WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 10, 2023 – 09:27 PM EDT

PDB ID	:	4K3N
Title	:	Phosphonic Arginine Mimetics as Inhibitors of the M17 Aminopeptidases from Plasmodium falciparum
Authors	:	McGowan, S.
Deposited on	:	2013-04-11
Resolution	:	2.00 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

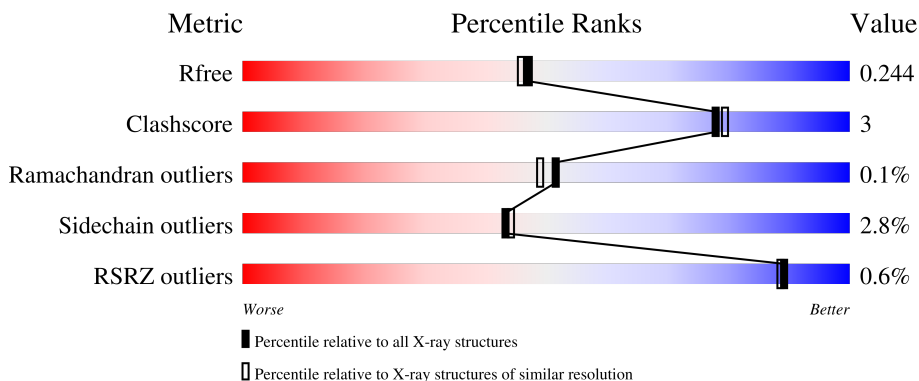|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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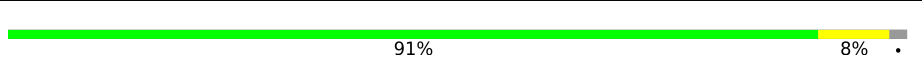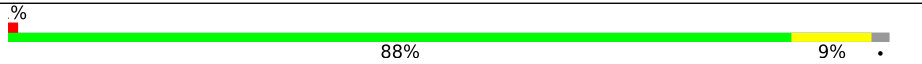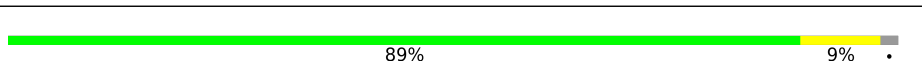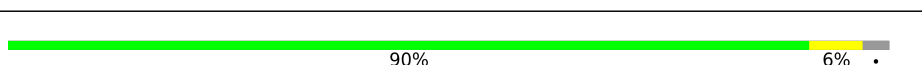*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		2.8%
RSRZ outliers		0.6%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	528	91% 8% •
1	B	528	.% 88% 9% •
1	C	528	89% 9% •
1	D	528	.% 89% 8% •
1	E	528	90% 6% •

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Mol	Chain	Length	Quality of chain
1	F	528	88% ... 8%
1	G	528	91% ... 7%
1	H	528	89% ... 8%
1	I	528	91% ... 7%
1	J	528	91% ... 6%
1	K	528	91% ... 5%
1	L	528	90% ... 7%

2   Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 49847 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 M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total 3995	C 2564	N 642	O 769	S 20	0	1	0
1	B	518	Total 3939	C 2529	N 638	O 752	S 20	0	0	0
1	C	518	Total 3960	C 2547	N 639	O 754	S 20	0	1	0
1	D	514	Total 3947	C 2539	N 635	O 753	S 20	0	0	0
1	E	510	Total 3905	C 2513	N 626	O 747	S 19	0	0	0
1	F	511	Total 3849	C 2472	N 624	O 734	S 19	0	0	0
1	G	519	Total 3993	C 2562	N 642	O 770	S 19	0	0	0
1	H	516	Total 3914	C 2513	N 632	O 750	S 19	0	0	0
1	I	518	Total 3964	C 2549	N 638	O 757	S 20	0	0	0
1	J	513	Total 3939	C 2536	N 636	O 747	S 20	0	0	0
1	K	509	Total 3906	C 2515	N 625	O 747	S 19	0	0	0
1	L	513	Total 3885	C 2494	N 628	O 744	S 19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	152	GLN	ASN	engineered mutation	UNP Q8IL11
A	515	GLN	ASN	engineered mutation	UNP Q8IL11
A	546	GLN	ASN	engineered mutation	UNP Q8IL11
A	606	HIS	-	expression tag	UNP Q8IL11
A	607	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
A	608	HIS	-	expression tag	UNP Q8IL11
A	609	HIS	-	expression tag	UNP Q8IL11
A	610	HIS	-	expression tag	UNP Q8IL11
A	611	HIS	-	expression tag	UNP Q8IL11
B	152	GLN	ASN	engineered mutation	UNP Q8IL11
B	515	GLN	ASN	engineered mutation	UNP Q8IL11
B	546	GLN	ASN	engineered mutation	UNP Q8IL11
B	606	HIS	-	expression tag	UNP Q8IL11
B	607	HIS	-	expression tag	UNP Q8IL11
B	608	HIS	-	expression tag	UNP Q8IL11
B	609	HIS	-	expression tag	UNP Q8IL11
B	610	HIS	-	expression tag	UNP Q8IL11
B	611	HIS	-	expression tag	UNP Q8IL11
C	152	GLN	ASN	engineered mutation	UNP Q8IL11
C	515	GLN	ASN	engineered mutation	UNP Q8IL11
C	546	GLN	ASN	engineered mutation	UNP Q8IL11
C	606	HIS	-	expression tag	UNP Q8IL11
C	607	HIS	-	expression tag	UNP Q8IL11
C	608	HIS	-	expression tag	UNP Q8IL11
C	609	HIS	-	expression tag	UNP Q8IL11
C	610	HIS	-	expression tag	UNP Q8IL11
C	611	HIS	-	expression tag	UNP Q8IL11
D	152	GLN	ASN	engineered mutation	UNP Q8IL11
D	515	GLN	ASN	engineered mutation	UNP Q8IL11
D	546	GLN	ASN	engineered mutation	UNP Q8IL11
D	606	HIS	-	expression tag	UNP Q8IL11
D	607	HIS	-	expression tag	UNP Q8IL11
D	608	HIS	-	expression tag	UNP Q8IL11
D	609	HIS	-	expression tag	UNP Q8IL11
D	610	HIS	-	expression tag	UNP Q8IL11
D	611	HIS	-	expression tag	UNP Q8IL11
E	152	GLN	ASN	engineered mutation	UNP Q8IL11
E	515	GLN	ASN	engineered mutation	UNP Q8IL11
E	546	GLN	ASN	engineered mutation	UNP Q8IL11
E	606	HIS	-	expression tag	UNP Q8IL11
E	607	HIS	-	expression tag	UNP Q8IL11
E	608	HIS	-	expression tag	UNP Q8IL11
E	609	HIS	-	expression tag	UNP Q8IL11
E	610	HIS	-	expression tag	UNP Q8IL11
E	611	HIS	-	expression tag	UNP Q8IL11
F	152	GLN	ASN	engineered mutation	UNP Q8IL11
F	515	GLN	ASN	engineered mutation	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP Q8IL11
G	152	GLN	ASN	engineered mutation	UNP Q8IL11
G	515	GLN	ASN	engineered mutation	UNP Q8IL11
G	546	GLN	ASN	engineered mutation	UNP Q8IL11
G	606	HIS	-	expression tag	UNP Q8IL11
G	607	HIS	-	expression tag	UNP Q8IL11
G	608	HIS	-	expression tag	UNP Q8IL11
G	609	HIS	-	expression tag	UNP Q8IL11
G	610	HIS	-	expression tag	UNP Q8IL11
G	611	HIS	-	expression tag	UNP Q8IL11
H	152	GLN	ASN	engineered mutation	UNP Q8IL11
H	515	GLN	ASN	engineered mutation	UNP Q8IL11
H	546	GLN	ASN	engineered mutation	UNP Q8IL11
H	606	HIS	-	expression tag	UNP Q8IL11
H	607	HIS	-	expression tag	UNP Q8IL11
H	608	HIS	-	expression tag	UNP Q8IL11
H	609	HIS	-	expression tag	UNP Q8IL11
H	610	HIS	-	expression tag	UNP Q8IL11
H	611	HIS	-	expression tag	UNP Q8IL11
I	152	GLN	ASN	engineered mutation	UNP Q8IL11
I	515	GLN	ASN	engineered mutation	UNP Q8IL11
I	546	GLN	ASN	engineered mutation	UNP Q8IL11
I	606	HIS	-	expression tag	UNP Q8IL11
I	607	HIS	-	expression tag	UNP Q8IL11
I	608	HIS	-	expression tag	UNP Q8IL11
I	609	HIS	-	expression tag	UNP Q8IL11
I	610	HIS	-	expression tag	UNP Q8IL11
I	611	HIS	-	expression tag	UNP Q8IL11
J	152	GLN	ASN	engineered mutation	UNP Q8IL11
J	515	GLN	ASN	engineered mutation	UNP Q8IL11
J	546	GLN	ASN	engineered mutation	UNP Q8IL11
J	606	HIS	-	expression tag	UNP Q8IL11
J	607	HIS	-	expression tag	UNP Q8IL11
J	608	HIS	-	expression tag	UNP Q8IL11
J	609	HIS	-	expression tag	UNP Q8IL11
J	610	HIS	-	expression tag	UNP Q8IL11

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Chain	Residue	Modelled	Actual	Comment	Reference
J	611	HIS	-	expression tag	UNP Q8IL11
K	152	GLN	ASN	engineered mutation	UNP Q8IL11
K	515	GLN	ASN	engineered mutation	UNP Q8IL11
K	546	GLN	ASN	engineered mutation	UNP Q8IL11
K	606	HIS	-	expression tag	UNP Q8IL11
K	607	HIS	-	expression tag	UNP Q8IL11
K	608	HIS	-	expression tag	UNP Q8IL11
K	609	HIS	-	expression tag	UNP Q8IL11
K	610	HIS	-	expression tag	UNP Q8IL11
K	611	HIS	-	expression tag	UNP Q8IL11
L	152	GLN	ASN	engineered mutation	UNP Q8IL11
L	515	GLN	ASN	engineered mutation	UNP Q8IL11
L	546	GLN	ASN	engineered mutation	UNP Q8IL11
L	606	HIS	-	expression tag	UNP Q8IL11
L	607	HIS	-	expression tag	UNP Q8IL11
L	608	HIS	-	expression tag	UNP Q8IL11
L	609	HIS	-	expression tag	UNP Q8IL11
L	610	HIS	-	expression tag	UNP Q8IL11
L	611	HIS	-	expression tag	UNP Q8IL11

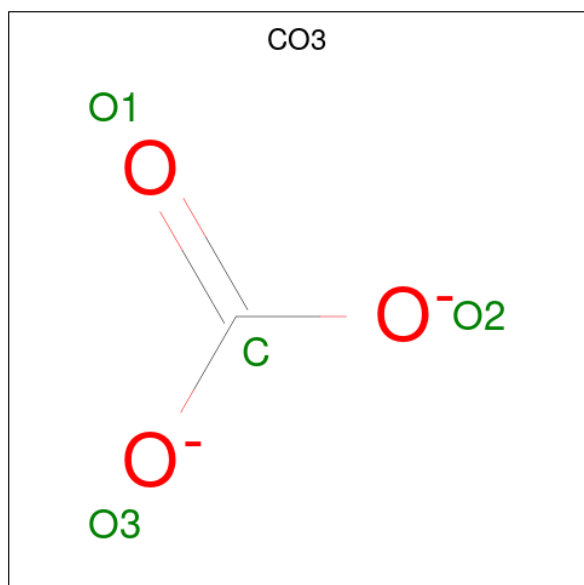- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	K	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0
3	B	1	Total 4	C 1	O 3	0	0
3	C	1	Total 4	C 1	O 3	0	0
3	D	1	Total 4	C 1	O 3	0	0
3	E	1	Total 4	C 1	O 3	0	0
3	F	1	Total 4	C 1	O 3	0	0
3	G	1	Total 4	C 1	O 3	0	0
3	H	1	Total 4	C 1	O 3	0	0
3	I	1	Total 4	C 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	J	1	Total 4	C 1	O 3	0	0
3	K	1	Total 4	C 1	O 3	0	0
3	L	1	Total 4	C 1	O 3	0	0

- Molecule 4 is {(R)-amino[4-(1H-pyrazol-1-yl)phenyl]methyl}phosphonic acid (three-letter code: 1OT) (formula: $C_{10}H_{12}N_3O_3P$).
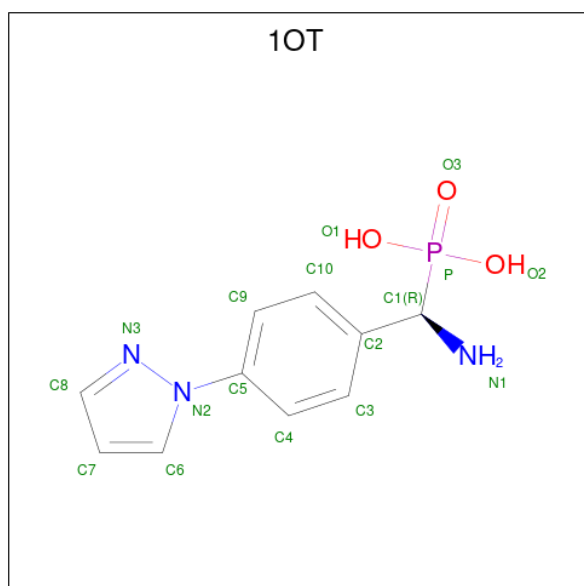
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	B	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	C	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	D	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	E	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	F	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	G	1	Total 17	C 10	N 3	O 3	P 1	0	0
4	H	1	Total 17	C 10	N 3	O 3	P 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	I	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	J	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	K	1	Total	C	N	O	P	0	0
			17	10	3	3	1		
4	L	1	Total	C	N	O	P	0	0
			17	10	3	3	1		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
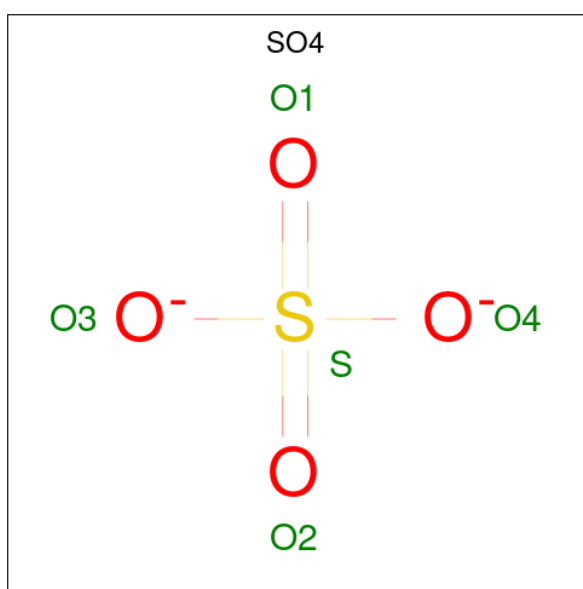
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	G	1	Total 5	O 4	S 1	0	0
5	G	1	Total 5	O 4	S 1	0	0
5	G	1	Total 5	O 4	S 1	0	0
5	H	1	Total 5	O 4	S 1	0	0
5	I	1	Total 5	O 4	S 1	0	0
5	I	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0
5	K	1	Total 5	O 4	S 1	0	0
5	K	1	Total 5	O 4	S 1	0	0
5	L	1	Total 5	O 4	S 1	0	0

