2.03	0.59
2:L:111:GLN:HE21	2:L:114:SER:HB2	1.68	0.59
1:B:53:ALA:HB1	1:B:130:ILE:HD11	1.85	0.58
1:C:53:ALA:HB1	1:C:130:ILE:HD11	1.85	0.58
1:G:53:ALA:HB1	1:G:130:ILE:HD11	1.85	0.58
2:I:111:GLN:HE21	2:I:114:SER:HB2	1.68	0.58
2:N:111:GLN:HE21	2:N:114:SER:HB2	1.68	0.58
2:N:2:SER:O	2:N:3:MET:HG2	2.03	0.58
1:F:53:ALA:HB1	1:F:130:ILE:HD11	1.85	0.58
1:A:202:ASP:OD1	1:A:238:HIS:HE1	1.87	0.58
2:I:2:SER:O	2:I:3:MET:HG2	2.03	0.58
2:M:111:GLN:HE21	2:M:114:SER:HB2	1.68	0.58
2:M:2:SER:O	2:M:3:MET:HG2	2.03	0.58
2:O:111:GLN:HE21	2:O:114:SER:HB2	1.68	0.58
2:J:2:SER:O	2:J:3:MET:HG2	2.03	0.58
1:C:202:ASP:OD1	1:C:238:HIS:HE1	1.87	0.58
1:D:202:ASP:OD1	1:D:238:HIS:HE1	1.87	0.58
2:P:111:GLN:HE21	2:P:114:SER:HB2	1.68	0.58
2:P:2:SER:O	2:P:3:MET:HG2	2.03	0.58
2:L:2:SER:O	2:L:3:MET:HG2	2.03	0.58
2:J:111:GLN:HE21	2:J:114:SER:HB2	1.68	0.57
1:A:105:LEU:HD21	1:D:146:LYS:HD2	1.86	0.57
1:B:202:ASP:OD1	1:B:238:HIS:HE1	1.87	0.57
1:G:202:ASP:OD1	1:G:238:HIS:HE1	1.87	0.57
1:H:442:GLY:O	1:H:446:ARG:HD3	2.05	0.57
2:K:111:GLN:HE21	2:K:114:SER:HB2	1.68	0.57
1:A:442:GLY:O	1:A:446:ARG:HD3	2.05	0.56
1:D:305:ARG:HD2	1:D:474:LYS:O	2.05	0.56
1:G:442:GLY:O	1:G:446:ARG:HD3	2.05	0.56
1:B:305:ARG:HD2	1:B:474:LYS:O	2.06	0.56
1:F:202:ASP:OD1	1:F:238:HIS:HE1	1.87	0.56
1:C:305:ARG:HD2	1:C:474:LYS:O	2.06	0.56
1:D:442:GLY:O	1:D:446:ARG:HD3	2.05	0.56
1:F:442:GLY:O	1:F:446:ARG:HD3	2.05	0.56
1:A:305:ARG:HD2	1:A:474:LYS:O	2.06	0.56
1:E:442:GLY:O	1:E:446:ARG:HD3	2.05	0.56
1:B:442:GLY:O	1:B:446:ARG:HD3	2.05	0.56
1:H:202:ASP:OD1	1:H:238:HIS:HE1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:ARG:HD2	1:G:474:LYS:O	2.06	0.56
1:C:442:GLY:O	1:C:446:ARG:HD3	2.05	0.56
1:E:202:ASP:OD1	1:E:238:HIS:HE1	1.87	0.56
1:E:146:LYS:HD2	1:H:105:LEU:HD21	1.88	0.56
1:H:305:ARG:HD2	1:H:474:LYS:O	2.06	0.56
2:N:91:ARG:HD2	2:N:118:HIS:HB2	1.88	0.56
1:E:305:ARG:HD2	1:E:474:LYS:O	2.06	0.55
2:P:91:ARG:HD2	2:P:118:HIS:HB2	1.88	0.55
2:O:91:ARG:HD2	2:O:118:HIS:HB2	1.88	0.55
1:F:305:ARG:HD2	1:F:474:LYS:O	2.06	0.55
2:M:91:ARG:HD2	2:M:118:HIS:HB2	1.88	0.55
2:I:91:ARG:HD2	2:I:118:HIS:HB2	1.88	0.55
2:J:30:ILE:O	2:J:34:ILE:HG12	2.07	0.55
2:M:30:ILE:O	2:M:34:ILE:HG12	2.08	0.55
2:K:91:ARG:HD2	2:K:118:HIS:HB2	1.88	0.54
2:I:30:ILE:O	2:I:34:ILE:HG12	2.08	0.54
2:N:30:ILE:O	2:N:34:ILE:HG12	2.08	0.54
1:B:200:THR:OG1	1:B:238:HIS:HD2	1.91	0.54
2:J:91:ARG:HD2	2:J:118:HIS:HB2	1.88	0.54
2:K:77:CYS:HA	2:K:82:GLN:HE22	1.73	0.54
2:L:30:ILE:O	2:L:34:ILE:HG12	2.08	0.53
1:F:200:THR:OG1	1:F:238:HIS:HD2	1.91	0.53
2:L:91:ARG:HD2	2:L:118:HIS:HB2	1.88	0.53
1:C:200:THR:OG1	1:C:238:HIS:HD2	1.91	0.53
2:P:30:ILE:O	2:P:34:ILE:HG12	2.08	0.53
1:B:383:HIS:H	1:B:386:HIS:CD2	2.23	0.53
1:A:146:LYS:HD2	1:D:105:LEU:HD21	1.91	0.53
2:P:77:CYS:HA	2:P:82:GLN:HE22	1.73	0.53
2:M:11:ARG:HD3	6:M:164:HOH:O	2.09	0.53
2:N:77:CYS:HA	2:N:82:GLN:HE22	1.73	0.53
1:D:200:THR:OG1	1:D:238:HIS:HD2	1.91	0.53
1:E:200:THR:OG1	1:E:238:HIS:HD2	1.91	0.53
2:I:77:CYS:HA	2:I:82:GLN:HE22	1.73	0.53
1:H:200:THR:OG1	1:H:238:HIS:HD2	1.91	0.53
2:J:77:CYS:HA	2:J:82:GLN:HE22	1.73	0.53
2:K:30:ILE:O	2:K:34:ILE:HG12	2.07	0.53
2:O:77:CYS:HA	2:O:82:GLN:HE22	1.73	0.53
1:C:383:HIS:H	1:C:386:HIS:CD2	2.23	0.53
2:O:30:ILE:O	2:O:34:ILE:HG12	2.08	0.53
1:G:200:THR:OG1	1:G:238:HIS:HD2	1.91	0.52
2:M:77:CYS:HA	2:M:82:GLN:HE22	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:77:CYS:HA	2:L:82:GLN:HE22	1.73	0.52
2:M:45:ASN:ND2	6:M:145:HOH:O	2.41	0.52
1:E:105:LEU:HD21	1:H:146:LYS:HD2	1.92	0.52
1:A:200:THR:OG1	1:A:238:HIS:HD2	1.91	0.51
1:A:229:GLN:HE21	1:A:236:LYS:H	1.58	0.51
1:A:285:ARG:NH2	6:A:487:HOH:O	2.43	0.51
1:C:105:LEU:HD21	1:F:146:LYS:HD2	1.92	0.51
1:H:239:TYR:HB3	1:H:266:MET:HB3	1.93	0.51
1:H:383:HIS:H	1:H:386:HIS:CD2	2.23	0.51
1:E:239:TYR:HB3	1:E:266:MET:HB3	1.93	0.51
1:E:312:ARG:HB2	1:E:345:PHE:HB3	1.93	0.51
1:C:229:GLN:HE21	1:C:236:LYS:H	1.58	0.51
1:H:312:ARG:HB2	1:H:345:PHE:HB3	1.93	0.51
1:E:229:GLN:HE21	1:E:236:LYS:H	1.58	0.51
1:D:312:ARG:HB2	1:D:345:PHE:HB3	1.93	0.50
1:E:383:HIS:H	1:E:386:HIS:CD2	2.23	0.50
1:B:93:GLU:CD	1:B:305:ARG:HH22	2.15	0.50
1:A:312:ARG:HB2	1:A:345:PHE:HB3	1.93	0.50
1:B:312:ARG:HB2	1:B:345:PHE:HB3	1.93	0.50
1:C:312:ARG:HB2	1:C:345:PHE:HB3	1.93	0.50
1:D:229:GLN:HE21	1:D:236:LYS:H	1.58	0.50
1:G:229:GLN:HE21	1:G:236:LYS:H	1.59	0.50
1:G:312:ARG:HB2	1:G:345:PHE:HB3	1.93	0.50
1:G:273:GLY:HA3	1:H:273:GLY:HA3	1.92	0.50
1:H:93:GLU:CD	1:H:305:ARG:HH22	2.15	0.50
1:B:239:TYR:HB3	1:B:266:MET:HB3	1.93	0.50
1:C:273:GLY:HA3	1:D:273:GLY:HA3	1.94	0.50
1:D:93:GLU:CD	1:D:305:ARG:HH22	2.15	0.50
1:F:312:ARG:HB2	1:F:345:PHE:HB3	1.93	0.50
1:H:229:GLN:HE21	1:H:236:LYS:H	1.59	0.50
1:A:239:TYR:HB3	1:A:266:MET:HB3	1.93	0.50
1:D:239:TYR:HB3	1:D:266:MET:HB3	1.93	0.50
1:D:383:HIS:H	1:D:386:HIS:CD2	2.23	0.49
1:C:93:GLU:CD	1:C:305:ARG:HH22	2.15	0.49
2:O:104:PHE:HZ	1:G:184:ASN:HD21	1.60	0.49
1:G:134:ARG:HA	1:G:308:GLY:O	2.13	0.49
1:A:93:GLU:CD	1:A:305:ARG:HH22	2.15	0.49
1:C:239:TYR:HB3	1:C:266:MET:HB3	1.93	0.49
1:F:229:GLN:HE21	1:F:236:LYS:H	1.58	0.49
1:A:383:HIS:H	1:A:386:HIS:CD2	2.23	0.49
1:E:93:GLU:CD	1:E:305:ARG:HH22	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:GLY:HA3	1:B:273:GLY:HA3	1.94	0.49
1:E:134:ARG:HA	1:E:308:GLY:O	2.13	0.49
1:E:273:GLY:HA3	1:F:273:GLY:HA3	1.93	0.49
1:G:93:GLU:CD	1:G:305:ARG:HH22	2.15	0.49
1:B:229:GLN:HE21	1:B:236:LYS:H	1.59	0.49
1:F:134:ARG:HA	1:F:308:GLY:O	2.13	0.49
1:D:134:ARG:HA	1:D:308:GLY:O	2.13	0.49
1:G:239:TYR:HB3	1:G:266:MET:HB3	1.93	0.49
1:F:93:GLU:CD	1:F:305:ARG:HH22	2.15	0.49
1:G:285:ARG:HG3	1:G:285:ARG:O	2.13	0.49
2:O:91:ARG:HD2	2:O:118:HIS:CB	2.43	0.49
1:A:134:ARG:HA	1:A:308:GLY:O	2.13	0.48
1:B:105:LEU:HD21	1:G:146:LYS:HD2	1.94	0.48
2:P:91:ARG:HD2	2:P:118:HIS:CB	2.43	0.48
1:F:239:TYR:HB3	1:F:266:MET:HB3	1.93	0.48
2:I:91:ARG:HD2	2:I:118:HIS:CB	2.43	0.48
2:L:91:ARG:HD2	2:L:118:HIS:CB	2.43	0.48
1:B:285:ARG:HG3	1:B:285:ARG:O	2.13	0.48
1:B:353:HIS:HD2	1:B:367:ASP:OD1	1.97	0.48
1:H:353:HIS:HD2	1:H:367:ASP:OD1	1.97	0.48
2:L:95:GLY:O	2:L:118:HIS:HE1	1.97	0.48
1:B:134:ARG:HA	1:B:308:GLY:O	2.13	0.48
2:P:95:GLY:O	2:P:118:HIS:HE1	1.97	0.48
1:F:285:ARG:O	1:F:285:ARG:HG3	2.13	0.48
1:A:295:ARG:HG3	6:A:521:HOH:O	2.13	0.48
1:C:134:ARG:HA	1:C:308:GLY:O	2.13	0.48
1:F:353:HIS:HD2	1:F:367:ASP:OD1	1.97	0.48
2:I:95:GLY:O	2:I:118:HIS:HE1	1.97	0.48
2:J:95:GLY:O	2:J:118:HIS:HE1	1.97	0.48
2:K:91:ARG:HD2	2:K:118:HIS:CB	2.43	0.48
2:O:95:GLY:O	2:O:118:HIS:HE1	1.97	0.48
1:B:184:ASN:HD21	2:J:104:PHE:HZ	1.57	0.48
1:D:353:HIS:HD2	1:D:367:ASP:OD1	1.97	0.48
1:C:285:ARG:O	1:C:285:ARG:HG3	2.13	0.48
1:C:353:HIS:HD2	1:C:367:ASP:OD1	1.97	0.48
1:C:146:LYS:HD2	1:F:105:LEU:HD21	1.96	0.48
1:H:134:ARG:HA	1:H:308:GLY:O	2.13	0.48
2:M:95:GLY:O	2:M:118:HIS:HE1	1.97	0.48
2:N:95:GLY:O	2:N:118:HIS:HE1	1.97	0.48
1:A:285:ARG:O	1:A:285:ARG:HG3	2.13	0.48
1:D:285:ARG:O	1:D:285:ARG:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:95:GLY:O	2:K:118:HIS:HE1	1.97	0.47
2:M:91:ARG:HD2	2:M:118:HIS:CB	2.43	0.47
2:N:91:ARG:HD2	2:N:118:HIS:CB	2.43	0.47
6:A:551:HOH:O	2:P:64:GLU:HG3	2.13	0.47
1:A:353:HIS:HD2	1:A:367:ASP:OD1	1.97	0.47
1:E:353:HIS:HD2	1:E:367:ASP:OD1	1.97	0.47
2:I:104:PHE:HZ	1:H:184:ASN:HD21	1.61	0.47
1:B:146:LYS:HD2	1:G:105:LEU:HD21	1.96	0.47
1:B:217:ARG:HB3	1:B:217:ARG:HE	1.45	0.47
1:E:285:ARG:O	1:E:285:ARG:HG3	2.13	0.47
1:D:167:ARG:HG2	1:D:168:PRO:O	2.15	0.47
1:H:285:ARG:O	1:H:285:ARG:HG3	2.13	0.47
1:B:167:ARG:HG2	1:B:168:PRO:O	2.15	0.47
1:B:171:GLY:HA2	1:B:199:PHE:O	2.15	0.47
2:J:91:ARG:HD2	2:J:118:HIS:CB	2.43	0.47
1:D:171:GLY:HA2	1:D:199:PHE:O	2.15	0.47
1:E:167:ARG:HG2	1:E:168:PRO:O	2.15	0.47
1:E:171:GLY:HA2	1:E:199:PHE:O	2.15	0.47
1:G:383:HIS:H	1:G:386:HIS:CD2	2.23	0.47
1:A:167:ARG:HG2	1:A:168:PRO:O	2.15	0.47
1:G:167:ARG:HG2	1:G:168:PRO:O	2.15	0.47
1:G:353:HIS:HD2	1:G:367:ASP:OD1	1.97	0.47
1:A:171:GLY:HA2	1:A:199:PHE:O	2.15	0.46
1:A:435:ARG:NH2	1:A:447:GLU:OE2	2.28	0.46
1:C:167:ARG:HG2	1:C:168:PRO:O	2.15	0.46
1:F:184:ASN:HD21	2:L:104:PHE:HZ	1.59	0.46
1:F:167:ARG:HG2	1:F:168:PRO:O	2.15	0.46
1:H:167:ARG:HG2	1:H:168:PRO:O	2.15	0.46
1:C:171:GLY:HA2	1:C:199:PHE:O	2.15	0.46
1:F:383:HIS:H	1:F:386:HIS:CD2	2.23	0.46
1:F:435:ARG:HH22	1:F:447:GLU:CD	2.16	0.46
1:G:171:GLY:HA2	1:G:199:PHE:O	2.15	0.46
1:H:171:GLY:HA2	1:H:199:PHE:O	2.15	0.46
1:F:171:GLY:HA2	1:F:199:PHE:O	2.15	0.45
1:D:207:ASN:O	1:D:217:ARG:NH1	2.49	0.45
2:N:12:PHE:HB3	2:N:116:ILE:HG13	1.99	0.45
2:M:12:PHE:HB3	2:M:116:ILE:HG13	1.99	0.45
2:I:12:PHE:HB3	2:I:116:ILE:HG13	1.99	0.45
1:A:207:ASN:O	1:A:217:ARG:NH1	2.49	0.45
1:B:435:ARG:NH2	1:B:447:GLU:OE2	2.28	0.45
2:J:12:PHE:HB3	2:J:116:ILE:HG13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:435:ARG:HH22	1:G:447:GLU:CD	2.16	0.45
1:B:207:ASN:O	1:B:217:ARG:NH1	2.49	0.44
2:N:77:CYS:HA	2:N:82:GLN:NE2	2.32	0.44
2:L:77:CYS:HA	2:L:82:GLN:NE2	2.32	0.44
2:O:77:CYS:HA	2:O:82:GLN:NE2	2.32	0.44
1:C:217:ARG:HE	1:C:217:ARG:HB3	1.45	0.44
1:H:207:ASN:O	1:H:217:ARG:NH1	2.49	0.44
1:H:295:ARG:HG3	1:H:295:ARG:H	1.64	0.44
1:C:14:LYS:HZ1	1:C:18:LYS:HG3	1.83	0.44
2:I:77:CYS:HA	2:I:82:GLN:NE2	2.32	0.44
2:K:12:PHE:HB3	2:K:116:ILE:HG13	1.99	0.44
1:E:217:ARG:HB3	1:E:217:ARG:HE	1.45	0.44
1:G:152:PRO:O	1:G:285:ARG:HD3	2.18	0.44
1:D:152:PRO:O	1:D:285:ARG:HD3	2.18	0.44
2:K:77:CYS:HA	2:K:82:GLN:NE2	2.32	0.44
1:G:62:SER:O	1:H:177:LYS:HB2	2.18	0.44
2:M:41:LEU:HD11	2:M:69:MET:HG3	2.00	0.44
1:B:18:LYS:HB2	1:B:18:LYS:HE2	1.89	0.44
1:C:152:PRO:O	1:C:285:ARG:HD3	2.18	0.44
1:H:18:LYS:HE2	1:H:18:LYS:HB2	1.89	0.44
2:J:77:CYS:HA	2:J:82:GLN:NE2	2.32	0.44
2:L:119:ARG:HG2	2:L:119:ARG:HH11	1.83	0.44
2:L:12:PHE:HB3	2:L:116:ILE:HG13	1.99	0.44
1:C:207:ASN:O	1:C:217:ARG:NH1	2.49	0.44
1:F:207:ASN:O	1:F:217:ARG:NH1	2.49	0.44
2:O:12:PHE:HB3	2:O:116:ILE:HG13	1.99	0.44
1:A:152:PRO:O	1:A:285:ARG:HD3	2.18	0.43
1:E:207:ASN:O	1:E:217:ARG:NH1	2.49	0.43
1:E:295:ARG:H	1:E:295:ARG:HG3	1.64	0.43
1:G:207:ASN:O	1:G:217:ARG:NH1	2.49	0.43
1:G:435:ARG:NH2	1:G:447:GLU:OE2	2.28	0.43
2:M:77:CYS:HA	2:M:82:GLN:NE2	2.32	0.43
1:F:152:PRO:O	1:F:285:ARG:HD3	2.18	0.43
1:H:217:ARG:HB3	1:H:217:ARG:HE	1.45	0.43
2:J:119:ARG:HH11	2:J:119:ARG:HG2	1.83	0.43
2:P:12:PHE:HB3	2:P:116:ILE:HG13	1.99	0.43
2:P:77:CYS:HA	2:P:82:GLN:NE2	2.32	0.43
1:B:229:GLN:NE2	1:B:236:LYS:H	2.17	0.43
1:B:152:PRO:O	1:B:285:ARG:HD3	2.18	0.43
1:H:152:PRO:O	1:H:285:ARG:HD3	2.18	0.43
2:K:41:LEU:HD13	2:K:73:PRO:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:119:ARG:HG2	2:P:119:ARG:HH11	1.83	0.43
2:P:41:LEU:HD11	2:P:69:MET:HG3	2.00	0.43
1:H:229:GLN:NE2	1:H:236:LYS:H	2.17	0.43
2:J:41:LEU:HD11	2:J:69:MET:HG3	2.00	0.43
2:L:41:LEU:HD13	2:L:73:PRO:HG3	2.01	0.43
1:C:229:GLN:NE2	1:C:236:LYS:H	2.17	0.43
2:N:119:ARG:HG2	2:N:119:ARG:HH11	1.83	0.43
2:P:41:LEU:HD13	2:P:73:PRO:HG3	2.01	0.43
1:E:152:PRO:O	1:E:285:ARG:HD3	2.18	0.43
1:D:353:HIS:HE1	1:D:355:GLU:OE2	2.02	0.43
2:L:41:LEU:HD11	2:L:69:MET:HG3	2.00	0.43
2:M:119:ARG:HG2	2:M:119:ARG:HH11	1.83	0.43
2:O:119:ARG:HG2	2:O:119:ARG:HH11	1.83	0.43
2:I:119:ARG:HH11	2:I:119:ARG:HG2	1.83	0.43
1:E:435:ARG:NH2	1:E:447:GLU:OE2	2.29	0.43
1:F:353:HIS:HE1	1:F:355:GLU:OE2	2.02	0.43
1:G:353:HIS:HE1	1:G:355:GLU:OE2	2.02	0.43
1:E:353:HIS:HE1	1:E:355:GLU:OE2	2.02	0.43
1:E:51:ASP:HA	1:E:87:ILE:CD1	2.49	0.43
1:H:353:HIS:HE1	1:H:355:GLU:OE2	2.02	0.43
2:M:10:ARG:HD3	6:M:170:HOH:O	2.19	0.43
1:A:353:HIS:HE1	1:A:355:GLU:OE2	2.02	0.42
1:B:133:LEU:O	1:B:307:HIS:HA	2.19	0.42
1:D:295:ARG:H	1:D:295:ARG:HG3	1.64	0.42
1:H:51:ASP:HA	1:H:87:ILE:CD1	2.49	0.42
2:O:41:LEU:HD11	2:O:69:MET:HG3	2.00	0.42
2:O:41:LEU:HD13	2:O:73:PRO:HG3	2.01	0.42
1:A:131:ARG:HD3	6:A:631:HOH:O	2.19	0.42
1:A:51:ASP:HA	1:A:87:ILE:CD1	2.50	0.42
1:D:51:ASP:HA	1:D:87:ILE:CD1	2.49	0.42
1:B:353:HIS:HE1	1:B:355:GLU:OE2	2.02	0.42
1:E:229:GLN:NE2	1:E:236:LYS:H	2.17	0.42
1:H:133:LEU:O	1:H:307:HIS:HA	2.19	0.42
2:K:41:LEU:HD11	2:K:69:MET:HG3	2.00	0.42
2:N:41:LEU:HD11	2:N:69:MET:HG3	2.00	0.42
1:A:133:LEU:O	1:A:307:HIS:HA	2.19	0.42
1:B:382:ILE:HA	1:B:386:HIS:CD2	2.55	0.42
2:N:41:LEU:HD13	2:N:73:PRO:HG3	2.01	0.42
1:C:133:LEU:O	1:C:307:HIS:HA	2.19	0.42
1:C:382:ILE:HA	1:C:386:HIS:CD2	2.55	0.42
1:D:152:PRO:HB2	1:D:153:HIS:CD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LEU:O	1:E:307:HIS:HA	2.19	0.42
1:F:382:ILE:HA	1:F:386:HIS:CD2	2.55	0.42
2:M:41:LEU:HD13	2:M:73:PRO:HG3	2.01	0.42
1:A:152:PRO:HB2	1:A:153:HIS:CD2	2.55	0.42
1:F:152:PRO:HB2	1:F:153:HIS:CD2	2.55	0.42
1:H:31:PRO:HB3	1:H:37:LEU:HD21	2.02	0.42
2:K:119:ARG:HH11	2:K:119:ARG:HG2	1.83	0.42
1:A:18:LYS:HB2	1:A:18:LYS:HE2	1.89	0.42
1:A:229:GLN:NE2	1:A:236:LYS:H	2.17	0.42
1:C:353:HIS:HE1	1:C:355:GLU:OE2	2.02	0.42
1:D:217:ARG:HB3	1:D:217:ARG:HE	1.45	0.42
1:E:152:PRO:HB2	1:E:153:HIS:CD2	2.55	0.42
1:F:31:PRO:HB3	1:F:37:LEU:HD21	2.02	0.42
2:I:41:LEU:HD13	2:I:73:PRO:HG3	2.01	0.42
2:J:4:LYS:NZ	2:J:4:LYS:HB3	2.35	0.42
1:B:152:PRO:HB2	1:B:153:HIS:CD2	2.55	0.42
1:B:295:ARG:H	1:B:295:ARG:HG3	1.64	0.42
1:D:18:LYS:HE2	1:D:18:LYS:HB2	1.89	0.42
1:G:133:LEU:O	1:G:307:HIS:HA	2.19	0.42
2:I:41:LEU:HD11	2:I:69:MET:HG3	2.00	0.42
1:B:51:ASP:HA	1:B:87:ILE:CD1	2.50	0.42
1:F:229:GLN:NE2	1:F:236:LYS:H	2.17	0.42
1:G:152:PRO:HB2	1:G:153:HIS:CD2	2.55	0.42
1:G:31:PRO:HB3	1:G:37:LEU:HD21	2.02	0.42
1:H:156:GLN:HG3	1:H:157:VAL:N	2.35	0.42
2:M:4:LYS:NZ	2:M:4:LYS:HB3	2.35	0.42
1:C:451:TRP:CH2	2:N:19:PRO:HD3	2.55	0.42
2:N:4:LYS:NZ	2:N:4:LYS:HB3	2.35	0.42
1:B:14:LYS:HZ1	1:B:18:LYS:HG3	1.85	0.42
1:D:156:GLN:HG3	1:D:157:VAL:N	2.35	0.42
1:D:229:GLN:NE2	1:D:236:LYS:H	2.17	0.42
1:E:31:PRO:HB3	1:E:37:LEU:HD21	2.02	0.42
1:E:451:TRP:CH2	2:O:19:PRO:HD3	2.55	0.42
1:D:451:TRP:CH2	2:J:19:PRO:HD3	2.55	0.42
1:A:451:TRP:CH2	2:M:19:PRO:HD3	2.55	0.42
1:A:319:ARG:HG2	1:A:368:TRP:CZ3	2.55	0.41
1:A:447:GLU:O	1:A:450:LYS:HB2	2.20	0.41
1:B:156:GLN:HG3	1:B:157:VAL:N	2.35	0.41
1:C:319:ARG:HG2	1:C:368:TRP:CZ3	2.55	0.41
1:D:133:LEU:O	1:D:307:HIS:HA	2.19	0.41
1:D:319:ARG:HG2	1:D:368:TRP:CZ3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:133:LEU:O	1:F:307:HIS:HA	2.19	0.41
1:F:447:GLU:O	1:F:450:LYS:HB2	2.20	0.41
1:G:451:TRP:CH2	2:P:19:PRO:HD3	2.55	0.41
1:G:51:ASP:HA	1:G:87:ILE:CD1	2.50	0.41
1:B:319:ARG:HG2	1:B:368:TRP:CZ3	2.55	0.41
1:E:382:ILE:HA	1:E:386:HIS:CD2	2.55	0.41
1:F:156:GLN:HG3	1:F:157:VAL:N	2.35	0.41
1:F:319:ARG:HG2	1:F:368:TRP:CZ3	2.55	0.41
1:G:447:GLU:O	1:G:450:LYS:HB2	2.20	0.41
1:B:451:TRP:CH2	2:I:19:PRO:HD3	2.55	0.41
2:L:4:LYS:NZ	2:L:4:LYS:HB3	2.35	0.41
1:G:382:ILE:HA	1:G:386:HIS:CD2	2.55	0.41
1:B:447:GLU:O	1:B:450:LYS:HB2	2.20	0.41
1:C:152:PRO:HB2	1:C:153:HIS:CD2	2.55	0.41
1:C:51:ASP:HA	1:C:87:ILE:CD1	2.50	0.41
1:D:382:ILE:HA	1:D:386:HIS:CD2	2.55	0.41
1:E:156:GLN:HG3	1:E:157:VAL:N	2.35	0.41
1:E:447:GLU:O	1:E:450:LYS:HB2	2.20	0.41
1:H:152:PRO:HB2	1:H:153:HIS:CD2	2.55	0.41
1:A:31:PRO:HB3	1:A:37:LEU:HD21	2.02	0.41
1:B:117:LEU:O	1:B:121:VAL:HG22	2.21	0.41
1:C:435:ARG:NH2	1:C:447:GLU:OE2	2.28	0.41
1:D:30:THR:HA	1:D:31:PRO:HD3	1.94	0.41
1:D:447:GLU:O	1:D:450:LYS:HB2	2.21	0.41
1:F:51:ASP:HA	1:F:87:ILE:CD1	2.49	0.41
1:H:447:GLU:O	1:H:450:LYS:HB2	2.21	0.41
2:J:41:LEU:HD13	2:J:73:PRO:HG3	2.01	0.41
2:J:39:HIS:CD2	2:J:75:PHE:O	2.74	0.41
1:H:451:TRP:CZ2	2:L:19:PRO:HD3	2.56	0.41
2:O:39:HIS:CD2	2:O:75:PHE:O	2.74	0.41
2:P:39:HIS:CD2	2:P:75:PHE:O	2.74	0.41
1:A:184:ASN:HD21	2:P:104:PHE:HZ	1.68	0.41
1:C:117:LEU:O	1:C:121:VAL:HG22	2.21	0.41
2:M:104:PHE:HZ	1:C:184:ASN:HD21	1.63	0.41
1:C:447:GLU:O	1:C:450:LYS:HB2	2.20	0.41
1:E:319:ARG:HG2	1:E:368:TRP:CZ3	2.55	0.41
1:F:451:TRP:CH2	2:K:19:PRO:HD3	2.55	0.41
1:H:117:LEU:O	1:H:121:VAL:HG22	2.21	0.41
1:H:451:TRP:CH2	2:L:19:PRO:HD3	2.55	0.41
1:B:451:TRP:CZ2	2:I:19:PRO:HD3	2.56	0.41
2:O:4:LYS:HB3	2:O:4:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:39:HIS:HA	2:P:40:PRO:HD3	1.92	0.41
1:A:117:LEU:O	1:A:121:VAL:HG22	2.21	0.41
1:E:117:LEU:O	1:E:121:VAL:HG22	2.21	0.41
1:E:62:SER:O	1:F:177:LYS:HB2	2.20	0.41
1:G:229:GLN:NE2	1:G:236:LYS:H	2.17	0.41
1:H:382:ILE:HA	1:H:386:HIS:CD2	2.55	0.41
1:B:166:GLY:HA2	2:I:112:THR:O	2.21	0.41
2:I:39:HIS:CD2	2:I:75:PHE:O	2.74	0.41
2:I:4:LYS:HB3	2:I:4:LYS:NZ	2.35	0.41
2:L:39:HIS:CD2	2:L:75:PHE:O	2.74	0.41
1:A:166:GLY:HA2	2:M:112:THR:O	2.21	0.41
1:A:382:ILE:HA	1:A:386:HIS:CD2	2.55	0.41
1:D:166:GLY:HA2	2:J:112:THR:O	2.21	0.41
1:D:31:PRO:HB3	1:D:37:LEU:HD21	2.02	0.41
1:D:435:ARG:HH22	1:D:447:GLU:CD	2.16	0.41
1:F:117:LEU:O	1:F:121:VAL:HG22	2.21	0.41
2:I:45:ASN:HD22	2:I:45:ASN:HA	1.77	0.41
2:P:45:ASN:HB2	2:P:67:TRP:CD2	2.56	0.41
1:C:156:GLN:HG3	1:C:157:VAL:N	2.35	0.41
1:H:435:ARG:HH22	1:H:447:GLU:CD	2.16	0.41
1:A:156:GLN:HG3	1:A:157:VAL:N	2.35	0.41
1:A:177:LYS:HB2	1:B:62:SER:O	2.21	0.41
1:A:451:TRP:CZ2	2:M:19:PRO:HD3	2.56	0.41
1:B:435:ARG:HH22	1:B:447:GLU:CD	2.16	0.41
1:C:31:PRO:HB3	1:C:37:LEU:HD21	2.02	0.41
2:K:45:ASN:HB2	2:K:67:TRP:CD2	2.56	0.41
2:M:45:ASN:HB2	2:M:67:TRP:CD2	2.56	0.41
2:M:39:HIS:CD2	2:M:75:PHE:O	2.74	0.41
1:C:451:TRP:CZ2	2:N:19:PRO:HD3	2.56	0.41
1:H:30:THR:HA	1:H:31:PRO:HD3	1.94	0.40
2:J:45:ASN:HB2	2:J:67:TRP:CD2	2.56	0.40
2:K:39:HIS:CD2	2:K:75:PHE:O	2.74	0.40
2:K:4:LYS:HB3	2:K:4:LYS:NZ	2.35	0.40
2:K:99:ILE:HB	2:K:118:HIS:HB3	2.04	0.40
2:N:39:HIS:CD2	2:N:75:PHE:O	2.74	0.40
1:E:451:TRP:CZ2	2:O:19:PRO:HD3	2.56	0.40
1:A:173:THR:HA	1:A:201:LYS:HG2	2.03	0.40
1:B:42:PHE:HE1	1:B:99:ALA:HB2	1.87	0.40
1:C:166:GLY:HA2	2:N:112:THR:O	2.21	0.40
1:G:18:LYS:HB2	1:G:18:LYS:HE2	1.89	0.40
1:G:42:PHE:HE1	1:G:99:ALA:HB2	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:451:TRP:CZ2	2:K:19:PRO:HD3	2.56	0.40
2:L:99:ILE:HB	2:L:118:HIS:HB3	2.04	0.40
2:O:45:ASN:HB2	2:O:67:TRP:CD2	2.56	0.40
1:A:295:ARG:HG3	1:A:295:ARG:H	1.64	0.40
1:D:24:TYR:CE1	1:D:81:LYS:HB2	2.57	0.40
1:G:24:TYR:CE1	1:G:81:LYS:HB2	2.57	0.40
1:G:319:ARG:HG2	1:G:368:TRP:CZ3	2.55	0.40
1:H:173:THR:HA	1:H:201:LYS:HG2	2.04	0.40
1:H:319:ARG:HG2	1:H:368:TRP:CZ3	2.55	0.40
2:I:6:LEU:HA	2:I:7:PRO:HD3	1.93	0.40
2:K:45:ASN:HA	2:K:45:ASN:HD22	1.77	0.40
2:K:6:LEU:HA	2:K:7:PRO:HD3	1.93	0.40
2:O:99:ILE:HB	2:O:118:HIS:HB3	2.04	0.40
1:B:181:SER:HB2	1:D:156:GLN:HE22	1.86	0.40
1:E:42:PHE:HE1	1:E:99:ALA:HB2	1.87	0.40
1:F:136:GLU:OE1	1:F:312:ARG:NH2	2.55	0.40
1:F:42:PHE:HE1	1:F:99:ALA:HB2	1.87	0.40
1:H:136:GLU:OE1	1:H:312:ARG:NH2	2.55	0.40
2:N:45:ASN:HB2	2:N:67:TRP:CD2	2.56	0.40
2:P:4:LYS:HB3	2:P:4:LYS:NZ	2.35	0.40
2:P:99:ILE:HB	2:P:118:HIS:HB3	2.04	0.40
1:B:31:PRO:HB3	1:B:37:LEU:HD21	2.02	0.40
1:E:136:GLU:OE1	1:E:312:ARG:NH2	2.55	0.40
1:E:469:PHE:CD2	1:F:128:LYS:HB3	2.57	0.40
1:G:156:GLN:HG3	1:G:157:VAL:N	2.35	0.40