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

1PE

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 9	C 6	O 3	0	0
6	A	1	Total 12	C 8	O 4	0	0
6	C	1	Total 13	C 9	O 4	0	0
6	C	1	Total 9	C 6	O 3	0	0
6	C	1	Total 7	C 5	O 2	0	0
6	D	1	Total 10	C 7	O 3	0	0
6	D	1	Total 9	C 6	O 3	0	0
6	D	1	Total 11	C 8	O 3	0	0
6	E	1	Total 12	C 8	O 4	0	0
6	E	1	Total 12	C 8	O 4	0	0
6	E	1	Total 8	C 5	O 3	0	0
6	F	1	Total 10	C 6	O 4	0	0
6	F	1	Total 10	C 6	O 4	0	0
6	F	1	Total 10	C 6	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total 11	C 7	O 4	0	0
6	G	1	Total 9	C 6	O 3	0	0
6	G	1	Total 6	C 4	O 2	0	0
6	G	1	Total 6	C 4	O 2	0	0
6	G	1	Total 15	C 10	O 5	0	0
6	I	1	Total 15	C 10	O 5	0	0
6	I	1	Total 11	C 8	O 3	0	0
6	I	1	Total 5	C 3	O 2	0	0
6	J	1	Total 11	C 7	O 4	0	0
6	J	1	Total 10	C 6	O 4	0	0
6	J	1	Total 11	C 8	O 3	0	0
6	J	1	Total 9	C 6	O 3	0	0
6	K	1	Total 12	C 8	O 4	0	0
6	K	1	Total 12	C 8	O 4	0	0
6	K	1	Total 11	C 7	O 4	0	0
6	K	1	Total 6	C 4	O 2	0	0
6	L	1	Total 10	C 6	O 4	0	0
6	L	1	Total 12	C 8	O 4	0	0
6	L	1	Total 8	C 5	O 3	0	0
6	L	1	Total 11	C 7	O 4	0	0

- Molecule 7 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula: $C_{18}H_{38}O_{10}$).

2PE
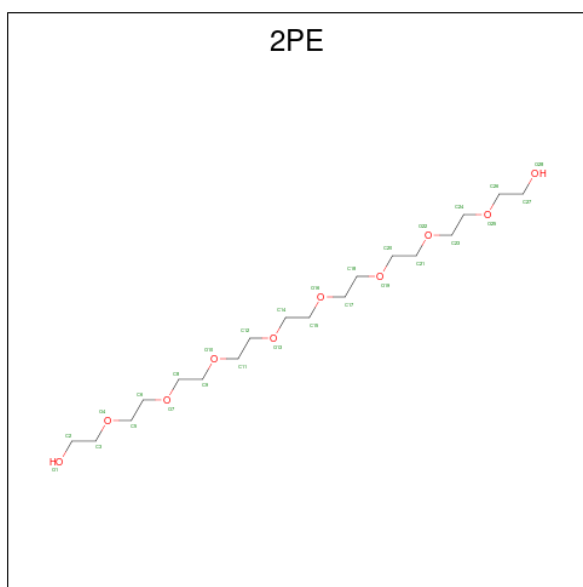
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total 26	C 17	O 9	0	0
7	B	1	Total 10	C 6	O 4	0	0
7	C	1	Total 9	C 6	O 3	0	0
7	D	1	Total 13	C 9	O 4	0	0
7	D	1	Total 5	C 3	O 2	0	0
7	D	1	Total 9	C 6	O 3	0	0
7	E	1	Total 9	C 6	O 3	0	0
7	F	1	Total 9	C 6	O 3	0	0
7	H	1	Total 25	C 16	O 9	0	0
7	H	1	Total 10	C 7	O 3	0	0
7	I	1	Total 8	C 5	O 3	0	0
7	J	1	Total 10	C 7	O 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	173	Total 173	O 173	0	0
8	B	125	Total 125	O 125	0	0
8	C	168	Total 168	O 168	0	0
8	D	150	Total 150	O 150	0	0
8	E	193	Total 193	O 193	0	0
8	F	117	Total 117	O 117	0	0
8	G	145	Total 145	O 145	0	0
8	H	129	Total 129	O 129	0	0
8	I	146	Total 146	O 146	0	0
8	J	137	Total 137	O 137	0	0
8	K	175	Total 175	O 175	0	0
8	L	126	Total 126	O 126	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.
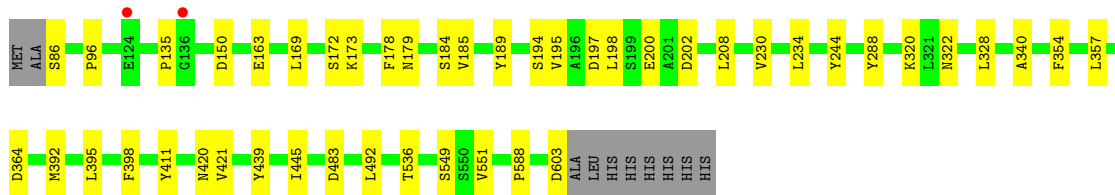
• Molecule 1: M17 leucyl aminopeptidase

Chain A:
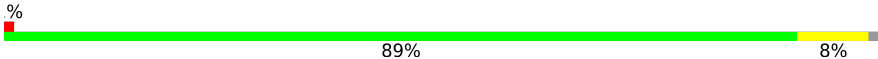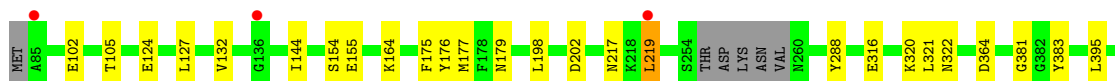

• Molecule 1: M17 leucyl aminopeptidase

Chain B:

• Molecule 1: M17 leucyl aminopeptidase

Chain C:

• Molecule 1: M17 leucyl aminopeptidase

Chain D:

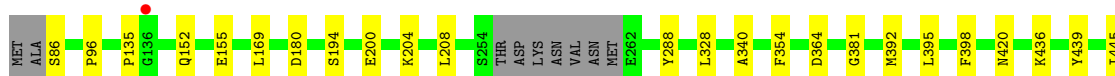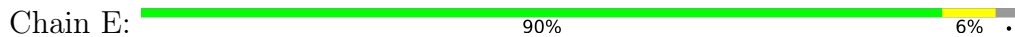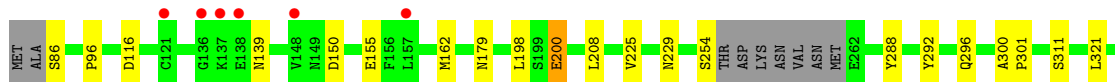F398 Y411 N420 S438 Y439 K451 D459 L492 L514 K518 Y533 T536 D543 K552 E564 W581 T597 L601 N602 D603 ALA LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain E:

90% 6% ·

MET ALA S86 P96 P135 G136 Q152 E155 L169 D180 S194 E200 K204 L208 S254 THR ASP LYS ASN VAL ASN MET E262 Y288 L328 A340 F354 D364 G381 M392 L395 F398 N420 K436 Y439 I445

K451 D459 L492 K518 T536 D543 S550 V551 V579 K589 N602 ASP ALA LEU HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain F:

%

88% 8% ·

MET ALA S86 P96 D116 C121 G136 K137 E138 N139 V148 N149 D150 E155 F156 L157 M162 N179 L198 S199 E200 L208 V225 N229 S254 THR ASP LYS ASN VAL ASN MET E262 Y288 Y292 Q296 A300 P301 S311 L321

I327 L328 A340 Y341 F354 K360 S361 D364 K386 M392 L395 F398 Y411 A428 Y439 I445 K451 Y480 L492 K512 I513 L514 Y533 T536 Q546 D603 ALA LEU HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain G:

91% 7% ··

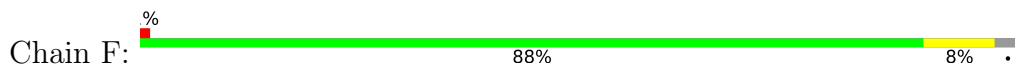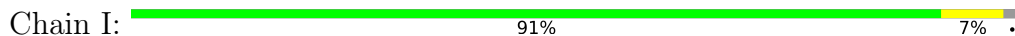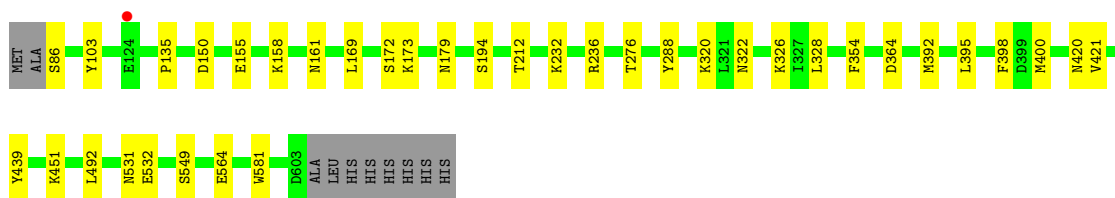MET A85 Y103 I117 C121 D150 K164 F165 L169 F178 N179 E200 K204 L208 L214 L222 Y270 Y288 E316 K320 L321 K326 I327 L328 F354 L357 K367 K386 M392 L395 F398 Y411 F425

K436 Y439 Y480 T488 L492 S555 Q567 P588 D603 ALA LEU HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain H:

89% 8% ··

MET ALA S86 N104 I117 N122 E125 P135 G136 K137 E138 S146 D150 S154 K164 F165 K173 H174 N181 Y189 S194 E200 A201 D202 R205 L208 H215 S254 T255 N258 VAL ASN M261 Y288 K320 L321 L328

K331 E335 A340 F354 L357 D364 F398 Y411 N420 V421 Y439 I445 T488 L492 S555 D603 ALA LEU HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain I:

91% 7% ·

MET ALA S86 Y103 E124 P135 D150 E155 K158 N161 L169 S172 K173 N179 S194 T212 K232 R236 T276 Y288 K320 L321 N322 K326 I327 L328 F354 D364 M392 L395 F398 D399 M400 N420 V421
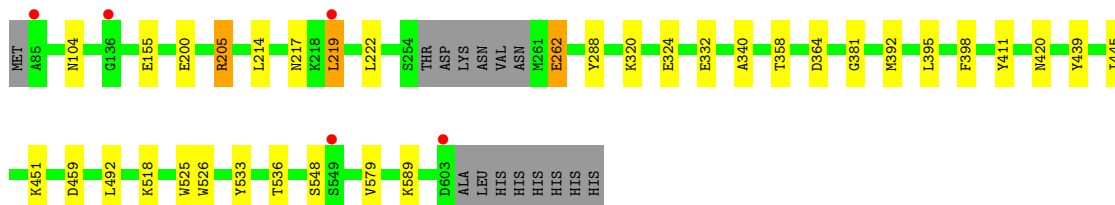
Y439 K451 L492 N531 E532 S549 E564 W581 D603 ALA LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain J:

91% 6%

MET A85 N104 G136 E155 E200 R205 L214 N217 K218 L219 L222 S254 THR ASP LYS ASN VAL ASN M261 E262 Y288 K320 E324 E332 A340 T358 D364 G381 M392 L395 F398 Y411 N420 Y439 I445
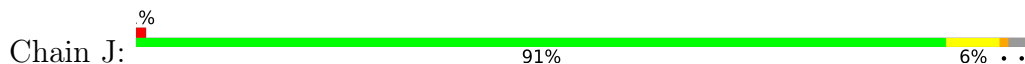
K451 D459 L492 K518 W525 W526 Y533 T536 S548 S549 V579 K589 D603 ALA LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain K:

91% 5%

MET ALA S86 P96 E102 T105 I117 V132 P135 GLY K137 S145 K164 L169 S172 K173 H174 M213 D216 S254 THR ASP LYS ASN VAL ASN MET E262 Y270 Y288 E316 K320 L328 A340 F354 G363 D364 F398

N420 Y439 I445 L492 L514 K518 S550 N602 ASP ALA LEU HIS HIS HIS HIS HIS HIS

• Molecule 1: M17 leucyl aminopeptidase

Chain L:

90% 7%

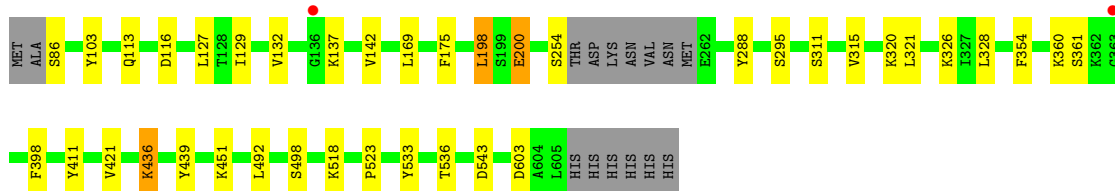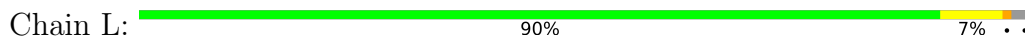MET ALA S86 Y103 Q113 D116 L127 T128 I129 V132 G136 K137 V142 L169 F175 L198 S199 E200 S254 THR ASP LYS ASN VAL ASN MET E262 Y288 S295 S311 V315 K320 L321 K326 I327 L328 F354 K360 S361 K362 G363

F398 Y411 V421 K436 Y439 K451 L492 S498 K518 P523 Y533 T536 D543 D603 A604 L605 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.72Å 177.08Å 229.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.11 – 2.00 62.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (45.11-2.00) 99.9 (62.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.196 , 0.240 0.205 , 0.244	Depositor DCC
R_{free} test set	23744 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 51.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49847	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 43.71 % 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 1.6963e-04. 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 1OT, ZN, SO4, CO3, 1PE, 2PE

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	0.37	0/4075	0.53	1/5525 (0.0%)
1	B	0.35	0/4017	0.53	0/5455
1	C	0.37	0/4041	0.53	0/5483
1	D	0.36	0/4024	0.53	0/5455
1	E	0.37	0/3982	0.53	0/5403
1	F	0.35	0/3925	0.53	1/5336 (0.0%)
1	G	0.39	0/4071	0.53	0/5521
1	H	0.35	0/3991	0.53	0/5422
1	I	0.36	0/4042	0.52	0/5484
1	J	0.36	0/4016	0.53	0/5443
1	K	0.37	0/3982	0.53	0/5400
1	L	0.37	0/3962	0.52	0/5384
All	All	0.37	0/48128	0.53	2/65311 (0.0%)

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	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	156	PHE	CG-CD1-CE1	5.96	127.35	120.80
1	F	139	ASN	N-CA-C	5.81	126.68	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	257	LYS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3995	0	3929	20	0
1	B	3939	0	3835	21	0
1	C	3960	0	3890	18	0
1	D	3947	0	3887	37	0
1	E	3905	0	3830	20	0
1	F	3849	0	3722	24	0
1	G	3993	0	3922	26	0
1	H	3914	0	3793	18	0
1	I	3964	0	3897	20	0
1	J	3939	0	3892	27	0
1	K	3906	0	3837	16	0
1	L	3885	0	3760	24	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	1	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	1	0
4	A	17	0	10	3	0
4	B	17	0	11	4	0
4	C	17	0	11	2	0
4	D	17	0	12	2	0
4	E	17	0	11	4	0
4	F	17	0	12	3	0
4	G	17	0	10	3	0
4	H	17	0	12	2	0
4	I	17	0	12	2	0
4	J	17	0	11	2	0
4	K	17	0	12	3	0
4	L	17	0	11	4	0
5	A	20	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	10	0	0	0	0
5	E	10	0	0	0	0
5	F	5	0	0	0	0
5	G	15	0	0	0	0
5	H	5	0	0	0	0
5	I	10	0	0	0	0
5	J	5	0	0	1	0
5	K	10	0	0	0	0
5	L	5	0	0	0	0
6	A	21	0	22	1	0
6	C	29	0	30	2	0
6	D	30	0	30	7	0
6	E	32	0	36	3	0
6	F	41	0	51	2	0
6	G	36	0	39	8	0
6	I	31	0	35	3	0
6	J	41	0	48	8	0
6	K	41	0	44	3	0
6	L	41	0	48	9	0
7	B	36	0	45	0	0
7	C	9	0	10	2	0
7	D	27	0	28	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	E	9	0	10	1	0
7	F	9	0	10	1	0
7	H	35	0	43	2	0
7	I	8	0	8	0	0
7	J	10	0	10	0	0
8	A	173	0	0	0	0
8	B	125	0	0	0	0
8	C	168	0	0	1	0
8	D	150	0	0	5	0
8	E	193	0	0	0	0
8	F	117	0	0	2	0
8	G	145	0	0	0	0
8	H	129	0	0	1	0
8	I	146	0	0	3	0
8	J	137	0	0	3	0
8	K	175	0	0	3	0
8	L	126	0	0	2	0
All	All	49847	0	46876	275	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 3.

All (275) 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:I:155:GLU:O	8:I:1103:HOH:O	1.97	0.82
1:I:161:ASN:ND2	8:I:1103:HOH:O	2.17	0.77
1:J:526:TRP:HB3	6:J:1009:1PE:H242	1.67	0.76
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.53	0.73
1:J:536:THR:OG1	8:J:1221:HOH:O	2.06	0.73
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.54	0.72
1:J:411:TYR:HE1	6:J:1006:1PE:H151	1.54	0.71
1:J:525:TRP:HA	6:J:1009:1PE:H132	1.70	0.71
1:J:392:MET:HE3	1:J:395:LEU:HD22	1.73	0.71
1:K:316:GLU:HG3	6:K:1007:1PE:H152	1.73	0.70
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.72	0.69
1:J:320:LYS:HB3	6:J:1006:1PE:H161	1.74	0.69
1:H:320:LYS:HB3	7:H:1006:2PE:H211	1.75	0.69
1:D:320:LYS:HZ1	7:D:1010:2PE:H121	1.59	0.67
1:J:533:TYR:O	1:J:536:THR:HG22	1.96	0.66
1:B:236:ARG:NE	1:B:240:GLU:OE2	2.21	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:GLN:HA	1:G:567:GLN:OE1	1.95	0.65
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.79	0.64
1:F:546:GLN:O	8:F:1209:HOH:O	2.15	0.64
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.62	0.62
1:G:316:GLU:HG3	6:G:1011:1PE:H231	1.80	0.62
1:J:411:TYR:CE1	6:J:1006:1PE:H151	2.32	0.62
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.81	0.62
1:D:320:LYS:HZ3	7:D:1010:2PE:H201	1.63	0.62
1:A:156:PHE:CD2	1:A:156:PHE:CZ	2.86	0.61
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.80	0.61
1:E:543:ASP:HB3	6:E:1009:1PE:H232	1.81	0.61
1:D:533:TYR:O	1:D:536:THR:HG22	2.01	0.61
1:B:230:VAL:HG12	1:B:234:LEU:HD23	1.84	0.60
1:A:366:LYS:HG2	1:A:420:ASN:HB3	1.84	0.60
1:J:451:LYS:HE3	6:J:1008:1PE:H261	1.82	0.60
1:L:492:LEU:HD11	4:L:1004:1OT:C7	2.33	0.59
1:F:321:LEU:HD11	1:F:411:TYR:HA	1.84	0.59
1:D:124:GLU:HA	1:D:179:ASN:HD22	1.67	0.59
1:G:214:LEU:HD21	1:G:222:LEU:HD22	1.84	0.59
1:G:411:TYR:HE1	6:G:1008:1PE:H132	1.68	0.59
1:D:411:TYR:HE1	6:D:1007:1PE:H232	1.68	0.59
1:L:320:LYS:NZ	6:L:1009:1PE:H252	2.18	0.58
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.85	0.58
1:D:492:LEU:HD11	4:D:1004:1OT:C7	2.34	0.58
1:L:320:LYS:HE2	6:L:1009:1PE:H141	1.86	0.58
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.86	0.58
1:F:514:LEU:HD22	6:F:1009:1PE:H142	1.85	0.58
1:A:392:MET:HE3	1:A:395:LEU:HD22	1.86	0.57
1:H:331:LYS:O	1:H:335:GLU:HG3	2.02	0.57
1:F:533:TYR:O	1:F:536:THR:HG22	2.04	0.57
1:A:173:LYS:NZ	1:D:217:ASN:OD1	2.36	0.57
1:B:538:ASN:O	1:B:545:ASN:ND2	2.38	0.57
1:E:451:LYS:HG2	6:E:1009:1PE:H231	1.85	0.57
1:F:451:LYS:HG2	6:F:1008:1PE:H141	1.87	0.57
1:L:320:LYS:HZ1	6:L:1009:1PE:H252	1.69	0.57
1:B:492:LEU:HD11	4:B:1004:1OT:H12	1.87	0.57
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.85	0.56
1:E:381:GLY:HA2	1:E:459:ASP:OD1	2.06	0.56
1:L:533:TYR:O	1:L:536:THR:HG22	2.05	0.56
1:B:492:LEU:HD11	4:B:1004:1OT:C7	2.35	0.56
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:320:LYS:NZ	7:D:1010:2PE:H121	2.21	0.55
1:E:492:LEU:HD11	4:E:1004:1OT:C7	2.35	0.55
1:K:96:PRO:HA	6:K:1010:1PE:H141	1.87	0.55
1:F:96:PRO:HA	7:F:1010:2PE:H111	1.88	0.55
1:H:492:LEU:HD11	4:H:1004:1OT:H12	1.88	0.55
1:C:172:SER:O	1:C:173:LYS:HD2	2.06	0.55
1:K:492:LEU:HD11	4:K:1004:1OT:H12	1.89	0.55
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.87	0.55
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.86	0.55
1:K:174:HIS:HB3	1:K:213:MET:HE2	1.88	0.55
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.87	0.55
1:F:392:MET:HE3	1:F:395:LEU:HD22	1.89	0.55
1:G:392:MET:HE3	1:G:395:LEU:HD22	1.89	0.55
1:B:392:MET:HE3	1:B:395:LEU:HD22	1.89	0.55
1:L:436:LYS:NZ	8:L:1226:HOH:O	2.17	0.55
1:D:451:LYS:NZ	6:D:1009:1PE:H242	2.22	0.54
1:K:492:LEU:HD11	4:K:1004:1OT:C7	2.38	0.54
1:A:178:PHE:CZ	1:D:155:GLU:HG2	2.39	0.54
1:G:320:LYS:HZ2	6:G:1011:1PE:H251	1.72	0.54
1:E:96:PRO:HA	7:E:1010:2PE:H182	1.90	0.54
1:G:492:LEU:HD11	4:G:1004:1OT:H12	1.90	0.54
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.90	0.54
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.90	0.53
1:A:176:TYR:HB3	8:D:1131:HOH:O	2.08	0.53
1:K:320:LYS:HD3	6:K:1007:1PE:H222	1.91	0.53
1:D:164:LYS:HE2	8:D:1240:HOH:O	2.08	0.53
1:G:326:LYS:HG2	1:G:328:LEU:HD12	1.91	0.53
1:I:392:MET:HE3	1:I:395:LEU:HD22	1.90	0.53
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.90	0.52
1:J:217:ASN:HB2	1:J:219:LEU:HD21	1.90	0.52
1:L:326:LYS:HE3	1:L:328:LEU:HD11	1.90	0.52
1:B:178:PHE:HZ	1:F:155:GLU:HG2	1.75	0.52
1:B:135:PRO:HA	1:B:194:SER:O	2.08	0.52
1:D:514:LEU:O	1:D:518:LYS:HG2	2.09	0.52
1:D:543:ASP:HB3	6:D:1009:1PE:H132	1.90	0.52
4:H:1004:1OT:H10	4:H:1004:1OT:O2	2.10	0.52
1:D:217:ASN:HB3	1:D:219:LEU:HD21	1.92	0.52
1:B:172:SER:O	1:B:173:LYS:HD2	2.10	0.51
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.92	0.51
1:J:492:LEU:HD11	4:J:1004:1OT:C7	2.40	0.51
1:D:175:PHE:HB3	8:D:1131:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.40	0.51
1:A:150:ASP:OD1	1:A:179:ASN:HB2	2.10	0.51
1:G:117:ILE:HG13	1:G:270:TYR:HB3	1.92	0.51
1:I:150:ASP:OD1	1:I:179:ASN:HB2	2.10	0.51
1:J:324:GLU:CG	1:J:358:THR:HB	2.41	0.51
1:L:103:TYR:HB2	6:L:1009:1PE:H161	1.93	0.50
1:A:321:LEU:HD11	1:A:411:TYR:HA	1.94	0.50
1:E:536:THR:HG21	1:E:551:VAL:HG23	1.94	0.50
1:G:320:LYS:NZ	6:G:1011:1PE:H251	2.26	0.50
1:H:254:SER:OG	1:H:255:THR:N	2.44	0.49
1:E:200:GLU:O	1:E:204:LYS:HG3	2.12	0.49
1:A:492:LEU:HD11	4:A:1004:1OT:H12	1.93	0.49
1:C:411:TYR:HE1	6:C:1007:1PE:H231	1.76	0.49
1:I:395:LEU:HD11	1:I:581:TRP:CG	2.48	0.49
1:J:104:ASN:N	5:J:1005:SO4:O2	2.40	0.49
1:D:217:ASN:HB2	1:D:219:LEU:HD11	1.95	0.49
1:C:364:ASP:O	1:C:420:ASN:HA	2.12	0.49
1:F:200:GLU:HG3	8:F:1122:HOH:O	2.13	0.49
1:G:178:PHE:CZ	1:J:155:GLU:HG2	2.42	0.49
1:J:548:SER:OG	8:J:1221:HOH:O	2.19	0.48
1:H:173:LYS:HB2	1:H:189:TYR:CE1	2.48	0.48
1:B:364:ASP:O	1:B:420:ASN:HA	2.13	0.48
1:C:392:MET:HE3	1:C:395:LEU:HD22	1.94	0.48
1:K:164:LYS:NZ	8:K:1188:HOH:O	2.46	0.48
1:H:364:ASP:O	1:H:420:ASN:HA	2.13	0.48
1:L:492:LEU:HD11	4:L:1004:1OT:H12	1.96	0.48
1:G:320:LYS:HD3	6:G:1011:1PE:H162	1.94	0.48
1:I:451:LYS:HE3	1:I:564:GLU:O	2.14	0.48
1:I:135:PRO:HA	1:I:194:SER:O	2.14	0.48
1:I:232:LYS:NZ	1:I:276:THR:O	2.46	0.48
1:G:121:CYS:HA	1:G:270:TYR:CE2	2.49	0.47
1:G:320:LYS:HZ2	6:G:1011:1PE:H161	1.79	0.47
1:A:316:GLU:HG3	6:A:1010:1PE:H131	1.95	0.47
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.95	0.47
4:B:1004:1OT:H10	4:B:1004:1OT:O2	2.14	0.47
1:J:364:ASP:O	1:J:420:ASN:HA	2.15	0.47
1:H:202:ASP:OD1	1:H:205:ARG:NH1	2.48	0.47
1:K:102:GLU:HG3	8:K:1272:HOH:O	2.15	0.47
1:L:543:ASP:HB3	6:L:1007:1PE:H221	1.96	0.47
1:F:492:LEU:HD11	4:F:1004:1OT:H12	1.96	0.47
1:G:103:TYR:CD1	6:G:1011:1PE:H252	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:367:LYS:HD3	1:G:480:TYR:CE2	2.50	0.47
1:H:104:ASN:HB3	8:H:1207:HOH:O	2.14	0.47
1:I:531:ASN:HB2	6:I:1009:1PE:H241	1.94	0.47
4:J:1004:1OT:H10	4:J:1004:1OT:O2	2.14	0.47
4:E:1004:1OT:H10	4:E:1004:1OT:O2	2.14	0.47
1:K:117:ILE:HG12	1:K:270:TYR:HB3	1.96	0.47
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.14	0.47
7:D:1012:2PE:H121	8:D:1222:HOH:O	2.15	0.47
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.97	0.46
1:D:451:LYS:HG2	6:D:1009:1PE:H251	1.97	0.46
1:A:492:LEU:HD11	4:A:1004:1OT:C7	2.45	0.46
1:L:451:LYS:HZ3	6:L:1007:1PE:H141	1.80	0.46
1:C:195:VAL:HG12	1:C:197:ASP:H	1.81	0.46
1:D:364:ASP:O	1:D:420:ASN:HA	2.15	0.46
1:E:392:MET:HE3	1:E:395:LEU:HD22	1.97	0.46
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.97	0.46
1:L:518:LYS:NZ	6:L:1008:1PE:H131	2.31	0.46
1:F:150:ASP:OD1	1:F:179:ASN:HB2	2.16	0.46
1:C:244:TYR:OH	1:C:588:PRO:O	2.32	0.46
1:C:536:THR:HG21	1:C:551:VAL:HG23	1.97	0.46
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.98	0.46
1:D:177:MET:HB3	8:D:1131:HOH:O	2.16	0.46
1:E:543:ASP:CB	6:E:1009:1PE:H232	2.45	0.46
3:D:1002:CO3:O1	4:D:1004:1OT:O3	2.33	0.45
1:I:172:SER:O	1:I:173:LYS:HD2	2.15	0.45
1:G:321:LEU:HD11	1:G:411:TYR:HA	1.97	0.45
1:F:492:LEU:HD11	4:F:1004:1OT:C7	2.46	0.45
1:J:320:LYS:NZ	6:J:1007:1PE:OH5	2.49	0.45
1:H:135:PRO:HA	1:H:194:SER:O	2.17	0.45
1:E:492:LEU:HD11	4:E:1004:1OT:H12	1.97	0.45
1:H:122:ASN:HD22	7:H:1007:2PE:H171	1.81	0.45
1:F:292:TYR:O	1:F:296:GLN:HG3	2.17	0.45
1:G:150:ASP:OD1	1:G:179:ASN:HB2	2.16	0.45
1:C:320:LYS:NZ	6:C:1006:1PE:OH6	2.50	0.45
1:C:150:ASP:OD1	1:C:179:ASN:HB2	2.17	0.44
1:D:411:TYR:CE1	6:D:1007:1PE:H232	2.51	0.44
1:L:321:LEU:HD11	1:L:411:TYR:HA	1.98	0.44
1:A:121:CYS:HA	1:A:270:TYR:CE2	2.53	0.44
1:D:451:LYS:HE3	1:D:564:GLU:O	2.17	0.44
1:K:364:ASP:O	1:K:420:ASN:HA	2.18	0.44
1:D:451:LYS:HZ2	6:D:1009:1PE:H242	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:518:LYS:HB2	1:E:518:LYS:HE2	1.56	0.44
1:G:164:LYS:HD3	1:G:165:PHE:CE1	2.52	0.44
1:I:532:GLU:HG3	1:J:205:ARG:HH22	1.82	0.44
4:K:1004:1OT:H10	4:K:1004:1OT:O1	2.18	0.44
1:H:150:ASP:O	1:H:154:SER:HB2	2.17	0.44
1:K:172:SER:HB2	1:K:213:MET:HE1	2.00	0.44
1:A:383:TYR:HE2	1:A:438:SER:HB2	1.83	0.44
1:B:173:LYS:HB2	1:B:189:TYR:CE1	2.52	0.44
1:B:287:TYR:CD2	1:B:594:ARG:HG2	2.53	0.43
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.99	0.43
1:I:103:TYR:HB3	6:I:1008:1PE:H142	2.00	0.43
1:I:320:LYS:HD3	6:I:1007:1PE:H161	2.00	0.43
1:C:135:PRO:HA	1:C:194:SER:O	2.19	0.43
1:C:492:LEU:HD11	4:C:1004:1OT:H12	2.00	0.43
4:C:1004:1OT:H10	4:C:1004:1OT:O2	2.17	0.43
1:H:117:ILE:HD11	1:H:146:SER:OG	2.18	0.43
1:L:518:LYS:HZ1	6:L:1008:1PE:H131	1.83	0.43
1:E:579:VAL:O	1:E:589:LYS:HD2	2.18	0.43
1:I:326:LYS:HE3	1:I:328:LEU:HD11	2.00	0.43
1:B:381:GLY:HA2	1:B:459:ASP:OD1	2.18	0.43
1:C:96:PRO:HA	7:C:1009:2PE:H172	2.00	0.43
1:D:127:LEU:HB2	1:D:219:LEU:HD22	1.99	0.43
1:E:536:THR:HG21	1:E:551:VAL:CG2	2.47	0.43
4:G:1004:1OT:H10	4:G:1004:1OT:O2	2.19	0.43
1:E:364:ASP:O	1:E:420:ASN:HA	2.19	0.43
1:I:492:LEU:HD11	4:I:1004:1OT:H12	2.01	0.43
1:L:360:LYS:HD2	1:L:361:SER:O	2.18	0.43
1:A:381:GLY:HA2	1:A:459:ASP:OD1	2.18	0.43
1:A:357:LEU:HB2	1:A:425:PHE:HB2	2.01	0.42
1:B:175:PHE:N	1:B:187:VAL:O	2.41	0.42
1:J:381:GLY:HA2	1:J:459:ASP:OD1	2.19	0.42
1:L:311:SER:O	1:L:315:VAL:HG23	2.19	0.42
1:D:219:LEU:H	1:D:219:LEU:HG	1.30	0.42
1:J:219:LEU:H	1:J:219:LEU:HG	1.16	0.42
1:E:392:MET:HE2	4:E:1004:1OT:C8	2.50	0.42
1:I:492:LEU:HD23	1:I:492:LEU:HA	1.82	0.42
1:D:198:LEU:HD22	1:D:202:ASP:HB3	2.02	0.42
1:L:498:SER:O	1:L:523:PRO:HG2	2.19	0.42
1:D:321:LEU:HD11	1:D:411:TYR:HA	2.01	0.42
1:D:383:TYR:HE2	1:D:438:SER:HB2	1.85	0.42
1:F:386:LYS:NZ	4:F:1004:1OT:O2	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:1004:1OT:O2	4:I:1004:1OT:H10	2.20	0.42
1:C:173:LYS:HB2	1:C:189:TYR:CE1	2.55	0.42
1:D:176:TYR:OH	1:D:217:ASN:OD1	2.20	0.42
1:D:381:GLY:HA2	1:D:459:ASP:OD1	2.20	0.42
1:F:360:LYS:HA	1:F:360:LYS:HD2	1.91	0.42
1:G:411:TYR:CE1	6:G:1008:1PE:H132	2.50	0.42
1:I:364:ASP:O	1:I:420:ASN:HA	2.19	0.42
1:L:200:GLU:HG3	8:L:1158:HOH:O	2.19	0.42
1:C:230:VAL:HG12	1:C:234:LEU:HD23	2.02	0.42
1:D:451:LYS:CG	6:D:1009:1PE:H251	2.50	0.42
1:D:597:THR:HG22	1:D:601:LEU:HD22	2.02	0.42
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.55	0.42
1:E:135:PRO:HA	1:E:194:SER:O	2.20	0.41
3:L:1002:CO3:O1	4:L:1004:1OT:O3	2.38	0.41
1:A:386:LYS:NZ	4:A:1004:1OT:O2	2.43	0.41
1:F:341:TYR:CE1	1:F:428:ALA:HB1	2.55	0.41
1:G:488:THR:HG21	1:G:555:SER:HA	2.02	0.41
1:J:332:GLU:HG3	8:J:1209:HOH:O	2.20	0.41
1:D:132:VAL:HG21	1:D:144:ILE:HD13	2.03	0.41
1:F:360:LYS:HD2	1:F:361:SER:N	2.34	0.41
1:G:386:LYS:NZ	4:G:1004:1OT:O2	2.38	0.41
1:J:451:LYS:HE3	6:J:1008:1PE:H151	2.02	0.41
1:D:395:LEU:HD11	1:D:581:TRP:CG	2.56	0.41
1:K:514:LEU:O	1:K:518:LYS:HG2	2.20	0.41
1:L:198:LEU:HD12	1:L:198:LEU:HA	1.84	0.41
1:I:158:LYS:HB2	8:I:1103:HOH:O	2.20	0.41
1:E:152:GLN:HG2	1:E:180:ASP:OD1	2.20	0.41
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.02	0.41
1:K:213:MET:HE3	8:K:1179:HOH:O	2.19	0.41
1:L:451:LYS:HE2	6:L:1007:1PE:H251	2.03	0.41
1:A:372:VAL:O	1:A:483:ASP:HA	2.21	0.41
1:D:102:GLU:HG2	1:D:105:THR:HG22	2.03	0.41
1:G:357:LEU:HB2	1:G:425:PHE:HB2	2.03	0.41
1:K:102:GLU:HG2	1:K:105:THR:HG22	2.02	0.41
1:A:114:VAL:HG12	1:A:274:ALA:HB1	2.03	0.41
1:B:386:LYS:NZ	4:B:1004:1OT:O2	2.42	0.41
7:C:1009:2PE:H141	8:C:1146:HOH:O	2.20	0.41
1:L:127:LEU:HD11	1:L:129:ILE:HD11	2.03	0.41
1:B:551:VAL:HG12	1:B:553:ALA:H	1.87	0.40
1:D:316:GLU:HG2	1:D:320:LYS:HE2	2.02	0.40
1:F:162:MET:HA	1:F:162:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:236:ARG:HH11	1:I:236:ARG:HD3	1.75	0.40
1:J:262:GLU:OE1	1:J:262:GLU:HA	2.21	0.40
1:F:360:LYS:HZ2	1:F:361:SER:HB2	1.86	0.40
1:B:165:PHE:CE2	1:B:173:LYS:HG2	2.56	0.40
1:D:320:LYS:HZ1	7:D:1010:2PE:C15	2.34	0.40
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.87	0.40
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.04	0.40
1:J:579:VAL:O	1:J:589:LYS:HD2	2.22	0.40
4:L:1004:1OT:O1	4:L:1004:1OT:H10	2.22	0.40
1:C:198:LEU:HD22	1:C:202:ASP:HB3	2.04	0.40
1:F:311:SER:HB2	1:F:327:ILE:HD12	2.03	0.40
1:G:492:LEU:HD23	1:G:492:LEU:HA	1.89	0.40
1:H:488:THR:HG21	1:H:555:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/528 (98%)	507 (98%)	11 (2%)	0	100	100
1	B	516/528 (98%)	503 (98%)	11 (2%)	2 (0%)	34	30
1	C	517/528 (98%)	505 (98%)	12 (2%)	0	100	100
1	D	510/528 (97%)	498 (98%)	12 (2%)	0	100	100
1	E	506/528 (96%)	495 (98%)	11 (2%)	0	100	100
1	F	507/528 (96%)	497 (98%)	10 (2%)	0	100	100
1	G	517/528 (98%)	507 (98%)	10 (2%)	0	100	100
1	H	512/528 (97%)	502 (98%)	9 (2%)	1 (0%)	47	44
1	I	516/528 (98%)	505 (98%)	11 (2%)	0	100	100
1	J	509/528 (96%)	498 (98%)	11 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	503/528 (95%)	494 (98%)	8 (2%)	1 (0%)	47	44
1	L	509/528 (96%)	500 (98%)	8 (2%)	1 (0%)	47	44
All	All	6140/6336 (97%)	6011 (98%)	124 (2%)	5 (0%)	51	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	GLU
1	L	137	LYS
1	B	257	LYS
1	B	258	ASN
1	K	363	GLY

5.3.2　Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	429/455 (94%)	417 (97%)	12 (3%)	43	44
1	B	415/455 (91%)	399 (96%)	16 (4%)	32	30
1	C	421/455 (92%)	405 (96%)	16 (4%)	33	31
1	D	421/455 (92%)	414 (98%)	7 (2%)	60	65
1	E	416/455 (91%)	409 (98%)	7 (2%)	60	65
1	F	401/455 (88%)	389 (97%)	12 (3%)	41	41
1	G	428/455 (94%)	415 (97%)	13 (3%)	41	41
1	H	411/455 (90%)	395 (96%)	16 (4%)	32	30
1	I	423/455 (93%)	413 (98%)	10 (2%)	49	51
1	J	420/455 (92%)	412 (98%)	8 (2%)	57	61
1	K	417/455 (92%)	409 (98%)	8 (2%)	57	61
1	L	407/455 (90%)	393 (97%)	14 (3%)	37	36
All	All	5009/5460 (92%)	4870 (97%)	139 (3%)	43	44