All (35) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:24:ARG:CZ	2:K:22:SER:N[2_554]	0.87	1.33
2:O:24:ARG:NE	2:K:22:SER:N[2_554]	1.02	1.18
2:O:24:ARG:NE	2:K:21:LEU:C[2_554]	1.09	1.11
2:O:24:ARG:NH1	2:K:22:SER:CA[2_554]	1.10	1.10
2:O:24:ARG:CZ	2:K:22:SER:CA[2_554]	1.17	1.03
2:O:81:GLN:NE2	2:K:24:ARG:NE[2_554]	1.17	1.03
2:O:24:ARG:CZ	2:K:21:LEU:C[2_554]	1.31	0.89
2:O:24:ARG:NH1	2:K:22:SER:N[2_554]	1.35	0.85
2:O:24:ARG:NH2	2:K:21:LEU:O[2_554]	1.37	0.83
2:O:24:ARG:NH1	2:K:22:SER:C[2_554]	1.43	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:460:ASP:OD2	2:L:92:SER:CA[2_554]	1.48	0.72
2:O:24:ARG:NH1	2:K:22:SER:O[2_554]	1.72	0.48
2:O:24:ARG:CZ	2:K:21:LEU:O[2_554]	1.76	0.44
2:O:24:ARG:CD	2:K:22:SER:N[2_554]	1.78	0.42
2:O:81:GLN:NE2	2:K:24:ARG:CZ[2_554]	1.80	0.40
2:O:24:ARG:NH2	2:K:21:LEU:C[2_554]	1.80	0.40
2:O:24:ARG:NE	2:K:21:LEU:O[2_554]	1.81	0.39
1:E:460:ASP:OD2	2:L:92:SER:CB[2_554]	1.81	0.39
2:O:81:GLN:NE2	2:K:24:ARG:CD[2_554]	1.81	0.39
2:O:24:ARG:CZ	2:K:22:SER:C[2_554]	1.82	0.38
2:O:24:ARG:NH1	2:K:22:SER:CB[2_554]	1.83	0.37
2:O:81:GLN:CD	2:K:24:ARG:NE[2_554]	1.86	0.34
2:O:24:ARG:NH2	2:K:22:SER:C[2_554]	1.87	0.33
2:I:28:ALA:CA	2:J:24:ARG:NH2[3_655]	1.88	0.32
2:O:24:ARG:NH1	2:K:22:SER:OG[2_554]	2.00	0.20
1:E:460:ASP:OD2	2:L:92:SER:C[2_554]	2.01	0.19
2:I:28:ALA:CB	2:J:24:ARG:NE[3_655]	2.03	0.17
2:O:24:ARG:NE	2:K:22:SER:CA[2_554]	2.03	0.17
2:O:81:GLN:CD	2:K:24:ARG:CZ[2_554]	2.05	0.15
2:O:24:ARG:NH2	2:K:22:SER:CA[2_554]	2.08	0.12
2:M:24:ARG:NH2	2:N:31:GLU:OE1[3_654]	2.08	0.12
2:O:24:ARG:NH2	2:K:22:SER:N[2_554]	2.15	0.05
1:E:460:ASP:OD2	2:L:92:SER:O[2_554]	2.16	0.04
2:O:24:ARG:NE	2:K:21:LEU:CA[2_554]	2.18	0.02
2:O:81:GLN:CG	2:K:24:ARG:NH2[2_554]	2.19	0.01