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	169	LEU
1	A	200	GLU
1	A	204	LYS
1	A	208	LEU
1	A	275	ASP
1	A	288	TYR
1	A	398	PHE
1	A	439	TYR
1	A	549	SER
1	A	552	LYS
1	A	588	PRO
1	A	603	ASP
1	B	125	GLU
1	B	169	LEU
1	B	199	SER
1	B	200	GLU
1	B	208	LEU
1	B	215	HIS
1	B	255	THR
1	B	272	ASN
1	B	288	TYR
1	B	328	LEU
1	B	357	LEU
1	B	398	PHE
1	B	400	MET
1	B	421	VAL
1	B	439	TYR
1	B	603	ASP
1	C	86	SER
1	C	163	GLU
1	C	169	LEU
1	C	184	SER
1	C	185	VAL
1	C	200	GLU
1	C	208	LEU
1	C	288	TYR
1	C	322	ASN
1	C	357	LEU
1	C	398	PHE
1	C	421	VAL
1	C	439	TYR
1	C	483	ASP

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Mol	Chain	Res	Type
1	C	549	SER
1	C	603	ASP
1	D	154	SER
1	D	219	LEU
1	D	288	TYR
1	D	322	ASN
1	D	398	PHE
1	D	439	TYR
1	D	552	LYS
1	E	86	SER
1	E	169	LEU
1	E	208	LEU
1	E	288	TYR
1	E	398	PHE
1	E	436	LYS
1	E	439	TYR
1	F	86	SER
1	F	116	ASP
1	F	198	LEU
1	F	200	GLU
1	F	208	LEU
1	F	225	VAL
1	F	229	ASN
1	F	254	SER
1	F	288	TYR
1	F	364	ASP
1	F	398	PHE
1	F	439	TYR
1	G	117	ILE
1	G	164	LYS
1	G	169	LEU
1	G	200	GLU
1	G	204	LYS
1	G	208	LEU
1	G	288	TYR
1	G	367	LYS
1	G	398	PHE
1	G	436	LYS
1	G	439	TYR
1	G	588	PRO
1	G	603	ASP
1	H	86	SER

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Mol	Chain	Res	Type
1	H	125	GLU
1	H	154	SER
1	H	164	LYS
1	H	173	LYS
1	H	181	ASN
1	H	200	GLU
1	H	208	LEU
1	H	215	HIS
1	H	254	SER
1	H	288	TYR
1	H	357	LEU
1	H	398	PHE
1	H	421	VAL
1	H	439	TYR
1	H	603	ASP
1	I	86	SER
1	I	169	LEU
1	I	212	THR
1	I	288	TYR
1	I	322	ASN
1	I	398	PHE
1	I	400	MET
1	I	421	VAL
1	I	439	TYR
1	I	549	SER
1	J	200	GLU
1	J	205	ARG
1	J	219	LEU
1	J	262	GLU
1	J	288	TYR
1	J	398	PHE
1	J	439	TYR
1	J	518	LYS
1	K	86	SER
1	K	132	VAL
1	K	145	SER
1	K	169	LEU
1	K	216	ASP
1	K	288	TYR
1	K	398	PHE
1	K	439	TYR
1	L	86	SER

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Mol	Chain	Res	Type
1	L	113	GLN
1	L	116	ASP
1	L	169	LEU
1	L	198	LEU
1	L	200	GLU
1	L	254	SER
1	L	288	TYR
1	L	295	SER
1	L	398	PHE
1	L	421	VAL
1	L	436	LYS
1	L	439	TYR
1	L	603	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	531	ASN
1	K	229	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 115 ligands modelled in this entry, 24 are monoatomic - leaving 91 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	$\#|Z| > 2$
7	2PE	B	1007	-	9,9,27	0.06	0	8,8,26	0.23	0
4	1OT	C	1004	2	16,18,18	2.63	5 (31%)	22,26,26	2.71	9 (40%)
7	2PE	H	1006	-	24,24,27	0.21	0	23,23,26	0.15	0
7	2PE	D	1010	-	12,12,27	0.20	0	11,11,26	0.15	0
5	SO4	B	1005	-	4,4,4	0.15	0	6,6,6	0.05	0
6	1PE	J	1008	-	10,10,15	0.55	0	9,9,14	0.27	0
6	1PE	L	1008	-	7,7,15	0.46	0	6,6,14	0.39	0
7	2PE	C	1009	-	8,8,27	0.16	0	7,7,26	0.24	0
6	1PE	F	1009	-	10,10,15	0.47	0	9,9,14	0.22	0
4	1OT	J	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.77	8 (36%)
5	SO4	K	1006	-	4,4,4	0.18	0	6,6,6	0.09	0
6	1PE	C	1008	-	6,6,15	0.50	0	5,5,14	0.26	0
3	CO3	I	1002	-	2,3,3	0.37	0	2,3,3	0.31	0
4	1OT	D	1004	2	16,18,18	2.79	5 (31%)	22,26,26	3.14	10 (45%)
3	CO3	L	1002	-	2,3,3	0.42	0	2,3,3	0.26	0
5	SO4	E	1005	-	4,4,4	0.13	0	6,6,6	0.15	0
6	1PE	K	1008	-	11,11,15	0.46	0	10,10,14	0.20	0
4	1OT	L	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.86	10 (45%)
7	2PE	I	1010	-	7,7,27	0.15	0	6,6,26	0.12	0
3	CO3	G	1002	-	2,3,3	0.43	0	2,3,3	0.35	0
3	CO3	B	1002	-	2,3,3	0.38	0	2,3,3	0.29	0
4	1OT	B	1004	2	16,18,18	2.72	5 (31%)	22,26,26	2.79	8 (36%)
6	1PE	E	1007	-	11,11,15	0.48	0	10,10,14	0.32	0
7	2PE	D	1012	-	8,8,27	0.18	0	7,7,26	0.17	0
7	2PE	H	1007	-	9,9,27	0.21	0	8,8,26	0.08	0
6	1PE	K	1007	-	11,11,15	0.52	0	10,10,14	0.44	0
6	1PE	E	1008	-	11,11,15	0.49	0	10,10,14	0.31	0
3	CO3	D	1002	-	2,3,3	0.42	0	2,3,3	0.33	0
3	CO3	E	1002	-	2,3,3	0.40	0	2,3,3	0.09	0
4	1OT	A	1004	2	16,18,18	2.70	5 (31%)	22,26,26	2.96	9 (40%)
5	SO4	D	1005	-	4,4,4	0.29	0	6,6,6	0.13	0
5	SO4	H	1005	-	4,4,4	0.12	0	6,6,6	0.17	0
5	SO4	E	1006	-	4,4,4	0.17	0	6,6,6	0.23	0
7	2PE	F	1010	-	8,8,27	0.21	0	7,7,26	0.22	0
7	2PE	B	1006	-	25,25,27	0.18	0	24,24,26	0.17	0
3	CO3	C	1002	-	2,3,3	0.41	0	2,3,3	0.19	0
5	SO4	D	1006	-	4,4,4	0.13	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	1PE	F	1008	-	9,9,15	0.47	0	8,8,14	0.18	0
7	2PE	D	1011	-	4,4,27	0.25	0	3,3,26	0.37	0
7	2PE	E	1010	-	8,8,27	0.14	0	7,7,26	0.19	0
5	SO4	C	1005	-	4,4,4	0.14	0	6,6,6	0.17	0
5	SO4	J	1005	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	G	1006	-	4,4,4	0.17	0	6,6,6	0.24	0
6	1PE	J	1006	-	10,10,15	0.43	0	9,9,14	0.44	0
6	1PE	F	1007	-	9,9,15	0.48	0	8,8,14	0.15	0
4	1OT	F	1004	2	16,18,18	2.68	5 (31%)	22,26,26	2.75	9 (40%)
5	SO4	L	1005	-	4,4,4	0.11	0	6,6,6	0.11	0
6	1PE	A	1010	-	11,11,15	0.51	0	10,10,14	0.15	0
6	1PE	G	1010	-	5,5,15	0.49	0	4,4,14	0.37	0
6	1PE	I	1007	-	14,14,15	0.39	0	13,13,14	0.49	0
6	1PE	G	1011	-	14,14,15	0.41	0	13,13,14	0.57	0
5	SO4	G	1005	-	4,4,4	0.19	0	6,6,6	0.25	0
6	1PE	L	1006	-	9,9,15	0.36	0	8,8,14	0.69	0
3	CO3	A	1002	-	2,3,3	0.41	0	2,3,3	0.29	0
6	1PE	D	1008	-	8,8,15	0.50	0	7,7,14	0.22	0
6	1PE	D	1007	-	9,9,15	0.44	0	8,8,14	0.43	0
6	1PE	L	1009	-	10,10,15	0.50	0	9,9,14	0.49	0
5	SO4	K	1005	-	4,4,4	0.24	0	6,6,6	0.16	0
6	1PE	K	1010	-	5,5,15	0.47	0	4,4,14	0.16	0
5	SO4	A	1005	-	4,4,4	0.09	0	6,6,6	0.27	0
6	1PE	L	1007	-	11,11,15	0.52	0	10,10,14	0.20	0
6	1PE	K	1009	-	10,10,15	0.47	0	9,9,14	0.15	0
5	SO4	A	1008	-	4,4,4	0.17	0	6,6,6	0.26	0
4	1OT	I	1004	2	16,18,18	2.57	5 (31%)	22,26,26	2.83	12 (54%)
6	1PE	D	1009	-	10,10,15	0.53	0	9,9,14	0.39	0
6	1PE	J	1009	-	8,8,15	0.54	0	7,7,14	0.38	0
3	CO3	J	1002	-	2,3,3	0.44	0	2,3,3	0.35	0
5	SO4	I	1006	-	4,4,4	0.20	0	6,6,6	0.18	0
7	2PE	J	1010	-	9,9,27	0.21	0	8,8,26	0.11	0
3	CO3	F	1002	-	2,3,3	0.45	0	2,3,3	0.21	0
5	SO4	A	1007	-	4,4,4	0.16	0	6,6,6	0.28	0
4	1OT	E	1004	2	16,18,18	2.72	5 (31%)	22,26,26	2.91	10 (45%)
6	1PE	I	1008	-	10,10,15	0.46	0	9,9,14	0.33	0
5	SO4	F	1005	-	4,4,4	0.12	0	6,6,6	0.07	0
5	SO4	A	1006	-	4,4,4	0.13	0	6,6,6	0.17	0
3	CO3	H	1002	-	2,3,3	0.43	0	2,3,3	0.46	0
6	1PE	C	1006	-	12,12,15	0.55	0	11,11,14	0.20	0
5	SO4	I	1005	-	4,4,4	0.16	0	6,6,6	0.07	0
6	1PE	C	1007	-	8,8,15	0.43	0	7,7,14	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	1PE	E	1009	-	7,7,15	0.43	0	6,6,14	0.36	0
6	1PE	F	1006	-	9,9,15	0.43	0	8,8,14	0.24	0
4	1OT	G	1004	2	16,18,18	2.66	5 (31%)	22,26,26	2.65	9 (40%)
6	1PE	I	1009	-	4,4,15	0.39	0	3,3,14	0.34	0
6	1PE	G	1008	-	8,8,15	0.41	0	7,7,14	0.36	0
4	1OT	H	1004	2	16,18,18	2.73	5 (31%)	22,26,26	2.63	7 (31%)
3	CO3	K	1002	-	2,3,3	0.34	0	2,3,3	0.12	0
6	1PE	G	1009	-	5,5,15	0.45	0	4,4,14	0.49	0
6	1PE	A	1009	-	8,8,15	0.43	0	7,7,14	0.27	0
4	1OT	K	1004	2	16,18,18	2.58	5 (31%)	22,26,26	2.73	10 (45%)
6	1PE	J	1007	-	9,9,15	0.52	0	8,8,14	0.32	0
5	SO4	G	1007	-	4,4,4	0.14	0	6,6,6	0.18	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
7	2PE	B	1007	-	-	4/7/7/25	-
4	1OT	C	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	L	1006	-	-	3/7/7/13	-
4	1OT	E	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	I	1008	-	-	3/8/8/13	-
7	2PE	H	1006	-	-	7/22/22/25	-
4	1OT	A	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	C	1006	-	-	1/10/10/13	-
6	1PE	D	1008	-	-	3/6/6/13	-
7	2PE	D	1010	-	-	7/10/10/25	-
6	1PE	C	1007	-	-	4/6/6/13	-
6	1PE	D	1007	-	-	4/7/7/13	-
6	1PE	E	1009	-	-	3/5/5/13	-
6	1PE	F	1006	-	-	1/7/7/13	-
6	1PE	J	1008	-	-	3/8/8/13	-
6	1PE	L	1008	-	-	3/5/5/13	-
6	1PE	L	1009	-	-	4/8/8/13	-
7	2PE	C	1009	-	-	3/6/6/25	-
4	1OT	G	1004	2	-	4/13/14/14	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	K	1010	-	-	2/3/3/13	-
7	2PE	H	1007	-	-	3/7/7/25	-
6	1PE	L	1007	-	-	6/9/9/13	-
6	1PE	F	1009	-	-	2/8/8/13	-
6	1PE	K	1009	-	-	1/8/8/13	-
6	1PE	I	1009	-	-	1/2/2/13	-
4	1OT	I	1004	2	-	5/13/14/14	0/2/2/2
7	2PE	F	1010	-	-	4/6/6/25	-
7	2PE	B	1006	-	-	9/23/23/25	-
6	1PE	D	1009	-	-	7/8/8/13	-
6	1PE	J	1009	-	-	3/6/6/13	-
4	1OT	J	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	G	1008	-	-	5/6/6/13	-
6	1PE	F	1008	-	-	2/7/7/13	-
4	1OT	H	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	G	1009	-	-	1/3/3/13	-
6	1PE	C	1008	-	-	2/4/4/13	-
6	1PE	A	1009	-	-	0/6/6/13	-
4	1OT	K	1004	2	-	5/13/14/14	0/2/2/2
7	2PE	D	1011	-	-	2/2/2/25	-
7	2PE	E	1010	-	-	3/6/6/25	-
4	1OT	D	1004	2	-	4/13/14/14	0/2/2/2
6	1PE	J	1007	-	-	0/7/7/13	-
6	1PE	K	1008	-	-	2/9/9/13	-
4	1OT	L	1004	2	-	4/13/14/14	0/2/2/2
7	2PE	I	1010	-	-	1/5/5/25	-
6	1PE	J	1006	-	-	6/8/8/13	-
7	2PE	J	1010	-	-	5/7/7/25	-
6	1PE	F	1007	-	-	4/7/7/13	-
4	1OT	B	1004	2	-	5/13/14/14	0/2/2/2
6	1PE	E	1007	-	-	4/9/9/13	-
4	1OT	F	1004	2	-	4/13/14/14	0/2/2/2
7	2PE	D	1012	-	-	3/6/6/25	-
6	1PE	A	1010	-	-	5/9/9/13	-
6	1PE	G	1010	-	-	3/3/3/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	1PE	I	1007	-	-	5/12/12/13	-
6	1PE	G	1011	-	-	6/12/12/13	-
6	1PE	K	1007	-	-	3/9/9/13	-
6	1PE	E	1008	-	-	3/9/9/13	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1004	1OT	P-O3	7.79	1.62	1.49
4	F	1004	1OT	P-O3	7.60	1.62	1.49
4	J	1004	1OT	P-O3	7.58	1.62	1.49
4	H	1004	1OT	P-O3	7.57	1.62	1.49
4	E	1004	1OT	P-O3	7.55	1.62	1.49
4	C	1004	1OT	P-O3	7.43	1.62	1.49
4	B	1004	1OT	P-O3	7.42	1.62	1.49
4	G	1004	1OT	P-O3	7.33	1.61	1.49
4	A	1004	1OT	P-O3	7.27	1.61	1.49
4	L	1004	1OT	P-O3	7.08	1.61	1.49
4	K	1004	1OT	P-O3	6.97	1.61	1.49
4	I	1004	1OT	P-O3	6.82	1.61	1.49
4	D	1004	1OT	P-O2	4.77	1.62	1.54
4	L	1004	1OT	P-O2	4.59	1.62	1.54
4	K	1004	1OT	P-O2	4.43	1.61	1.54
4	F	1004	1OT	P-O2	4.33	1.61	1.54
4	E	1004	1OT	P-O2	4.31	1.61	1.54
4	G	1004	1OT	P-O2	4.30	1.61	1.54
4	A	1004	1OT	P-O2	4.29	1.61	1.54
4	B	1004	1OT	P-O2	4.27	1.61	1.54
4	I	1004	1OT	P-O2	4.23	1.61	1.54
4	C	1004	1OT	P-O2	4.22	1.61	1.54
4	B	1004	1OT	P-O1	-4.14	1.48	1.54
4	H	1004	1OT	P-O1	-4.10	1.48	1.54
4	H	1004	1OT	P-O2	3.98	1.61	1.54
4	I	1004	1OT	P-O1	-3.94	1.48	1.54
4	E	1004	1OT	P-O1	-3.93	1.48	1.54
4	J	1004	1OT	P-O2	3.92	1.61	1.54
4	A	1004	1OT	P-O1	-3.85	1.48	1.54
4	L	1004	1OT	C5-N2	-3.83	1.33	1.44
4	E	1004	1OT	C5-N2	-3.81	1.33	1.44
4	A	1004	1OT	C5-N2	-3.69	1.33	1.44
4	C	1004	1OT	P-O1	-3.69	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	1004	1OT	P-O1	-3.68	1.49	1.54
4	B	1004	1OT	C5-N2	-3.67	1.33	1.44
4	J	1004	1OT	C5-N2	-3.67	1.33	1.44
4	D	1004	1OT	C5-N2	-3.66	1.33	1.44
4	G	1004	1OT	C5-N2	-3.66	1.33	1.44
4	F	1004	1OT	C5-N2	-3.65	1.33	1.44
4	K	1004	1OT	C5-N2	-3.65	1.33	1.44
4	H	1004	1OT	C5-N2	-3.64	1.33	1.44
4	C	1004	1OT	C5-N2	-3.55	1.33	1.44
4	F	1004	1OT	P-O1	-3.53	1.49	1.54
4	I	1004	1OT	C5-N2	-3.47	1.34	1.44
4	G	1004	1OT	P-O1	-3.42	1.49	1.54
4	A	1004	1OT	C2-C1	-3.35	1.47	1.52
4	K	1004	1OT	C2-C1	-3.35	1.47	1.52
4	H	1004	1OT	C2-C1	-3.32	1.47	1.52
4	D	1004	1OT	P-O1	-3.30	1.49	1.54
4	G	1004	1OT	C2-C1	-3.29	1.47	1.52
4	J	1004	1OT	P-O1	-3.26	1.49	1.54
4	J	1004	1OT	C2-C1	-3.19	1.47	1.52
4	I	1004	1OT	C2-C1	-3.17	1.47	1.52
4	L	1004	1OT	C2-C1	-3.12	1.48	1.52
4	K	1004	1OT	P-O1	-3.06	1.50	1.54
4	D	1004	1OT	C2-C1	-3.00	1.48	1.52
4	E	1004	1OT	C2-C1	-2.97	1.48	1.52
4	B	1004	1OT	C2-C1	-2.97	1.48	1.52
4	F	1004	1OT	C2-C1	-2.76	1.48	1.52
4	C	1004	1OT	C2-C1	-2.69	1.48	1.52