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	465/467 (100%)	455 (98%)	10 (2%)	0	100	100
1	B	465/467 (100%)	455 (98%)	10 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
1	D	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
1	E	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
1	F	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
1	G	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
1	H	465/467 (100%)	455 (98%)	10 (2%)	0	100 100
2	I	107/109 (98%)	98 (92%)	9 (8%)	0	100 100
2	J	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17 16
2	K	107/109 (98%)	98 (92%)	9 (8%)	0	100 100
2	L	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17 16
2	M	107/109 (98%)	98 (92%)	9 (8%)	0	100 100
2	N	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17 16
2	O	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	17 16
2	P	107/109 (98%)	98 (92%)	9 (8%)	0	100 100
All	All	4576/4608 (99%)	4424 (97%)	148 (3%)	4 (0%)	51 60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	L	3	MET
2	N	121	GLY
2	J	121	GLY
2	O	121	GLY

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	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	B	377/377 (100%)	355 (94%)	22 (6%)	20 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	D	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	E	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	F	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	G	377/377 (100%)	355 (94%)	22 (6%)	20 23
1	H	377/377 (100%)	355 (94%)	22 (6%)	20 23
2	I	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	J	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	K	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	L	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	M	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	N	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	O	99/99 (100%)	90 (91%)	9 (9%)	9 9
2	P	99/99 (100%)	90 (91%)	9 (9%)	9 9
All	All	3808/3808 (100%)	3560 (94%)	248 (6%)	17 19

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LYS
1	A	36	LEU
1	A	41	ARG
1	A	78	ASP
1	A	127	PHE
1	A	134	ARG
1	A	156	GLN
1	A	167	ARG
1	A	203	ASP
1	A	213	ARG
1	A	215	ARG
1	A	217	ARG
1	A	219	LEU
1	A	239	TYR
1	A	241	ASN
1	A	295	ARG
1	A	303	ARG
1	A	319	ARG

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Mol	Chain	Res	Type
1	A	339	LYS
1	A	341	SER
1	A	392	GLU
1	A	450	LYS
2	M	4	LYS
2	M	23	ASP
2	M	24	ARG
2	M	36	GLN
2	M	91	ARG
2	M	100	ARG
2	M	106	ASN
2	M	119	ARG
2	M	122	ARG
1	B	14	LYS
1	B	36	LEU
1	B	41	ARG
1	B	78	ASP
1	B	127	PHE
1	B	134	ARG
1	B	156	GLN
1	B	167	ARG
1	B	203	ASP
1	B	213	ARG
1	B	215	ARG
1	B	217	ARG
1	B	219	LEU
1	B	239	TYR
1	B	241	ASN
1	B	295	ARG
1	B	303	ARG
1	B	319	ARG
1	B	339	LYS
1	B	341	SER
1	B	392	GLU
1	B	450	LYS
2	I	4	LYS
2	I	23	ASP
2	I	24	ARG
2	I	36	GLN
2	I	91	ARG
2	I	100	ARG
2	I	106	ASN

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Mol	Chain	Res	Type
2	I	119	ARG
2	I	122	ARG
1	C	14	LYS
1	C	36	LEU
1	C	41	ARG
1	C	78	ASP
1	C	127	PHE
1	C	134	ARG
1	C	156	GLN
1	C	167	ARG
1	C	203	ASP
1	C	213	ARG
1	C	215	ARG
1	C	217	ARG
1	C	219	LEU
1	C	239	TYR
1	C	241	ASN
1	C	295	ARG
1	C	303	ARG
1	C	319	ARG
1	C	339	LYS
1	C	341	SER
1	C	392	GLU
1	C	450	LYS
2	N	4	LYS
2	N	23	ASP
2	N	24	ARG
2	N	36	GLN
2	N	91	ARG
2	N	100	ARG
2	N	106	ASN
2	N	119	ARG
2	N	122	ARG
1	D	14	LYS
1	D	36	LEU
1	D	41	ARG
1	D	78	ASP
1	D	127	PHE
1	D	134	ARG
1	D	156	GLN
1	D	167	ARG
1	D	203	ASP