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1004	1OT	C4-C5-N2	7.13	125.38	119.15
4	A	1004	1OT	C4-C5-N2	6.15	124.53	119.15
4	L	1004	1OT	C6-N2-N3	6.10	116.06	111.94
4	E	1004	1OT	C6-N2-N3	6.01	115.99	111.94
4	L	1004	1OT	C7-C6-N2	-5.84	102.63	107.08
4	D	1004	1OT	C5-N2-N3	5.79	123.94	118.80
4	J	1004	1OT	C6-N2-N3	5.78	115.84	111.94
4	K	1004	1OT	C7-C6-N2	-5.75	102.70	107.08
4	F	1004	1OT	C7-C6-N2	-5.74	102.71	107.08
4	G	1004	1OT	C7-C6-N2	-5.72	102.72	107.08
4	I	1004	1OT	C4-C5-N2	5.63	124.07	119.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1004	1OT	C4-C5-N2	5.63	124.07	119.15
4	B	1004	1OT	C7-C6-N2	-5.60	102.82	107.08
4	A	1004	1OT	C7-C6-N2	-5.59	102.82	107.08
4	J	1004	1OT	C7-C6-N2	-5.59	102.82	107.08
4	K	1004	1OT	C6-N2-N3	5.59	115.71	111.94
4	H	1004	1OT	C7-C6-N2	-5.56	102.85	107.08
4	C	1004	1OT	C7-C6-N2	-5.53	102.86	107.08
4	A	1004	1OT	C6-N2-N3	5.53	115.67	111.94
4	I	1004	1OT	C7-C6-N2	-5.53	102.87	107.08
4	F	1004	1OT	C6-N2-N3	5.52	115.66	111.94
4	E	1004	1OT	C7-C6-N2	-5.48	102.91	107.08
4	C	1004	1OT	C6-N2-N3	5.38	115.57	111.94
4	B	1004	1OT	C4-C5-N2	5.37	123.85	119.15
4	G	1004	1OT	C6-N2-N3	5.33	115.53	111.94
4	B	1004	1OT	C6-N2-N3	5.31	115.52	111.94
4	H	1004	1OT	C6-N2-N3	5.28	115.50	111.94
4	A	1004	1OT	C5-N2-N3	5.20	123.41	118.80
4	L	1004	1OT	C4-C5-N2	5.12	123.63	119.15
4	B	1004	1OT	C5-N2-N3	5.11	123.33	118.80
4	I	1004	1OT	C5-N2-N3	5.06	123.29	118.80
4	D	1004	1OT	C6-N2-N3	5.04	115.34	111.94
4	J	1004	1OT	C4-C5-N2	4.99	123.51	119.15
4	E	1004	1OT	C5-N2-N3	4.97	123.21	118.80
4	I	1004	1OT	C6-N2-N3	4.92	115.26	111.94
4	F	1004	1OT	C5-N2-N3	4.85	123.10	118.80
4	D	1004	1OT	C7-C6-N2	-4.83	103.40	107.08
4	C	1004	1OT	C4-C5-N2	4.74	123.30	119.15
4	C	1004	1OT	C5-N2-N3	4.65	122.93	118.80
4	J	1004	1OT	C5-N2-N3	4.61	122.89	118.80
4	F	1004	1OT	C4-C5-N2	4.55	123.13	119.15
4	H	1004	1OT	C5-N2-N3	4.50	122.80	118.80
4	D	1004	1OT	C10-C2-C1	-4.44	115.65	120.77
4	K	1004	1OT	C5-N2-N3	4.37	122.68	118.80
4	H	1004	1OT	C4-C5-N2	4.32	122.93	119.15
4	L	1004	1OT	C5-N2-N3	4.13	122.47	118.80
4	G	1004	1OT	C4-C5-N2	4.08	122.72	119.15
4	K	1004	1OT	C4-C5-N2	4.07	122.71	119.15
4	G	1004	1OT	C5-N2-N3	3.95	122.31	118.80
4	A	1004	1OT	C10-C2-C1	-3.84	116.34	120.77
4	D	1004	1OT	C4-C5-C9	-3.55	116.07	121.33
4	I	1004	1OT	C4-C5-C9	-3.54	116.09	121.33
4	F	1004	1OT	C4-C5-C9	-3.53	116.09	121.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1004	1OT	C10-C2-C1	-3.51	116.72	120.77
4	D	1004	1OT	C3-C2-C1	3.43	124.73	120.77
4	G	1004	1OT	C4-C5-C9	-3.42	116.26	121.33
4	C	1004	1OT	C4-C5-C9	-3.41	116.28	121.33
4	J	1004	1OT	C10-C2-C1	-3.40	116.85	120.77
4	H	1004	1OT	C4-C5-C9	-3.39	116.30	121.33
4	L	1004	1OT	C10-C2-C1	-3.38	116.87	120.77
4	B	1004	1OT	C4-C5-C9	-3.32	116.41	121.33
4	K	1004	1OT	C4-C5-C9	-3.32	116.41	121.33
4	J	1004	1OT	C4-C5-C9	-3.22	116.56	121.33
4	L	1004	1OT	C4-C5-C9	-3.21	116.58	121.33
4	I	1004	1OT	C10-C2-C1	-3.11	117.18	120.77
4	A	1004	1OT	C4-C5-C9	-3.11	116.73	121.33
4	E	1004	1OT	C4-C5-C9	-3.06	116.80	121.33
4	F	1004	1OT	C10-C2-C1	-2.96	117.35	120.77
4	B	1004	1OT	C10-C2-C1	-2.92	117.41	120.77
4	G	1004	1OT	C10-C2-C1	-2.79	117.56	120.77
4	H	1004	1OT	C10-C9-C5	2.70	123.00	119.07
4	C	1004	1OT	O1-P-O3	-2.64	106.81	113.45
4	A	1004	1OT	C10-C9-C5	2.61	122.87	119.07
4	B	1004	1OT	C10-C9-C5	2.57	122.80	119.07
4	F	1004	1OT	C10-C9-C5	2.50	122.71	119.07
4	K	1004	1OT	C10-C2-C1	-2.50	117.89	120.77
4	G	1004	1OT	C10-C9-C5	2.49	122.69	119.07
4	H	1004	1OT	C10-C2-C1	-2.45	117.94	120.77
4	I	1004	1OT	C10-C9-C5	2.45	122.63	119.07
4	D	1004	1OT	C4-C3-C2	-2.44	118.74	121.20
4	C	1004	1OT	C10-C2-C1	-2.43	117.97	120.77
4	D	1004	1OT	C3-C4-C5	2.43	122.60	119.07
4	D	1004	1OT	C10-C9-C5	2.43	122.60	119.07
4	I	1004	1OT	C3-C4-C5	2.42	122.59	119.07
4	J	1004	1OT	C10-C9-C5	2.39	122.54	119.07
4	E	1004	1OT	C10-C9-C5	2.37	122.51	119.07
4	C	1004	1OT	C10-C9-C5	2.33	122.45	119.07
4	L	1004	1OT	C10-C9-C5	2.31	122.43	119.07
4	E	1004	1OT	C3-C2-C1	2.28	123.40	120.77
4	C	1004	1OT	C3-C4-C5	2.27	122.37	119.07
4	K	1004	1OT	C3-C4-C5	2.23	122.32	119.07
4	K	1004	1OT	C10-C9-C5	2.21	122.29	119.07
4	I	1004	1OT	O1-P-O3	-2.21	107.90	113.45
4	E	1004	1OT	C8-N3-N2	-2.20	102.10	103.70
4	B	1004	1OT	C3-C2-C1	2.16	123.27	120.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1004	1OT	C3-C4-C5	2.16	122.21	119.07
4	K	1004	1OT	O2-P-O3	-2.15	108.04	113.45
4	G	1004	1OT	C9-C5-N2	2.14	121.02	119.15
4	A	1004	1OT	C3-C2-C1	2.14	123.23	120.77
4	E	1004	1OT	O1-P-O3	-2.12	108.11	113.45
4	I	1004	1OT	C3-C2-C1	2.11	123.20	120.77
4	L	1004	1OT	O1-P-O3	-2.11	108.15	113.45
4	I	1004	1OT	C4-C3-C2	-2.10	119.08	121.20
4	G	1004	1OT	C3-C4-C5	2.10	122.12	119.07
4	A	1004	1OT	C4-C3-C2	-2.09	119.09	121.20
4	F	1004	1OT	C3-C2-C1	2.08	123.17	120.77
4	K	1004	1OT	C4-C3-C2	-2.07	119.11	121.20
4	L	1004	1OT	C3-C4-C5	2.07	122.08	119.07
4	J	1004	1OT	C3-C2-C1	2.07	123.15	120.77
4	I	1004	1OT	P-C1-C2	2.02	115.63	111.70
4	L	1004	1OT	C3-C2-C1	2.00	123.08	120.77

There are no chirality outliers.

All (210) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1004	1OT	P-C1-C2-C10
4	D	1004	1OT	P-C1-C2-C3
4	E	1004	1OT	P-C1-C2-C10
4	F	1004	1OT	P-C1-C2-C10
4	F	1004	1OT	P-C1-C2-C3
4	J	1004	1OT	P-C1-C2-C10
4	J	1004	1OT	P-C1-C2-C3
4	L	1004	1OT	P-C1-C2-C10
6	G	1011	1PE	OH6-C15-C25-OH5
7	H	1006	2PE	O16-C17-C18-O19
6	F	1007	1PE	OH6-C15-C25-OH5
6	K	1010	1PE	OH5-C14-C24-OH4
6	I	1007	1PE	OH4-C13-C23-OH3
6	I	1008	1PE	OH4-C13-C23-OH3
6	L	1009	1PE	OH6-C15-C25-OH5
6	G	1011	1PE	OH5-C14-C24-OH4
7	C	1009	2PE	C14-C15-O16-C17
7	F	1010	2PE	C11-C12-O13-C14
6	I	1007	1PE	OH6-C15-C25-OH5
6	L	1007	1PE	OH5-C14-C24-OH4
7	D	1011	2PE	C14-C15-O16-C17

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Mol	Chain	Res	Type	Atoms
6	D	1007	1PE	OH5-C14-C24-OH4
4	A	1004	1OT	P-C1-C2-C10
4	A	1004	1OT	P-C1-C2-C3
4	B	1004	1OT	P-C1-C2-C10
4	B	1004	1OT	P-C1-C2-C3
4	C	1004	1OT	P-C1-C2-C10
4	C	1004	1OT	P-C1-C2-C3
4	E	1004	1OT	P-C1-C2-C3
4	G	1004	1OT	P-C1-C2-C10
4	G	1004	1OT	P-C1-C2-C3
4	H	1004	1OT	P-C1-C2-C10
4	H	1004	1OT	P-C1-C2-C3
4	I	1004	1OT	P-C1-C2-C10
4	I	1004	1OT	P-C1-C2-C3
4	K	1004	1OT	P-C1-C2-C10
4	K	1004	1OT	P-C1-C2-C3
4	L	1004	1OT	P-C1-C2-C3
6	L	1006	1PE	OH6-C15-C25-OH5
6	E	1009	1PE	OH4-C13-C23-OH3
6	F	1007	1PE	OH5-C14-C24-OH4
6	I	1009	1PE	OH5-C14-C24-OH4
6	L	1007	1PE	OH6-C15-C25-OH5
7	D	1011	2PE	O13-C14-C15-O16
7	J	1010	2PE	O13-C14-C15-O16
6	D	1007	1PE	OH4-C13-C23-OH3
7	D	1010	2PE	O10-C11-C12-O13
6	F	1008	1PE	OH5-C14-C24-OH4
6	G	1010	1PE	OH6-C15-C25-OH5
6	C	1008	1PE	OH5-C14-C24-OH4
6	C	1007	1PE	OH4-C13-C23-OH3
6	J	1008	1PE	OH6-C15-C25-OH5
6	D	1009	1PE	OH6-C15-C25-OH5
6	L	1006	1PE	OH7-C16-C26-OH6
6	J	1006	1PE	OH5-C14-C24-OH4
6	F	1009	1PE	OH4-C13-C23-OH3
6	K	1007	1PE	OH6-C15-C25-OH5
6	J	1008	1PE	OH5-C14-C24-OH4
6	J	1006	1PE	OH6-C15-C25-OH5
6	G	1010	1PE	C24-C14-OH5-C25
7	D	1012	2PE	C18-C17-O16-C15
6	E	1009	1PE	OH5-C14-C24-OH4
6	D	1007	1PE	C12-C22-OH3-C23

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Mol	Chain	Res	Type	Atoms
6	A	1010	1PE	C13-C23-OH3-C22
6	J	1006	1PE	C14-C24-OH4-C13
6	D	1009	1PE	C23-C13-OH4-C24
7	B	1007	2PE	O13-C14-C15-O16
6	I	1007	1PE	C12-C22-OH3-C23
6	K	1010	1PE	C14-C24-OH4-C13
6	L	1008	1PE	C24-C14-OH5-C25
6	C	1008	1PE	C15-C25-OH5-C14
6	E	1007	1PE	OH6-C15-C25-OH5
6	C	1007	1PE	C12-C22-OH3-C23
6	E	1009	1PE	C23-C13-OH4-C24
7	H	1006	2PE	C14-C15-O16-C17
7	H	1007	2PE	C14-C15-O16-C17
7	H	1006	2PE	C17-C18-O19-C20
6	J	1006	1PE	C16-C26-OH6-C15
6	L	1009	1PE	C15-C25-OH5-C14
7	B	1006	2PE	C2-C3-O4-C5
6	J	1006	1PE	C15-C25-OH5-C14
6	L	1008	1PE	C23-C13-OH4-C24
7	H	1006	2PE	C24-C23-O22-C21
6	L	1007	1PE	C24-C14-OH5-C25
6	L	1009	1PE	C25-C15-OH6-C26
6	D	1008	1PE	C14-C24-OH4-C13
7	D	1010	2PE	C11-C12-O13-C14
6	F	1008	1PE	C16-C26-OH6-C15
6	D	1009	1PE	C16-C26-OH6-C15
7	B	1006	2PE	C17-C18-O19-C20
6	F	1007	1PE	C15-C25-OH5-C14
7	B	1006	2PE	C20-C21-O22-C23
7	D	1012	2PE	C14-C15-O16-C17
7	D	1010	2PE	O13-C14-C15-O16
7	B	1007	2PE	O16-C17-C18-O19
6	D	1008	1PE	OH5-C14-C24-OH4
6	K	1007	1PE	C14-C24-OH4-C13
6	L	1009	1PE	C14-C24-OH4-C13
7	B	1006	2PE	C23-C24-O25-C26
7	H	1006	2PE	C21-C20-O19-C18
6	G	1008	1PE	C24-C14-OH5-C25
7	B	1006	2PE	O1-C2-C3-O4
6	G	1011	1PE	C14-C24-OH4-C13
6	I	1008	1PE	C13-C23-OH3-C22
7	D	1010	2PE	O16-C17-C18-O19

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Mol	Chain	Res	Type	Atoms
6	I	1007	1PE	C25-C15-OH6-C26
6	J	1008	1PE	C25-C15-OH6-C26
6	F	1009	1PE	C25-C15-OH6-C26
6	I	1008	1PE	C14-C24-OH4-C13
6	A	1010	1PE	OH4-C13-C23-OH3
7	B	1006	2PE	O22-C23-C24-O25
7	H	1007	2PE	C18-C17-O16-C15
6	G	1008	1PE	C13-C23-OH3-C22
6	J	1006	1PE	OH7-C16-C26-OH6
6	G	1011	1PE	C16-C26-OH6-C15
6	L	1007	1PE	C15-C25-OH5-C14
7	H	1006	2PE	C23-C24-O25-C26
6	G	1008	1PE	OH5-C14-C24-OH4
7	D	1010	2PE	C21-C20-O19-C18
7	I	1010	2PE	C14-C15-O16-C17
6	G	1011	1PE	OH7-C16-C26-OH6
6	E	1008	1PE	OH5-C14-C24-OH4
6	K	1009	1PE	C25-C15-OH6-C26
6	E	1007	1PE	C12-C22-OH3-C23
6	J	1009	1PE	C23-C13-OH4-C24
7	E	1010	2PE	C21-C20-O19-C18
6	K	1008	1PE	OH6-C15-C25-OH5
6	G	1011	1PE	C24-C14-OH5-C25
7	F	1010	2PE	C8-C9-O10-C11
7	B	1006	2PE	C15-C14-O13-C12
7	B	1007	2PE	C14-C15-O16-C17
7	J	1010	2PE	C18-C17-O16-C15
6	D	1009	1PE	C24-C14-OH5-C25
6	E	1008	1PE	C12-C22-OH3-C23
6	C	1007	1PE	OH5-C14-C24-OH4
6	L	1006	1PE	C16-C26-OH6-C15
4	A	1004	1OT	C9-C5-N2-C6
4	A	1004	1OT	C4-C5-N2-C6
4	B	1004	1OT	C9-C5-N2-C6
4	B	1004	1OT	C4-C5-N2-C6
4	C	1004	1OT	C9-C5-N2-C6
4	C	1004	1OT	C4-C5-N2-C6
4	D	1004	1OT	C9-C5-N2-C6
4	D	1004	1OT	C4-C5-N2-C6
4	E	1004	1OT	C9-C5-N2-C6
4	E	1004	1OT	C4-C5-N2-C6
4	F	1004	1OT	C9-C5-N2-C6

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Mol	Chain	Res	Type	Atoms
4	F	1004	1OT	C4-C5-N2-C6
4	G	1004	1OT	C9-C5-N2-C6
4	G	1004	1OT	C4-C5-N2-C6
4	H	1004	1OT	C9-C5-N2-C6
4	H	1004	1OT	C4-C5-N2-C6
4	I	1004	1OT	C9-C5-N2-C6
4	I	1004	1OT	C4-C5-N2-C6
4	J	1004	1OT	C9-C5-N2-C6
4	J	1004	1OT	C4-C5-N2-C6
4	K	1004	1OT	C9-C5-N2-C6
4	K	1004	1OT	C4-C5-N2-C6
4	L	1004	1OT	C9-C5-N2-C6
4	L	1004	1OT	C4-C5-N2-C6
7	D	1010	2PE	C18-C17-O16-C15
6	D	1009	1PE	C15-C25-OH5-C14
6	J	1009	1PE	C14-C24-OH4-C13
6	D	1009	1PE	OH5-C14-C24-OH4
7	B	1006	2PE	C18-C17-O16-C15
6	A	1010	1PE	C25-C15-OH6-C26
6	D	1008	1PE	C13-C23-OH3-C22
7	J	1010	2PE	C15-C14-O13-C12
6	I	1007	1PE	OH5-C14-C24-OH4
7	C	1009	2PE	C18-C17-O16-C15
6	K	1008	1PE	C15-C25-OH5-C14
6	F	1006	1PE	C24-C14-OH5-C25
7	H	1007	2PE	C12-C11-O10-C9
6	G	1008	1PE	C23-C13-OH4-C24
6	A	1010	1PE	OH6-C15-C25-OH5
7	F	1010	2PE	C15-C14-O13-C12
6	J	1009	1PE	C15-C25-OH5-C14
6	E	1007	1PE	OH5-C14-C24-OH4
6	A	1010	1PE	C15-C25-OH5-C14
6	D	1007	1PE	C23-C13-OH4-C24
7	C	1009	2PE	C11-C12-O13-C14
6	E	1008	1PE	C23-C13-OH4-C24
7	D	1010	2PE	C15-C14-O13-C12
6	L	1007	1PE	C14-C24-OH4-C13
6	K	1007	1PE	C12-C22-OH3-C23
7	D	1012	2PE	C15-C14-O13-C12
6	E	1007	1PE	OH4-C13-C23-OH3
7	B	1006	2PE	O16-C17-C18-O19
6	D	1009	1PE	C14-C24-OH4-C13

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Mol	Chain	Res	Type	Atoms
6	G	1010	1PE	C15-C25-OH5-C14
6	F	1007	1PE	C25-C15-OH6-C26
6	L	1007	1PE	C12-C22-OH3-C23
7	H	1006	2PE	O22-C23-C24-O25
7	J	1010	2PE	C17-C18-O19-C20
6	G	1009	1PE	C15-C25-OH5-C14
7	J	1010	2PE	C21-C20-O19-C18
4	A	1004	1OT	N1-C1-C2-C3
4	B	1004	1OT	N1-C1-C2-C3
4	C	1004	1OT	N1-C1-C2-C3
4	H	1004	1OT	N1-C1-C2-C3
4	I	1004	1OT	N1-C1-C2-C3
4	K	1004	1OT	N1-C1-C2-C3
6	L	1008	1PE	C14-C24-OH4-C13
6	C	1007	1PE	C23-C13-OH4-C24
7	B	1007	2PE	C11-C12-O13-C14
7	F	1010	2PE	O10-C11-C12-O13
6	G	1008	1PE	OH4-C13-C23-OH3
6	C	1006	1PE	C12-C22-OH3-C23
7	E	1010	2PE	C18-C17-O16-C15
7	E	1010	2PE	O16-C17-C18-O19

There are no ring outliers.