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Mol	Chain	Res	Type
1	D	213	ARG
1	D	215	ARG
1	D	217	ARG
1	D	219	LEU
1	D	239	TYR
1	D	241	ASN
1	D	295	ARG
1	D	303	ARG
1	D	319	ARG
1	D	339	LYS
1	D	341	SER
1	D	392	GLU
1	D	450	LYS
2	J	4	LYS
2	J	23	ASP
2	J	24	ARG
2	J	36	GLN
2	J	91	ARG
2	J	100	ARG
2	J	106	ASN
2	J	119	ARG
2	J	122	ARG
1	E	14	LYS
1	E	36	LEU
1	E	41	ARG
1	E	78	ASP
1	E	127	PHE
1	E	134	ARG
1	E	156	GLN
1	E	167	ARG
1	E	203	ASP
1	E	213	ARG
1	E	215	ARG
1	E	217	ARG
1	E	219	LEU
1	E	239	TYR
1	E	241	ASN
1	E	295	ARG
1	E	303	ARG
1	E	319	ARG
1	E	339	LYS
1	E	341	SER

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Mol	Chain	Res	Type
1	E	392	GLU
1	E	450	LYS
2	O	4	LYS
2	O	23	ASP
2	O	24	ARG
2	O	36	GLN
2	O	91	ARG
2	O	100	ARG
2	O	106	ASN
2	O	119	ARG
2	O	122	ARG
1	F	14	LYS
1	F	36	LEU
1	F	41	ARG
1	F	78	ASP
1	F	127	PHE
1	F	134	ARG
1	F	156	GLN
1	F	167	ARG
1	F	203	ASP
1	F	213	ARG
1	F	215	ARG
1	F	217	ARG
1	F	219	LEU
1	F	239	TYR
1	F	241	ASN
1	F	295	ARG
1	F	303	ARG
1	F	319	ARG
1	F	339	LYS
1	F	341	SER
1	F	392	GLU
1	F	450	LYS
2	K	4	LYS
2	K	23	ASP
2	K	24	ARG
2	K	36	GLN
2	K	91	ARG
2	K	100	ARG
2	K	106	ASN
2	K	119	ARG
2	K	122	ARG

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Mol	Chain	Res	Type
1	G	14	LYS
1	G	36	LEU
1	G	41	ARG
1	G	78	ASP
1	G	127	PHE
1	G	134	ARG
1	G	156	GLN
1	G	167	ARG
1	G	203	ASP
1	G	213	ARG
1	G	215	ARG
1	G	217	ARG
1	G	219	LEU
1	G	239	TYR
1	G	241	ASN
1	G	295	ARG
1	G	303	ARG
1	G	319	ARG
1	G	339	LYS
1	G	341	SER
1	G	392	GLU
1	G	450	LYS
2	P	4	LYS
2	P	23	ASP
2	P	24	ARG
2	P	36	GLN
2	P	91	ARG
2	P	100	ARG
2	P	106	ASN
2	P	119	ARG
2	P	122	ARG
1	H	14	LYS
1	H	36	LEU
1	H	41	ARG
1	H	78	ASP
1	H	127	PHE
1	H	134	ARG
1	H	156	GLN
1	H	167	ARG
1	H	203	ASP
1	H	213	ARG
1	H	215	ARG

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Mol	Chain	Res	Type
1	H	217	ARG
1	H	219	LEU
1	H	239	TYR
1	H	241	ASN
1	H	295	ARG
1	H	303	ARG
1	H	319	ARG
1	H	339	LYS
1	H	341	SER
1	H	392	GLU
1	H	450	LYS
2	L	4	LYS
2	L	23	ASP
2	L	24	ARG
2	L	36	GLN
2	L	91	ARG
2	L	100	ARG
2	L	106	ASN
2	L	119	ARG
2	L	122	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	153	HIS
1	A	156	GLN
1	A	212	GLN
1	A	226	HIS
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	353	HIS
1	A	386	HIS
1	A	401	GLN
2	M	39	HIS
2	M	45	ASN
2	M	82	GLN
2	M	106	ASN
2	M	118	HIS

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Mol	Chain	Res	Type
1	B	153	HIS
1	B	156	GLN
1	B	212	GLN
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	353	HIS
1	B	386	HIS
1	B	401	GLN
2	I	39	HIS
2	I	45	ASN
2	I	82	GLN
2	I	106	ASN
2	I	111	GLN
2	I	118	HIS
1	C	153	HIS
1	C	156	GLN
1	C	212	GLN
1	C	229	GLN
1	C	238	HIS
1	C	241	ASN
1	C	267	HIS
1	C	277	ASN
1	C	304	GLN
1	C	353	HIS
1	C	386	HIS
1	C	401	GLN
2	N	39	HIS
2	N	45	ASN
2	N	82	GLN
2	N	106	ASN
2	N	111	GLN
2	N	118	HIS
1	D	153	HIS
1	D	156	GLN
1	D	212	GLN
1	D	229	GLN
1	D	238	HIS
1	D	241	ASN

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Mol	Chain	Res	Type
1	D	267	HIS
1	D	277	ASN
1	D	304	GLN
1	D	353	HIS
1	D	386	HIS
1	D	401	GLN
2	J	39	HIS
2	J	45	ASN
2	J	82	GLN
2	J	106	ASN
2	J	111	GLN
2	J	118	HIS
1	E	153	HIS
1	E	156	GLN
1	E	212	GLN
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	353	HIS
1	E	386	HIS
1	E	401	GLN
2	O	36	GLN
2	O	39	HIS
2	O	45	ASN
2	O	82	GLN
2	O	106	ASN
2	O	111	GLN
2	O	118	HIS
1	F	153	HIS
1	F	156	GLN
1	F	212	GLN
1	F	229	GLN
1	F	238	HIS
1	F	241	ASN
1	F	267	HIS
1	F	277	ASN
1	F	304	GLN
1	F	353	HIS
1	F	386	HIS

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Mol	Chain	Res	Type
1	F	401	GLN
2	K	39	HIS
2	K	45	ASN
2	K	82	GLN
2	K	106	ASN
2	K	111	GLN
2	K	118	HIS
1	G	153	HIS
1	G	156	GLN
1	G	212	GLN
1	G	229	GLN
1	G	238	HIS
1	G	241	ASN
1	G	267	HIS
1	G	277	ASN
1	G	304	GLN
1	G	353	HIS
1	G	386	HIS
1	G	401	GLN
2	P	39	HIS
2	P	45	ASN
2	P	82	GLN
2	P	106	ASN
2	P	111	GLN
2	P	118	HIS
1	H	153	HIS
1	H	156	GLN
1	H	212	GLN
1	H	229	GLN
1	H	238	HIS
1	H	241	ASN
1	H	267	HIS
1	H	277	ASN
1	H	304	GLN
1	H	353	HIS
1	H	386	HIS
1	H	401	GLN
2	L	39	HIS
2	L	45	ASN
2	L	82	GLN
2	L	106	ASN
2	L	111	GLN

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Mol	Chain	Res	Type
2	L	118	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	CAP	D	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.13	6 (30%)
4	CAP	F	476	3	15,20,20	2.13	7 (46%)	20,31,31	2.14	5 (25%)
5	FMT	D	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	CAP	G	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
4	CAP	B	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
5	FMT	G	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	E	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	C	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	A	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	B	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
5	FMT	H	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-
4	CAP	H	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	CAP	A	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	5 (25%)
4	CAP	C	476	3	15,20,20	2.14	7 (46%)	20,31,31	2.14	6 (30%)
4	CAP	E	476	3	15,20,20	2.13	7 (46%)	20,31,31	2.14	6 (30%)
5	FMT	F	478	1,3	0,2,2	0.00	-	0,1,1	0.00	-

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
4	CAP	D	476	3	-	6/23/29/29	-
4	CAP	B	476	3	-	6/23/29/29	-
4	CAP	F	476	3	-	6/23/29/29	-
4	CAP	H	476	3	-	6/23/29/29	-
4	CAP	A	476	3	-	6/23/29/29	-
4	CAP	C	476	3	-	6/23/29/29	-
4	CAP	E	476	3	-	6/23/29/29	-
4	CAP	G	476	3	-	6/23/29/29	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	476	CAP	P2-O5	-3.93	1.47	1.60
4	B	476	CAP	P2-O5	-3.93	1.47	1.60
4	G	476	CAP	P2-O5	-3.93	1.47	1.60
4	A	476	CAP	P2-O5	-3.92	1.47	1.60
4	H	476	CAP	P2-O5	-3.92	1.47	1.60
4	C	476	CAP	P2-O5	-3.92	1.47	1.60
4	F	476	CAP	P2-O5	-3.91	1.47	1.60
4	E	476	CAP	P2-O5	-3.91	1.47	1.60
4	D	476	CAP	O2-C2	-3.39	1.37	1.43
4	F	476	CAP	O2-C2	-3.37	1.37	1.43
4	B	476	CAP	O2-C2	-3.36	1.37	1.43
4	H	476	CAP	O2-C2	-3.36	1.37	1.43
4	A	476	CAP	O2-C2	-3.35	1.37	1.43
4	C	476	CAP	O2-C2	-3.35	1.37	1.43
4	G	476	CAP	O2-C2	-3.34	1.37	1.43
4	E	476	CAP	O2-C2	-3.31	1.37	1.43
4	G	476	CAP	P1-O1	-3.16	1.50	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	476	CAP	P1-O1	-3.15	1.50	1.60
4	B	476	CAP	P1-O1	-3.15	1.50	1.60
4	A	476	CAP	P1-O1	-3.15	1.50	1.60
4	F	476	CAP	P1-O1	-3.14	1.50	1.60
4	H	476	CAP	P1-O1	-3.14	1.50	1.60
4	D	476	CAP	P1-O1	-3.13	1.50	1.60
4	C	476	CAP	P1-O1	-3.13	1.50	1.60
4	G	476	CAP	O4-C4	-2.76	1.37	1.43
4	E	476	CAP	O4-C4	-2.74	1.37	1.43
4	A	476	CAP	O4-C4	-2.73	1.37	1.43
4	C	476	CAP	O4-C4	-2.73	1.37	1.43
4	H	476	CAP	O4-C4	-2.72	1.37	1.43
4	B	476	CAP	O4-C4	-2.72	1.37	1.43
4	D	476	CAP	O4-C4	-2.71	1.37	1.43
4	F	476	CAP	O4-C4	-2.71	1.37	1.43
4	E	476	CAP	P2-O4P	2.58	1.58	1.50
4	F	476	CAP	P2-O4P	2.58	1.58	1.50
4	G	476	CAP	P2-O4P	2.58	1.58	1.50
4	B	476	CAP	P2-O4P	2.57	1.58	1.50
4	A	476	CAP	P2-O4P	2.57	1.58	1.50
4	C	476	CAP	P2-O4P	2.57	1.58	1.50
4	H	476	CAP	P2-O4P	2.57	1.58	1.50
4	D	476	CAP	P2-O4P	2.55	1.58	1.50
4	E	476	CAP	P1-O1P	2.32	1.58	1.50
4	H	476	CAP	P1-O1P	2.31	1.58	1.50
4	D	476	CAP	P1-O1P	2.31	1.58	1.50
4	G	476	CAP	P1-O1P	2.30	1.58	1.50
4	A	476	CAP	P1-O1P	2.30	1.58	1.50
4	C	476	CAP	P1-O1P	2.28	1.57	1.50
4	B	476	CAP	P1-O1P	2.28	1.57	1.50
4	F	476	CAP	P1-O1P	2.28	1.57	1.50
4	B	476	CAP	O3-C3	-2.24	1.38	1.42
4	H	476	CAP	O3-C3	-2.24	1.38	1.42
4	C	476	CAP	O3-C3	-2.23	1.38	1.42
4	G	476	CAP	O3-C3	-2.23	1.38	1.42
4	D	476	CAP	O3-C3	-2.22	1.38	1.42
4	A	476	CAP	O3-C3	-2.22	1.38	1.42
4	E	476	CAP	O3-C3	-2.22	1.38	1.42
4	F	476	CAP	O3-C3	-2.22	1.38	1.42

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	476	CAP	C5-C4-C3	5.27	122.71	111.94
4	H	476	CAP	C5-C4-C3	5.27	122.71	111.94
4	G	476	CAP	C5-C4-C3	5.26	122.69	111.94
4	C	476	CAP	C5-C4-C3	5.25	122.68	111.94
4	A	476	CAP	C5-C4-C3	5.25	122.67	111.94
4	E	476	CAP	C5-C4-C3	5.25	122.67	111.94
4	B	476	CAP	C5-C4-C3	5.24	122.65	111.94
4	D	476	CAP	C5-C4-C3	5.23	122.63	111.94
4	H	476	CAP	O4-C4-C3	-4.12	100.54	108.78
4	E	476	CAP	O4-C4-C3	-4.12	100.55	108.78
4	B	476	CAP	O4-C4-C3	-4.11	100.56	108.78
4	D	476	CAP	O4-C4-C3	-4.11	100.56	108.78
4	G	476	CAP	O4-C4-C3	-4.10	100.58	108.78
4	A	476	CAP	O4-C4-C3	-4.10	100.58	108.78
4	F	476	CAP	O4-C4-C3	-4.10	100.59	108.78
4	C	476	CAP	O4-C4-C3	-4.08	100.62	108.78
4	F	476	CAP	C2-C3-C4	2.77	119.63	114.00
4	A	476	CAP	C2-C3-C4	2.74	119.57	114.00
4	H	476	CAP	C2-C3-C4	2.74	119.56	114.00
4	G	476	CAP	C2-C3-C4	2.73	119.56	114.00
4	C	476	CAP	C2-C3-C4	2.73	119.56	114.00
4	B	476	CAP	C2-C3-C4	2.73	119.55	114.00
4	D	476	CAP	C2-C3-C4	2.73	119.55	114.00
4	E	476	CAP	C2-C3-C4	2.72	119.54	114.00
4	B	476	CAP	P2-O5-C5	2.40	124.92	118.30
4	D	476	CAP	P2-O5-C5	2.40	124.91	118.30
4	A	476	CAP	P2-O5-C5	2.40	124.90	118.30
4	G	476	CAP	P2-O5-C5	2.40	124.90	118.30
4	F	476	CAP	P2-O5-C5	2.40	124.89	118.30
4	E	476	CAP	P2-O5-C5	2.40	124.89	118.30
4	C	476	CAP	P2-O5-C5	2.39	124.88	118.30
4	H	476	CAP	P2-O5-C5	2.38	124.84	118.30
4	C	476	CAP	O5-C5-C4	2.22	115.28	109.36
4	F	476	CAP	O5-C5-C4	2.22	115.28	109.36
4	E	476	CAP	O5-C5-C4	2.22	115.28	109.36
4	G	476	CAP	O5-C5-C4	2.21	115.27	109.36
4	A	476	CAP	O5-C5-C4	2.21	115.25	109.36
4	H	476	CAP	O5-C5-C4	2.21	115.25	109.36
4	B	476	CAP	O5-C5-C4	2.19	115.21	109.36
4	D	476	CAP	O5-C5-C4	2.19	115.20	109.36
4	E	476	CAP	O3P-P1-O2P	2.01	115.30	107.64
4	C	476	CAP	O3P-P1-O2P	2.00	115.28	107.64
4	D	476	CAP	O3P-P1-O2P	2.00	115.28	107.64

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	476	CAP	C2-C3-C4-C5
4	F	476	CAP	C2-C3-C4-O4
4	F	476	CAP	O3-C3-C4-O4
4	G	476	CAP	C2-C3-C4-C5
4	G	476	CAP	C2-C3-C4-O4
4	G	476	CAP	O3-C3-C4-O4
4	B	476	CAP	C2-C3-C4-C5
4	B	476	CAP	C2-C3-C4-O4
4	B	476	CAP	O3-C3-C4-O4
4	A	476	CAP	C2-C3-C4-C5
4	A	476	CAP	C2-C3-C4-O4
4	A	476	CAP	O3-C3-C4-O4
4	C	476	CAP	C2-C3-C4-C5
4	C	476	CAP	C2-C3-C4-O4
4	C	476	CAP	O3-C3-C4-O4
4	D	476	CAP	C2-C3-C4-C5
4	D	476	CAP	C2-C3-C4-O4
4	D	476	CAP	O3-C3-C4-O4
4	H	476	CAP	C2-C3-C4-C5
4	H	476	CAP	C2-C3-C4-O4
4	H	476	CAP	O3-C3-C4-O4
4	E	476	CAP	C2-C3-C4-C5
4	E	476	CAP	C2-C3-C4-O4
4	E	476	CAP	O3-C3-C4-O4
4	F	476	CAP	O2-C2-C3-C4
4	G	476	CAP	O2-C2-C3-C4
4	B	476	CAP	O2-C2-C3-C4
4	A	476	CAP	O2-C2-C3-C4
4	C	476	CAP	O2-C2-C3-C4
4	D	476	CAP	O2-C2-C3-C4
4	H	476	CAP	O2-C2-C3-C4
4	E	476	CAP	O2-C2-C3-C4
4	F	476	CAP	O3-C3-C4-C5
4	G	476	CAP	O3-C3-C4-C5
4	B	476	CAP	O3-C3-C4-C5
4	A	476	CAP	O3-C3-C4-C5
4	C	476	CAP	O3-C3-C4-C5
4	D	476	CAP	O3-C3-C4-C5
4	H	476	CAP	O3-C3-C4-C5
4	E	476	CAP	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	F	476	CAP	C4-C5-O5-P2
4	G	476	CAP	C4-C5-O5-P2
4	B	476	CAP	C4-C5-O5-P2
4	A	476	CAP	C4-C5-O5-P2
4	C	476	CAP	C4-C5-O5-P2
4	D	476	CAP	C4-C5-O5-P2
4	H	476	CAP	C4-C5-O5-P2
4	E	476	CAP	C4-C5-O5-P2

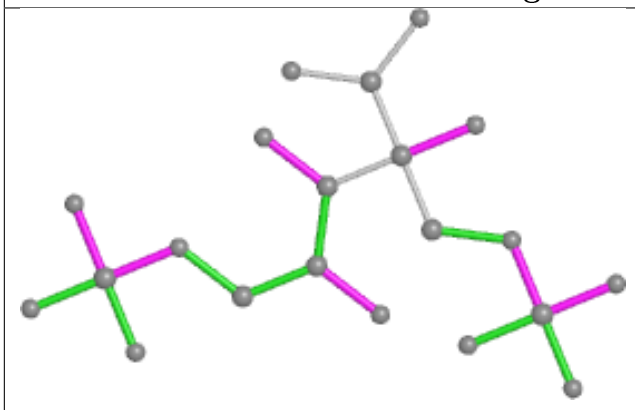
There are no ring outliers.

8 monomers are involved in 8 short contacts:

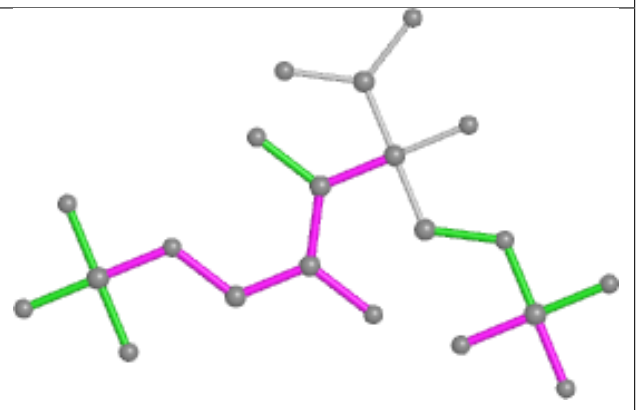
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	476	CAP	1	0
4	F	476	CAP	1	0
4	G	476	CAP	1	0
4	B	476	CAP	1	0
4	H	476	CAP	1	0
4	A	476	CAP	1	0
4	C	476	CAP	1	0
4	E	476	CAP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

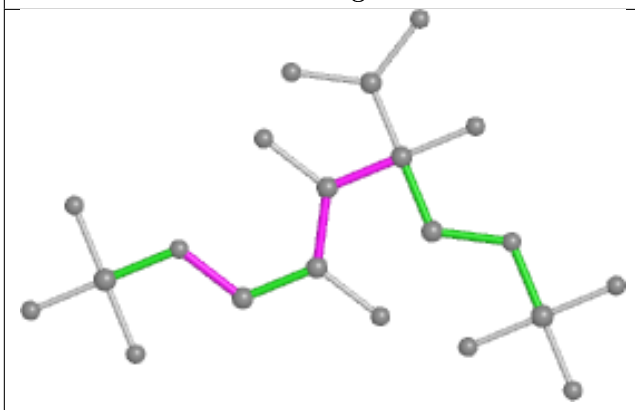
Ligand CAP D 476



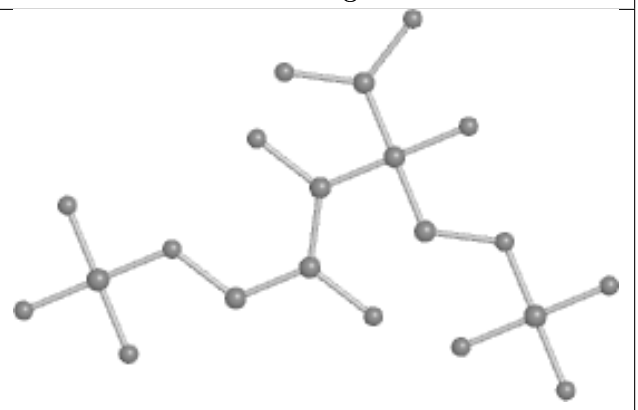
Bond lengths



Bond angles

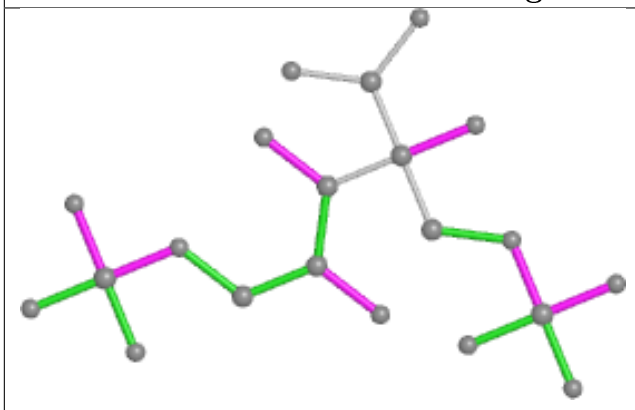


Torsions

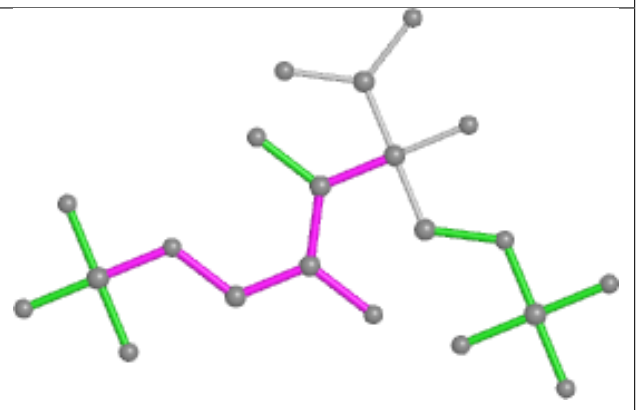


Rings

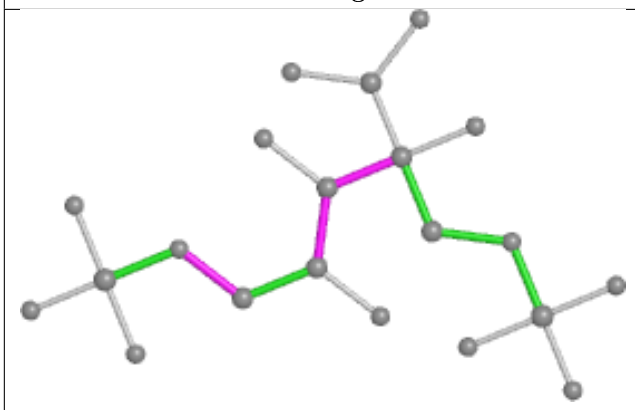
Ligand CAP F 476



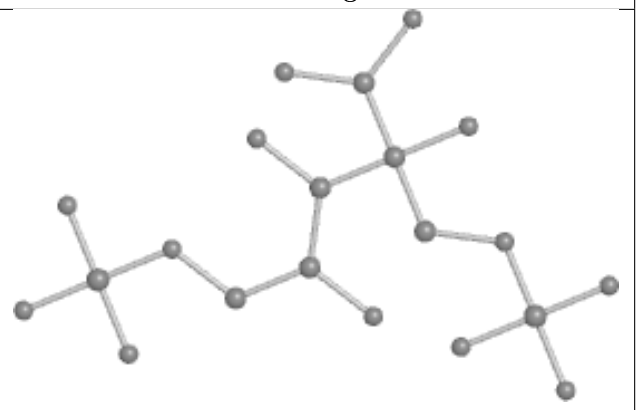
Bond lengths



Bond angles

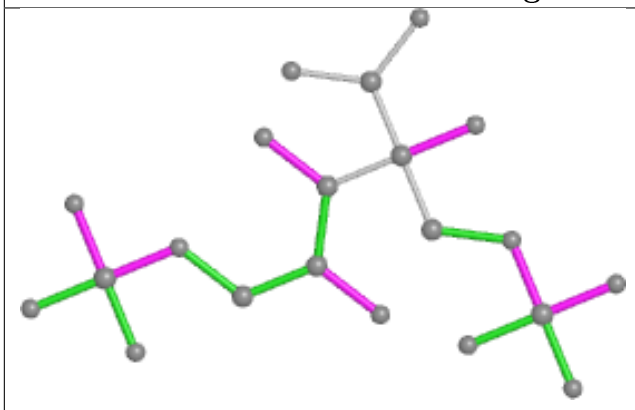


Torsions

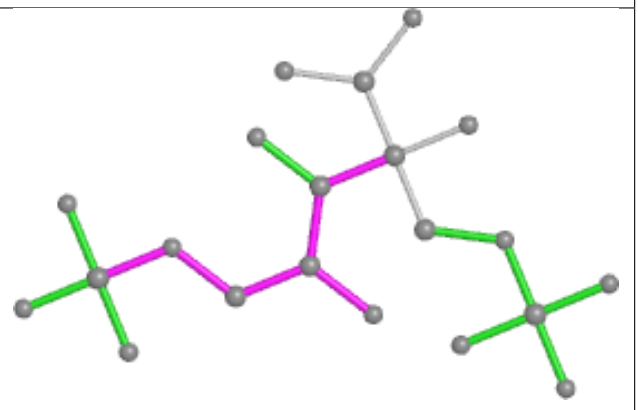


Rings

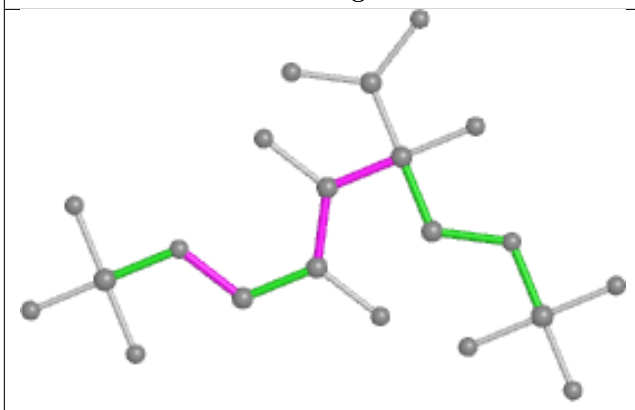
Ligand CAP G 476



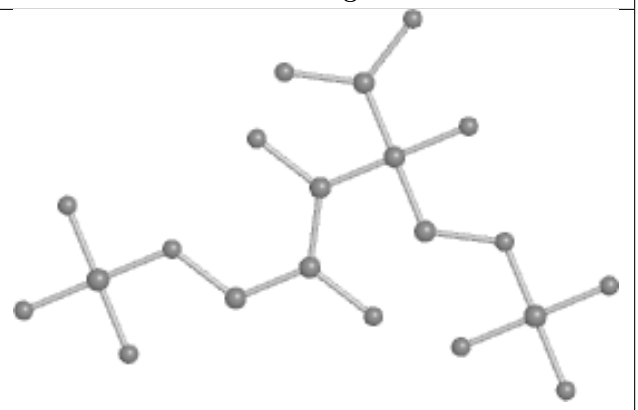
Bond lengths



Bond angles

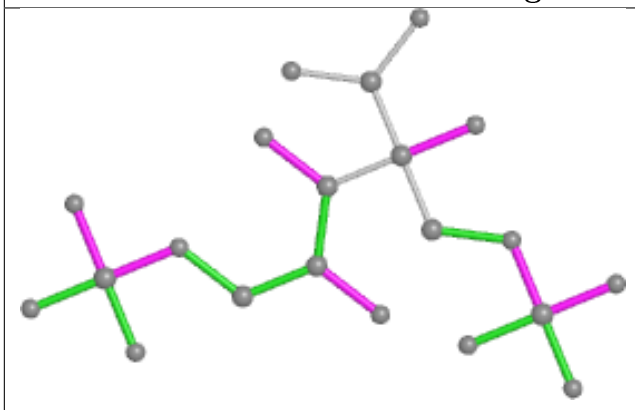


Torsions

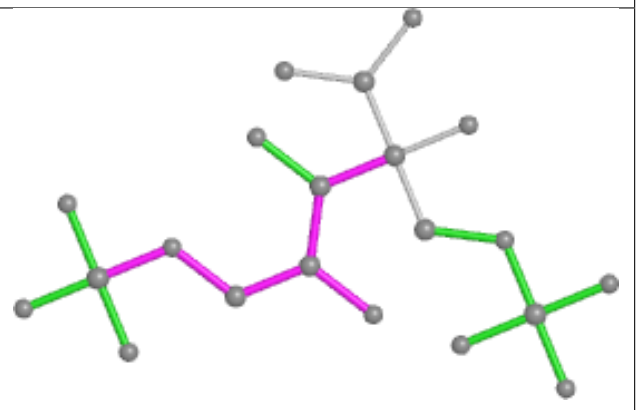


Rings

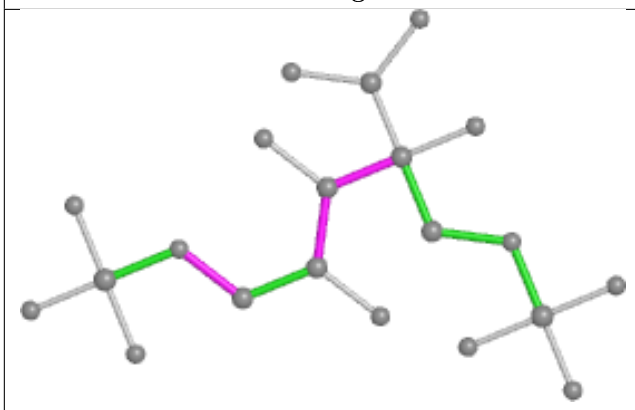
Ligand CAP B 476



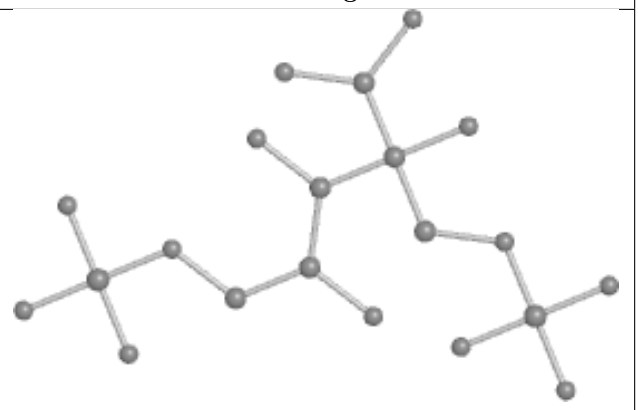
Bond lengths



Bond angles

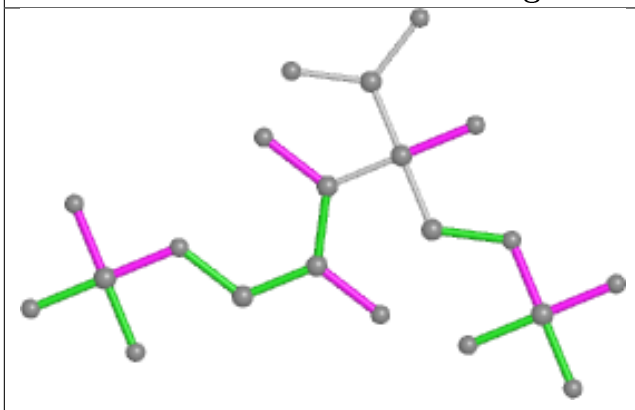


Torsions

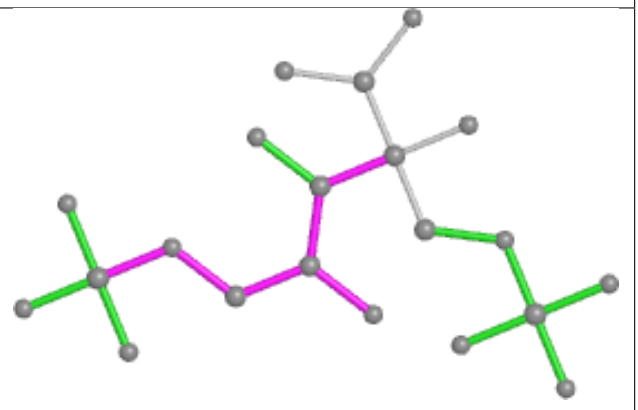


Rings

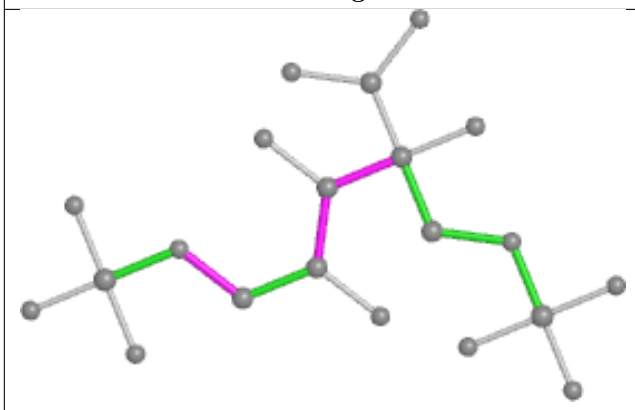
Ligand CAP H 476



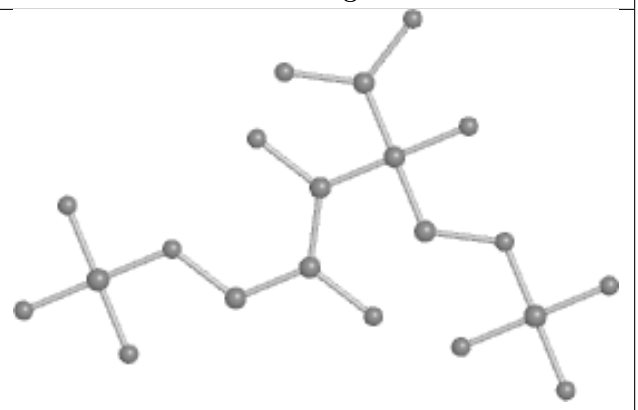
Bond lengths



Bond angles

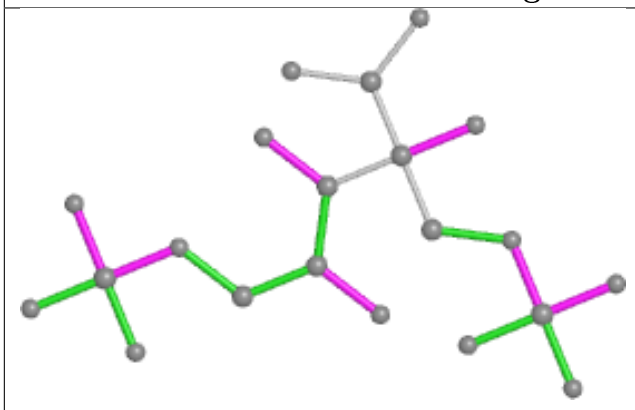


Torsions

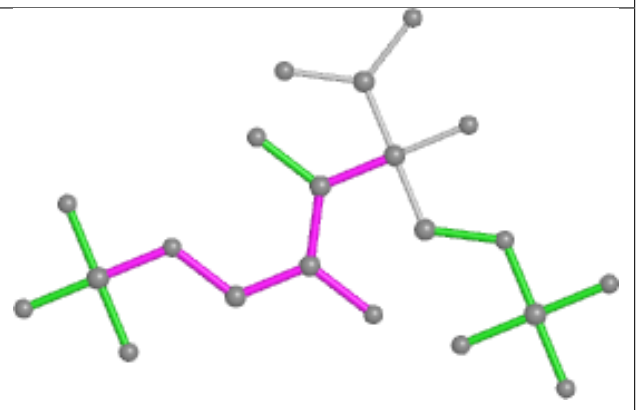


Rings

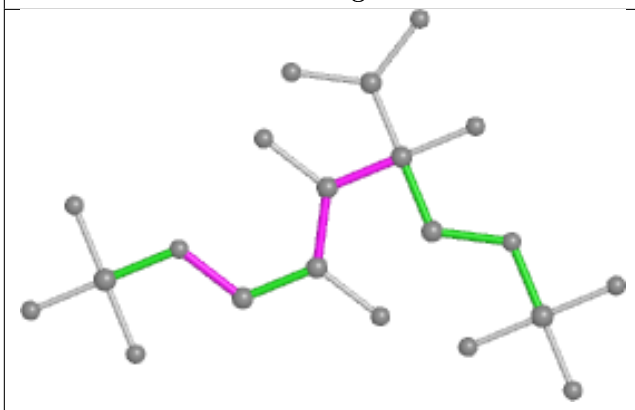
Ligand CAP A 476



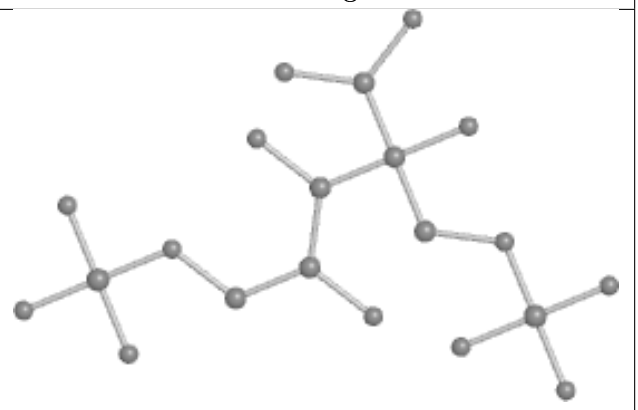
Bond lengths



Bond angles

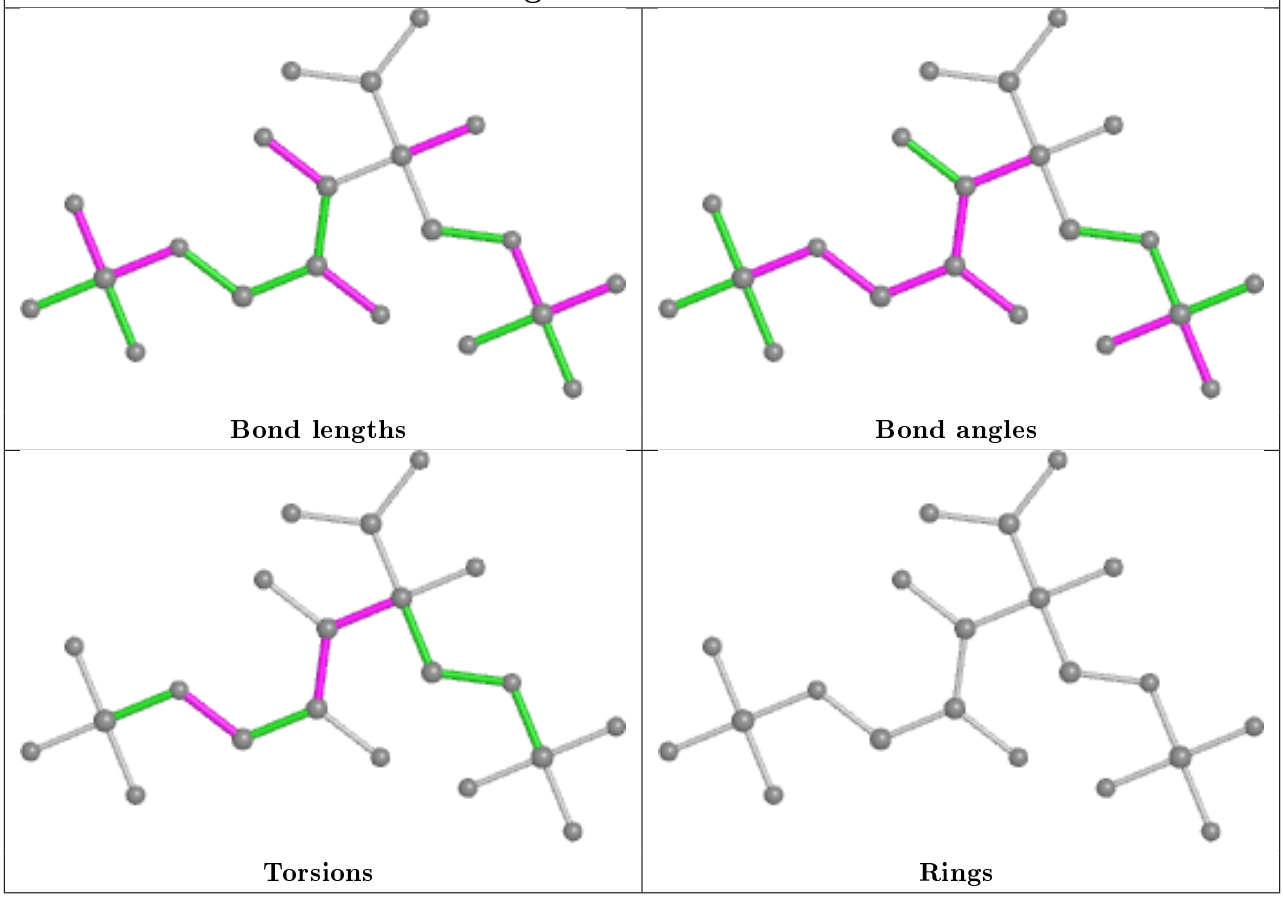


Torsions

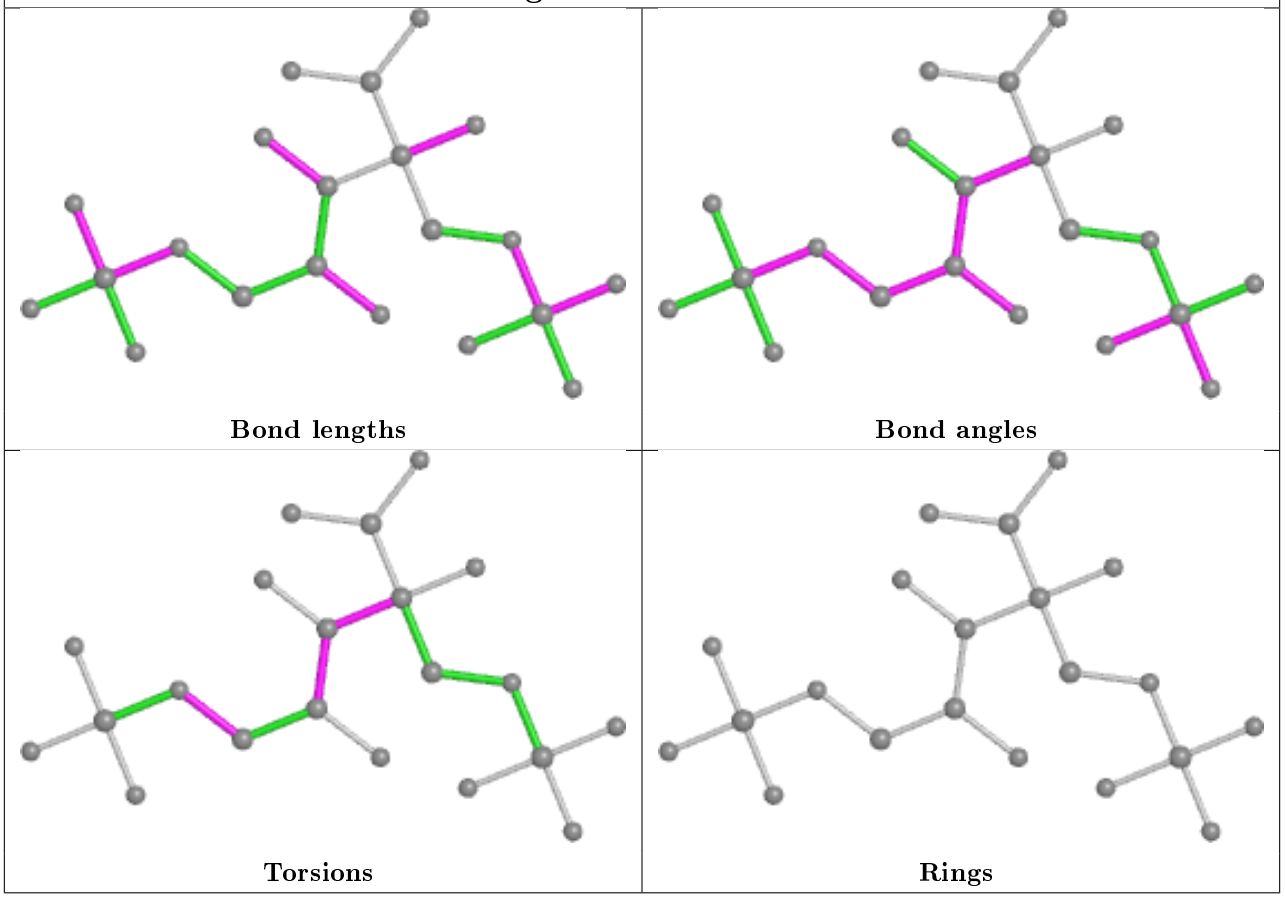


Rings

Ligand CAP C 476



Ligand CAP E 476



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	464/467 (99%)	-0.74	3 (0%)	89	88	11, 18, 36, 62	0
1	B	464/467 (99%)	-0.74	2 (0%)	92	91	11, 18, 36, 62	0
1	C	464/467 (99%)	-0.76	2 (0%)	92	91	11, 18, 36, 62	0
1	D	464/467 (99%)	-0.76	1 (0%)	95	94	11, 18, 36, 62	0
1	E	464/467 (99%)	-0.78	1 (0%)	95	94	11, 18, 36, 62	0
1	F	464/467 (99%)	-0.79	4 (0%)	84	83	11, 18, 36, 62	0
1	G	464/467 (99%)	-0.82	3 (0%)	89	88	11, 18, 36, 62	0
1	H	464/467 (99%)	-0.83	1 (0%)	95	94	11, 18, 36, 62	0
2	I	108/109 (99%)	-0.32	3 (2%)	53	51	16, 28, 60, 80	0
2	J	108/109 (99%)	-0.08	5 (4%)	32	31	16, 28, 60, 80	0
2	K	108/109 (99%)	-0.14	3 (2%)	53	51	16, 28, 60, 80	0
2	L	108/109 (99%)	-0.13	6 (5%)	24	23	16, 28, 60, 80	0
2	M	108/109 (99%)	-0.33	2 (1%)	66	65	16, 28, 60, 80	0
2	N	108/109 (99%)	-0.27	2 (1%)	66	65	16, 28, 60, 80	0
2	O	108/109 (99%)	-0.07	6 (5%)	24	23	16, 28, 60, 80	0
2	P	108/109 (99%)	-0.21	5 (4%)	32	31	16, 28, 60, 80	0
All	All	4576/4608 (99%)	-0.67	49 (1%)	80	79	11, 19, 45, 80	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	121	GLY	11.1
2	L	121	GLY	10.5
2	J	121	GLY	9.9
2	O	2	SER	9.6
2	M	121	GLY	8.7

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Mol	Chain	Res	Type	RSRZ
2	L	2	SER	6.6
2	P	121	GLY	5.8
2	K	2	SER	5.3
1	B	438	TYR	5.2
2	P	2	SER	5.0
2	M	2	SER	4.8
2	O	76	ALA	4.7
2	N	121	GLY	4.7
2	K	121	GLY	4.6
1	F	438	TYR	4.3
2	J	2	SER	3.9
2	J	77	CYS	3.7
2	O	3	MET	3.6
1	C	438	TYR	3.5
2	L	77	CYS	3.3
1	G	439	ARG	3.2
1	G	94	GLU	3.2
2	L	24	ARG	3.1
1	F	94	GLU	3.1
1	F	439	ARG	3.0
1	D	438	TYR	3.0
1	A	438	TYR	2.9
1	E	438	TYR	2.9
1	G	438	TYR	2.9
2	J	92	SER	2.9
2	K	24	ARG	2.8
2	O	92	SER	2.7
1	C	439	ARG	2.7
2	N	2	SER	2.5
2	J	24	ARG	2.4
2	I	2	SER	2.4
1	B	439	ARG	2.3
2	P	24	ARG	2.3
2	L	76	ALA	2.3
1	H	438	TYR	2.2
1	A	439	ARG	2.2
1	A	28	ASP	2.2
2	L	78	ALA	2.2
2	I	121	GLY	2.2
2	I	77	CYS	2.2
2	P	77	CYS	2.1
1	F	12	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	3	MET	2.0
2	O	23	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates 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, 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
3	MG	F	477	1/1	0.92	0.14	19,19,19,19	0
3	MG	B	477	1/1	0.94	0.19	19,19,19,19	0
3	MG	D	477	1/1	0.94	0.09	19,19,19,19	0
3	MG	C	477	1/1	0.95	0.18	19,19,19,19	0
3	MG	E	477	1/1	0.95	0.16	19,19,19,19	0
5	FMT	E	478	3/3	0.96	0.09	13,13,14,15	0
4	CAP	C	476	21/21	0.97	0.09	13,16,20,21	0
3	MG	H	477	1/1	0.97	0.07	19,19,19,19	0
3	MG	G	477	1/1	0.97	0.12	19,19,19,19	0
4	CAP	H	476	21/21	0.97	0.08	13,16,20,21	0
4	CAP	E	476	21/21	0.97	0.09	13,16,20,21	0
3	MG	A	477	1/1	0.97	0.16	19,19,19,19	0
5	FMT	B	478	3/3	0.97	0.11	13,13,14,15	0
4	CAP	F	476	21/21	0.98	0.08	13,16,20,21	0
5	FMT	C	478	3/3	0.98	0.09	13,13,14,15	0
5	FMT	A	478	3/3	0.98	0.09	13,13,14,15	0
4	CAP	B	476	21/21	0.98	0.09	13,16,20,21	0
5	FMT	G	478	3/3	0.98	0.07	13,13,14,15	0
4	CAP	A	476	21/21	0.98	0.08	13,16,20,21	0
4	CAP	G	476	21/21	0.98	0.07	13,16,20,21	0
4	CAP	D	476	21/21	0.98	0.07	13,16,20,21	0

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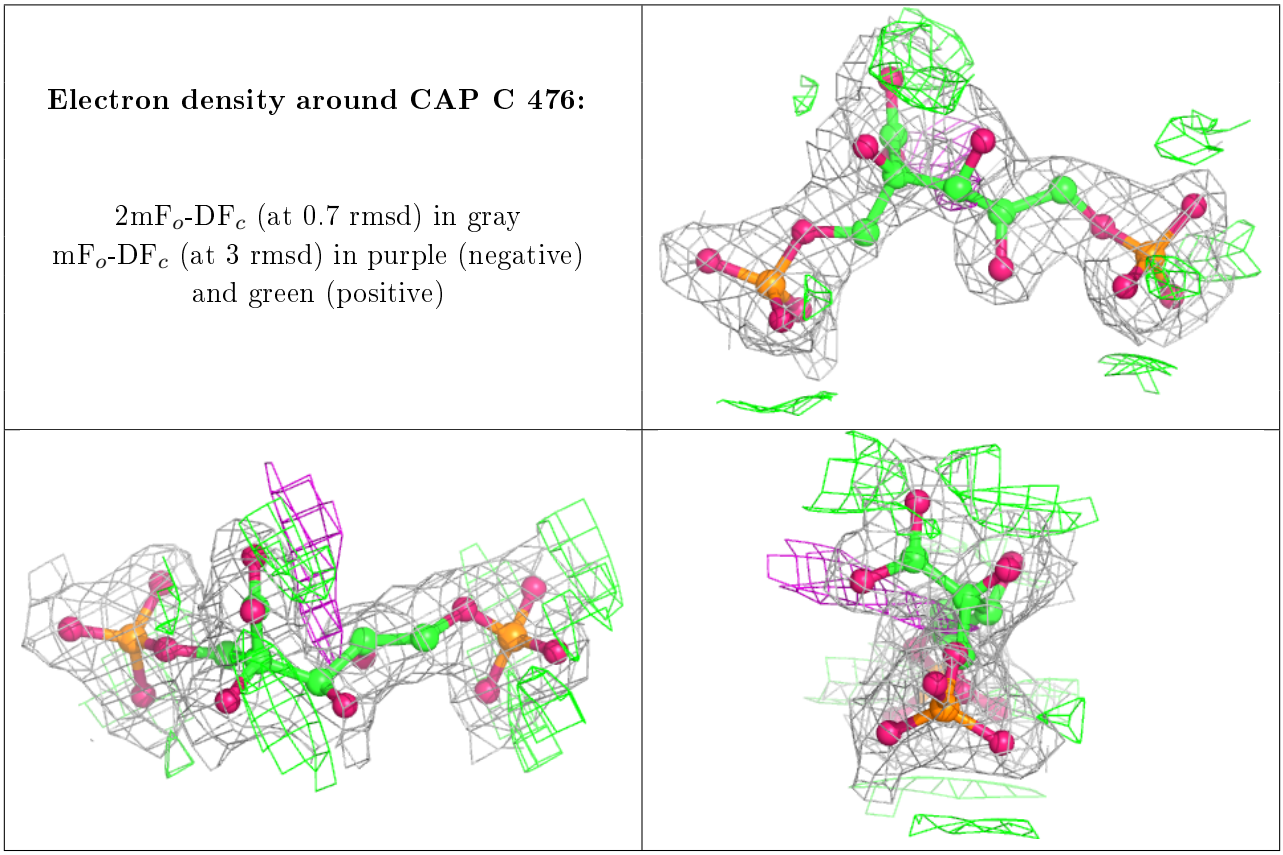
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	FMT	H	478	3/3	0.99	0.07	13,13,14,15	0
5	FMT	D	478	3/3	0.99	0.07	13,13,14,15	0
5	FMT	F	478	3/3	0.99	0.07	13,13,14,15	0

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

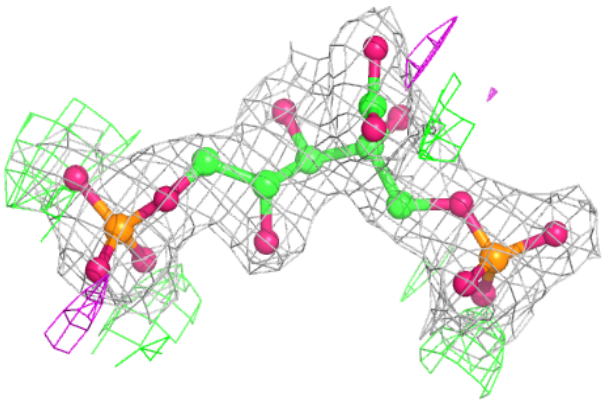
Electron density around CAP C 476:

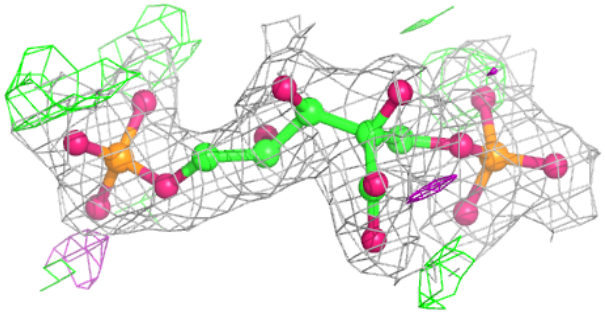
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

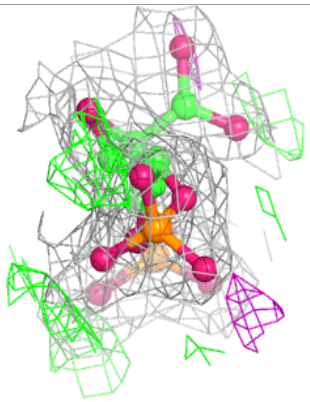


Electron density around CAP H 476:

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

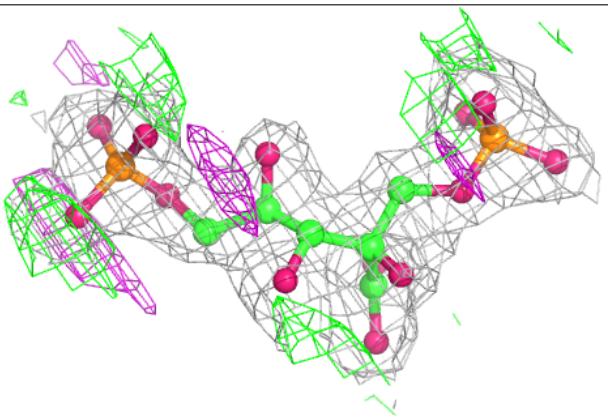


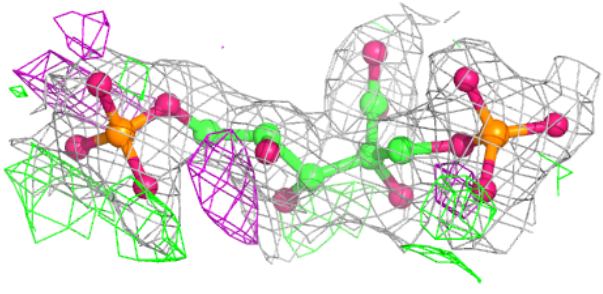


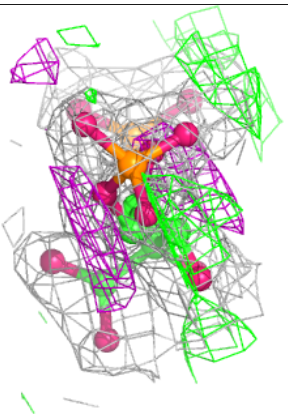


Electron density around CAP E 476:

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

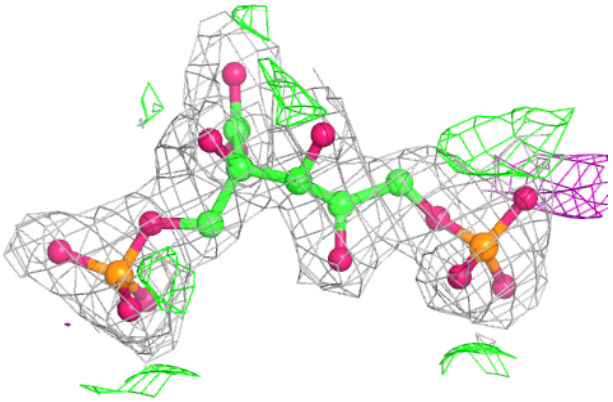


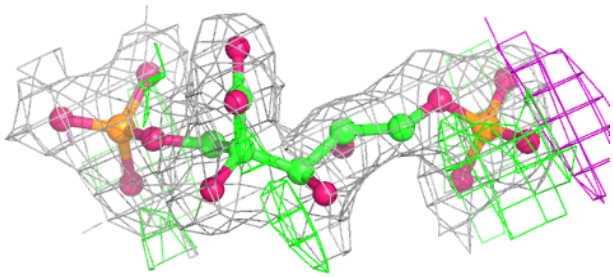


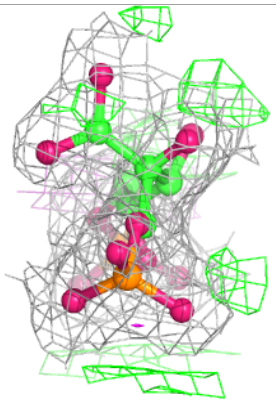


Electron density around CAP F 476:

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

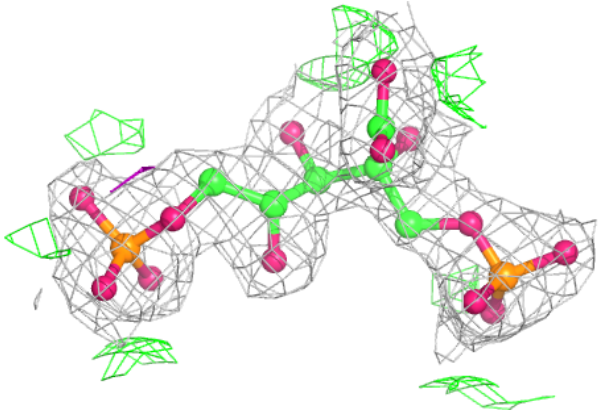


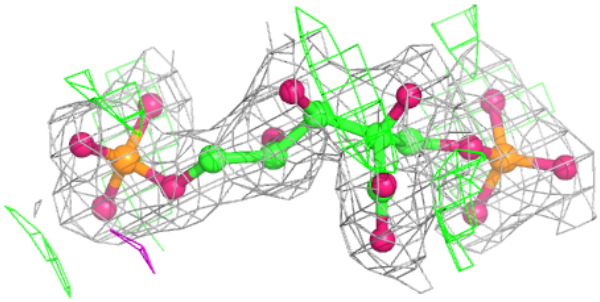


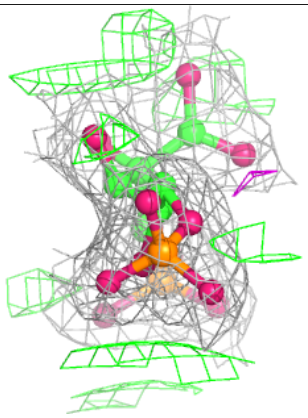


Electron density around CAP B 476:

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

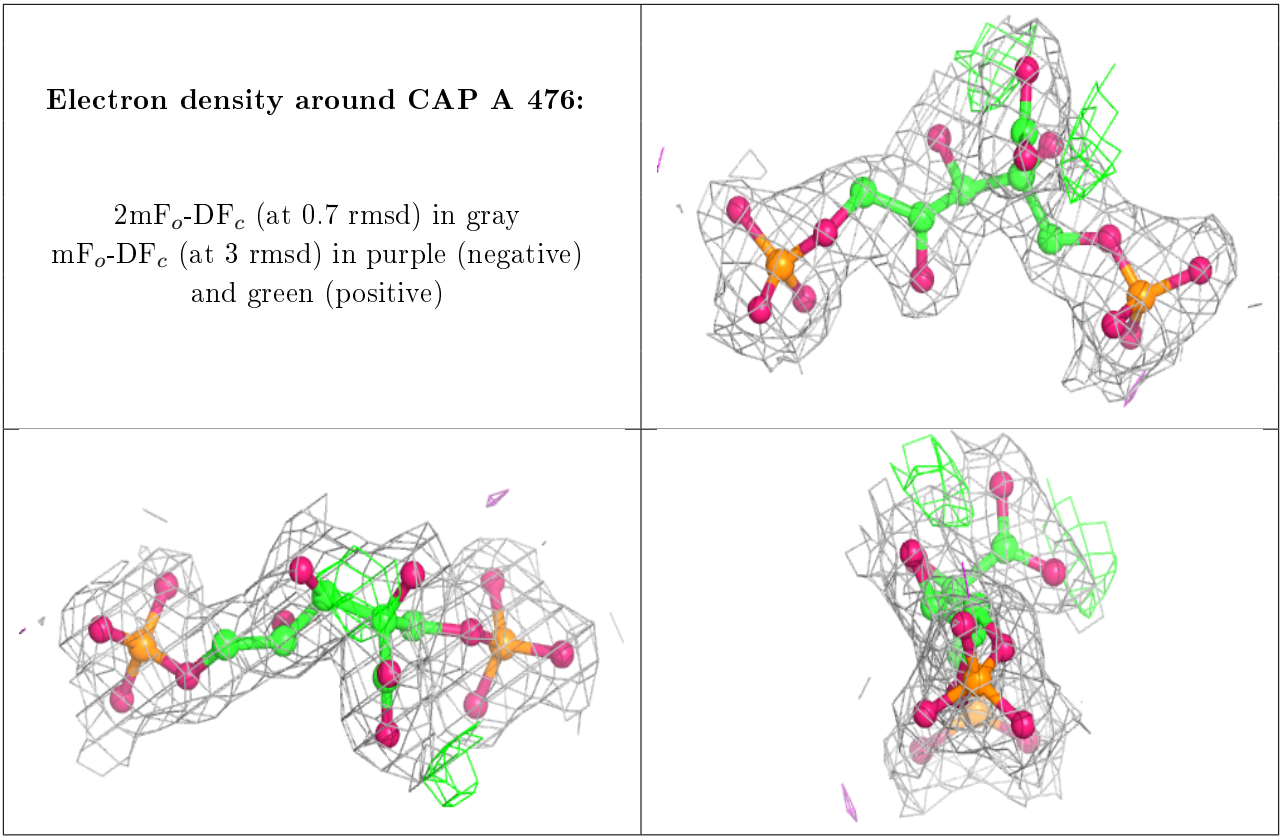






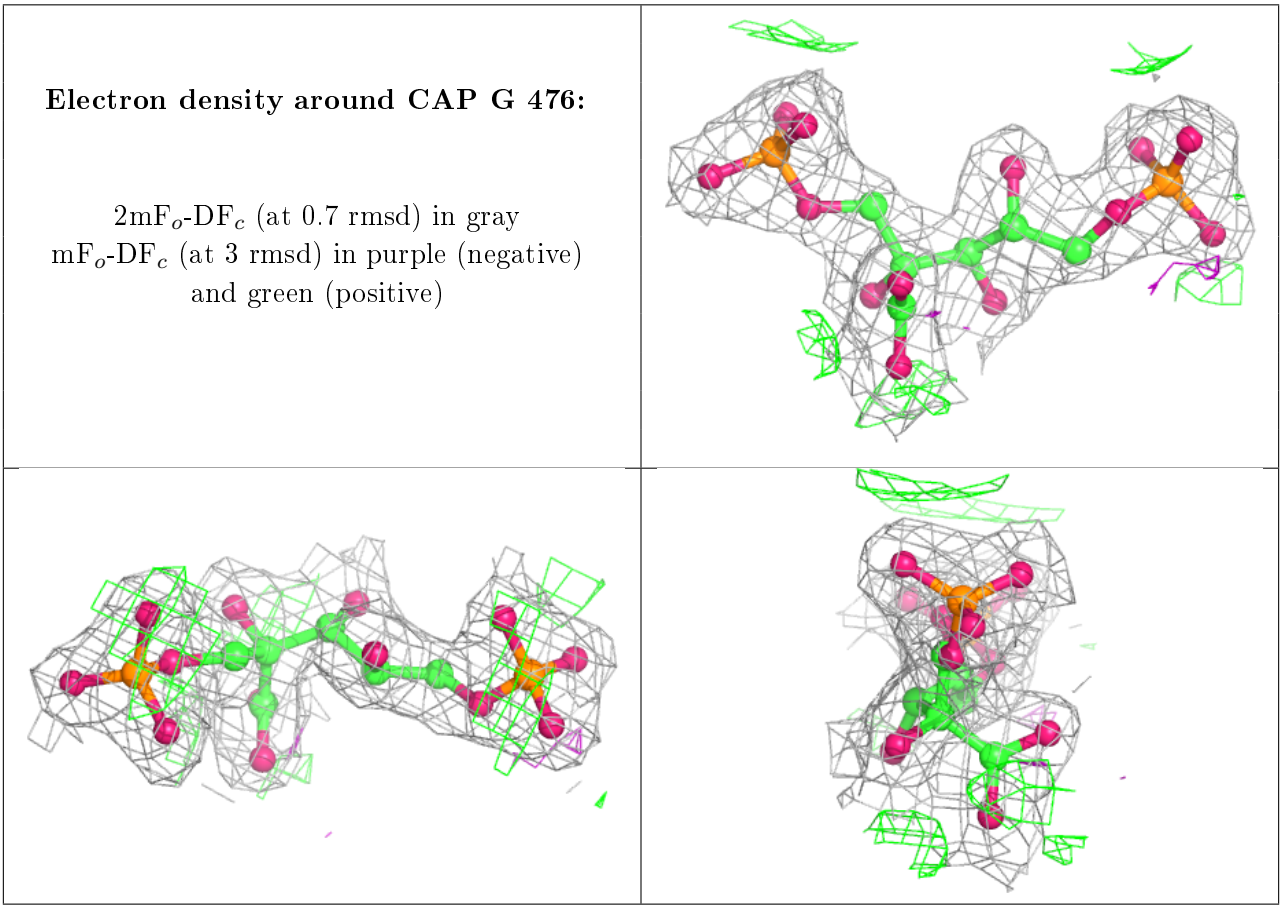
Electron density around CAP A 476:

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



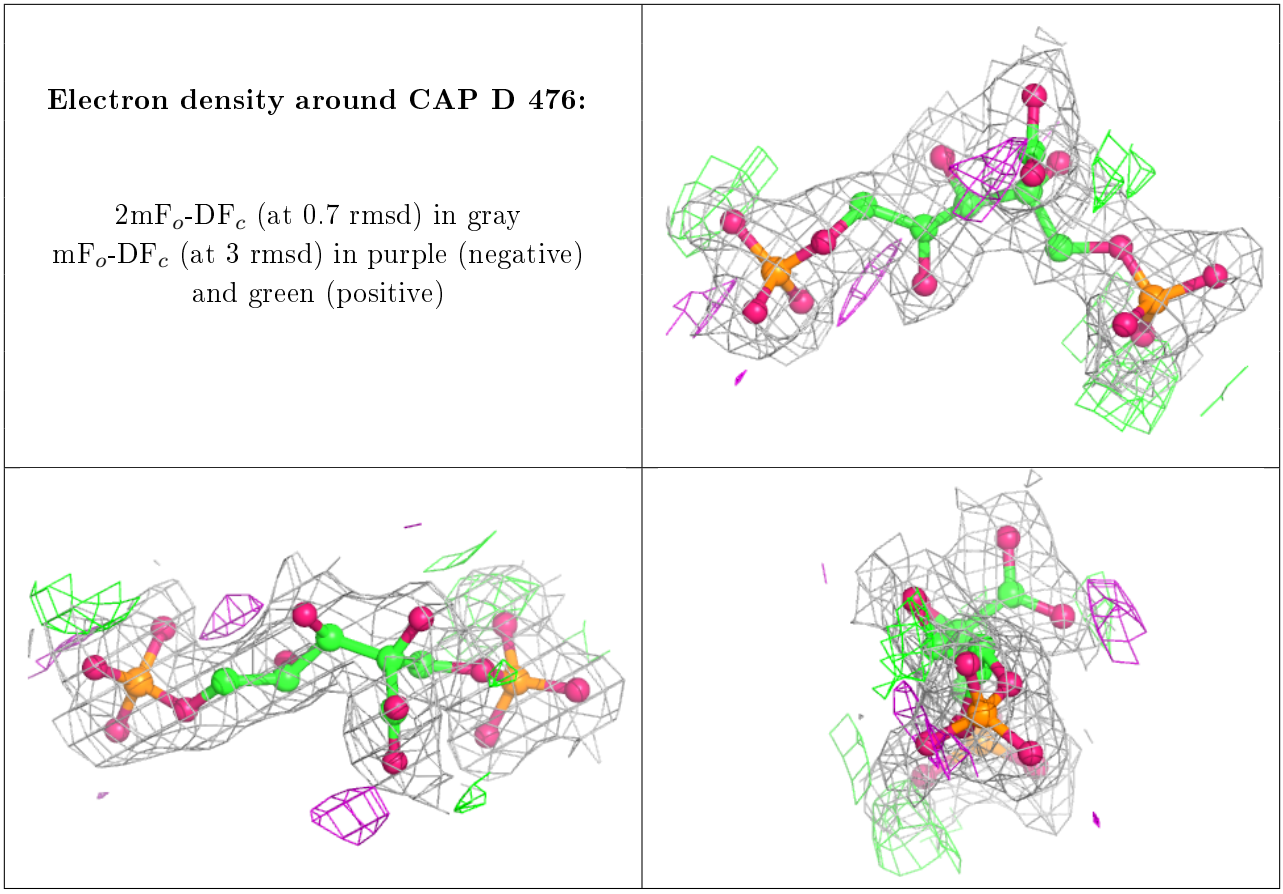
Electron density around CAP G 476:

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



Electron density around CAP D 476:

$2mF_o$-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

There are no such residues in this entry.