44 monomers are involved in 92 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1004	1OT	2	0
7	H	1006	2PE	1	0
7	D	1010	2PE	4	0
6	J	1008	1PE	2	0
6	L	1008	1PE	2	0
7	C	1009	2PE	2	0
6	F	1009	1PE	1	0
4	J	1004	1OT	2	0
4	D	1004	1OT	2	0
3	L	1002	CO3	1	0
4	L	1004	1OT	4	0
4	B	1004	1OT	4	0
7	D	1012	2PE	1	0
7	H	1007	2PE	1	0
6	K	1007	1PE	2	0
3	D	1002	CO3	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	1OT	3	0
7	F	1010	2PE	1	0
6	F	1008	1PE	1	0
7	E	1010	2PE	1	0
5	J	1005	SO4	1	0
6	J	1006	1PE	3	0
4	F	1004	1OT	3	0
6	A	1010	1PE	1	0
6	I	1007	1PE	1	0
6	G	1011	1PE	6	0
6	D	1007	1PE	2	0
6	L	1009	1PE	4	0
6	K	1010	1PE	1	0
6	L	1007	1PE	3	0
4	I	1004	1OT	2	0
6	D	1009	1PE	5	0
6	J	1009	1PE	2	0
4	E	1004	1OT	4	0
6	I	1008	1PE	1	0
6	C	1006	1PE	1	0
6	C	1007	1PE	1	0
6	E	1009	1PE	3	0
4	G	1004	1OT	3	0
6	I	1009	1PE	1	0
6	G	1008	1PE	2	0
4	H	1004	1OT	2	0
4	K	1004	1OT	3	0
6	J	1007	1PE	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 2PE B 1007

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT C 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE H 1006

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE D 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE C 1009

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT J 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT D 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT L 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE I 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT B 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE D 1012

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE H 1007

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT A 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE F 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE B 1006

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE D 1011

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE E 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT F 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT I 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 2PE J 1010

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT E 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT G 1004

Bond lengths

Bond angles

Torsions

Rings

Ligand 1OT H 1004

Bond lengths

Bond angles

Torsions

Rings

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	\<RSRZ\>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	519/528 (98%)	-0.34	1 (0%)	95	94	6, 13, 30, 50	0
1	B	518/528 (98%)	-0.21	6 (1%)	79	78	5, 14, 43, 65	1 (0%)
1	C	518/528 (98%)	-0.33	2 (0%)	92	92	4, 12, 33, 48	0
1	D	514/528 (97%)	-0.39	4 (0%)	86	85	5, 12, 31, 54	0
1	E	510/528 (96%)	-0.47	2 (0%)	92	92	4, 11, 25, 50	0
1	F	511/528 (96%)	-0.20	7 (1%)	75	74	6, 16, 37, 69	0
1	G	519/528 (98%)	-0.34	0	100	100	5, 12, 31, 52	0
1	H	516/528 (97%)	-0.26	2 (0%)	92	92	5, 14, 41, 63	1 (0%)
1	I	518/528 (98%)	-0.34	1 (0%)	95	94	4, 13, 33, 56	0
1	J	513/528 (97%)	-0.40	5 (0%)	82	81	4, 13, 32, 57	0
1	K	509/528 (96%)	-0.47	2 (0%)	92	92	5, 12, 26, 52	0
1	L	513/528 (97%)	-0.27	2 (0%)	92	92	5, 14, 35, 52	0
All	All	6178/6336 (97%)	-0.33	34 (0%)	89	88	4, 13, 34, 69	2 (0%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	259	VAL	5.9
1	H	136	GLY	4.0
1	B	257	LYS	3.8
1	J	136	GLY	3.7
1	J	85	ALA	3.5
1	F	136	GLY	3.4
1	B	136	GLY	3.4
1	L	136	GLY	3.4
1	F	121	CYS	3.4
1	K	550	SER	3.1
1	D	85	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	136	GLY	2.9
1	E	136	GLY	2.7
1	J	603	ASP	2.7
1	F	137	LYS	2.7
1	B	260	ASN	2.7
1	F	148	VAL	2.6
1	F	361	SER	2.5
1	B	256	ASP	2.5
1	D	603	ASP	2.5
1	C	136	GLY	2.5
1	B	144	ILE	2.3
1	F	138	GLU	2.3
1	A	362	LYS	2.3
1	K	363	GLY	2.3
1	I	124	GLU	2.3
1	J	219	LEU	2.2
1	E	550	SER	2.2
1	L	363	GLY	2.1
1	F	157	LEU	2.1
1	C	124	GLU	2.1
1	H	181	ASN	2.1
1	D	219	LEU	2.0
1	J	549	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	1PE	L	1008	8/16	0.67	0.20	48,51,53,53	0
6	1PE	J	1009	9/16	0.73	0.25	26,32,38,39	0
6	1PE	J	1008	11/16	0.75	0.23	26,32,42,42	0
6	1PE	A	1010	12/16	0.75	0.23	32,38,46,48	0
6	1PE	D	1008	9/16	0.75	0.22	46,49,60,60	0
6	1PE	L	1009	11/16	0.76	0.20	36,39,43,45	0
6	1PE	C	1008	7/16	0.77	0.35	42,43,44,45	0
6	1PE	K	1010	6/16	0.77	0.18	23,28,37,39	0
6	1PE	L	1007	12/16	0.78	0.18	28,35,39,41	0
6	1PE	J	1007	10/16	0.80	0.22	28,32,39,41	0
6	1PE	F	1009	11/16	0.81	0.29	46,51,55,56	0
6	1PE	G	1011	15/16	0.81	0.22	26,38,47,51	0
6	1PE	E	1009	8/16	0.81	0.22	29,42,43,43	0
7	2PE	H	1007	10/28	0.81	0.19	36,45,53,53	0
7	2PE	J	1010	10/28	0.81	0.22	18,47,48,48	0
6	1PE	F	1007	10/16	0.82	0.18	40,42,49,51	0
7	2PE	I	1010	8/28	0.82	0.18	32,39,48,49	0
6	1PE	D	1009	11/16	0.82	0.19	23,35,40,43	0
6	1PE	E	1007	12/16	0.83	0.15	29,32,34,34	0
7	2PE	E	1010	9/28	0.84	0.19	36,39,42,46	0
7	2PE	D	1010	13/28	0.84	0.20	28,38,49,51	0
7	2PE	H	1006	25/28	0.85	0.15	21,31,39,44	0
6	1PE	C	1006	13/16	0.85	0.17	12,34,44,45	0
6	1PE	K	1007	12/16	0.85	0.17	31,37,40,41	0
6	1PE	K	1009	11/16	0.85	0.17	30,33,36,38	0
7	2PE	D	1012	9/28	0.86	0.21	36,42,45,47	0
7	2PE	B	1006	26/28	0.86	0.18	17,43,51,51	0
6	1PE	I	1007	15/16	0.86	0.21	20,31,40,40	0
7	2PE	B	1007	10/28	0.87	0.17	45,49,53,55	0
6	1PE	F	1008	10/16	0.87	0.17	26,32,35,36	0
6	1PE	G	1008	9/16	0.88	0.15	17,25,29,30	0
5	SO4	A	1008	5/5	0.88	0.18	26,35,41,48	0
7	2PE	C	1009	9/28	0.88	0.15	29,32,38,39	0
7	2PE	F	1010	9/28	0.88	0.14	35,38,39,42	0
6	1PE	C	1007	9/16	0.90	0.13	13,22,29,31	0
6	1PE	E	1008	12/16	0.90	0.16	19,23,39,39	0
5	SO4	E	1006	5/5	0.90	0.27	46,53,54,62	0
6	1PE	I	1008	11/16	0.90	0.14	18,24,31,33	0
6	1PE	G	1010	6/16	0.91	0.14	30,32,32,33	0
7	2PE	D	1011	5/28	0.91	0.25	21,21,28,28	0
5	SO4	C	1005	5/5	0.91	0.26	41,47,51,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	1OT	F	1004	17/17	0.92	0.15	10,24,32,32	0
4	1OT	H	1004	17/17	0.92	0.15	10,24,37,37	0
6	1PE	L	1006	10/16	0.92	0.15	19,25,29,35	0
6	1PE	I	1009	5/16	0.92	0.15	14,20,20,21	0
6	1PE	J	1006	11/16	0.92	0.16	20,25,35,37	0
4	1OT	L	1004	17/17	0.92	0.15	7,25,34,34	0
5	SO4	G	1007	5/5	0.92	0.16	43,48,51,56	0
6	1PE	D	1007	10/16	0.92	0.12	17,24,28,32	0
6	1PE	F	1006	10/16	0.92	0.13	29,32,36,37	0
4	1OT	J	1004	17/17	0.93	0.17	15,21,43,44	0
6	1PE	A	1009	9/16	0.93	0.09	18,21,25,34	0
5	SO4	B	1005	5/5	0.93	0.18	67,68,68,69	0
4	1OT	I	1004	17/17	0.93	0.14	9,24,37,37	0
5	SO4	A	1007	5/5	0.93	0.19	38,42,45,49	0
5	SO4	G	1006	5/5	0.94	0.21	40,41,45,49	0
4	1OT	K	1004	17/17	0.94	0.15	12,20,40,40	0
5	SO4	I	1006	5/5	0.94	0.24	53,55,56,60	0
5	SO4	J	1005	5/5	0.94	0.28	51,51,55,56	0
5	SO4	L	1005	5/5	0.94	0.17	33,40,45,48	0
4	1OT	E	1004	17/17	0.94	0.15	14,20,41,42	0
2	ZN	J	1003	1/1	0.94	0.16	53,53,53,53	0
6	1PE	K	1008	12/16	0.94	0.14	16,25,38,39	0
4	1OT	G	1004	17/17	0.94	0.13	8,20,32,35	0
4	1OT	A	1004	17/17	0.94	0.12	5,20,33,34	0
4	1OT	B	1004	17/17	0.94	0.12	9,18,39,41	0
5	SO4	D	1006	5/5	0.94	0.23	44,51,54,55	0
4	1OT	C	1004	17/17	0.94	0.13	9,18,36,37	0
4	1OT	D	1004	17/17	0.95	0.13	12,21,39,39	0
5	SO4	G	1005	5/5	0.95	0.18	32,32,33,40	0
5	SO4	I	1005	5/5	0.95	0.30	50,51,54,55	0
2	ZN	C	1003	1/1	0.96	0.13	41,41,41,41	0
5	SO4	E	1005	5/5	0.96	0.22	42,45,49,50	0
5	SO4	A	1006	5/5	0.96	0.20	45,46,50,50	0
5	SO4	F	1005	5/5	0.96	0.21	44,46,49,51	0
2	ZN	H	1003	1/1	0.96	0.15	46,46,46,46	0
6	1PE	G	1009	6/16	0.96	0.19	21,22,26,33	0
5	SO4	K	1006	5/5	0.96	0.22	42,45,47,53	0
3	CO3	J	1002	4/4	0.97	0.11	5,6,11,15	0
2	ZN	F	1001	1/1	0.97	0.11	39,39,39,39	0
3	CO3	C	1002	4/4	0.98	0.12	8,10,12,17	0
3	CO3	D	1002	4/4	0.98	0.09	6,7,10,12	0
3	CO3	E	1002	4/4	0.98	0.11	8,10,11,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CO3	F	1002	4/4	0.98	0.12	7,12,14,15	0
3	CO3	G	1002	4/4	0.98	0.10	7,8,8,17	0
3	CO3	H	1002	4/4	0.98	0.10	4,10,10,12	0
3	CO3	I	1002	4/4	0.98	0.11	7,8,8,15	0
2	ZN	B	1001	1/1	0.98	0.08	36,36,36,36	0
3	CO3	K	1002	4/4	0.98	0.07	8,12,13,18	0
3	CO3	L	1002	4/4	0.98	0.12	6,8,10,12	0
2	ZN	F	1003	1/1	0.98	0.12	51,51,51,51	0
2	ZN	H	1001	1/1	0.98	0.10	36,36,36,36	0
2	ZN	B	1003	1/1	0.98	0.14	38,38,38,38	0
2	ZN	A	1003	1/1	0.98	0.10	46,46,46,46	0
2	ZN	K	1003	1/1	0.98	0.19	46,46,46,46	0
2	ZN	L	1003	1/1	0.98	0.13	45,45,45,45	0
3	CO3	B	1002	4/4	0.98	0.12	5,6,7,11	0
2	ZN	G	1001	1/1	0.99	0.06	39,39,39,39	0
2	ZN	G	1003	1/1	0.99	0.11	39,39,39,39	0
2	ZN	D	1001	1/1	0.99	0.09	36,36,36,36	0
5	SO4	D	1005	5/5	0.99	0.08	9,9,11,12	0
2	ZN	D	1003	1/1	0.99	0.14	45,45,45,45	0
2	ZN	I	1001	1/1	0.99	0.12	40,40,40,40	0
2	ZN	E	1001	1/1	0.99	0.10	36,36,36,36	0
2	ZN	K	1001	1/1	0.99	0.12	35,35,35,35	0
2	ZN	E	1003	1/1	0.99	0.17	49,49,49,49	0
2	ZN	L	1001	1/1	0.99	0.09	41,41,41,41	0
2	ZN	C	1001	1/1	0.99	0.13	41,41,41,41	0
5	SO4	H	1005	5/5	0.99	0.09	7,8,10,11	0
5	SO4	A	1005	5/5	0.99	0.07	6,7,11,13	0
3	CO3	A	1002	4/4	0.99	0.09	7,10,12,18	0
2	ZN	A	1001	1/1	0.99	0.07	37,37,37,37	0
5	SO4	K	1005	5/5	0.99	0.08	9,11,11,12	0
2	ZN	I	1003	1/1	1.00	0.15	42,42,42,42	0
2	ZN	J	1001	1/1	1.00	0.07	36,36,36,36	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 2PE H 1007:

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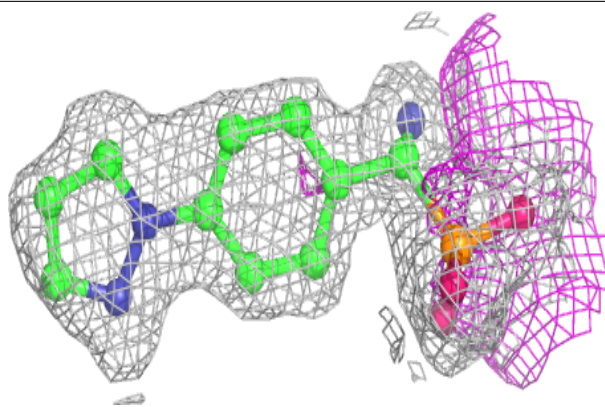$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 2PE J 1010:

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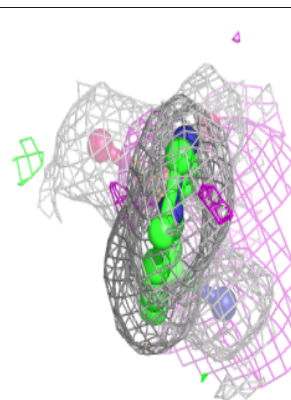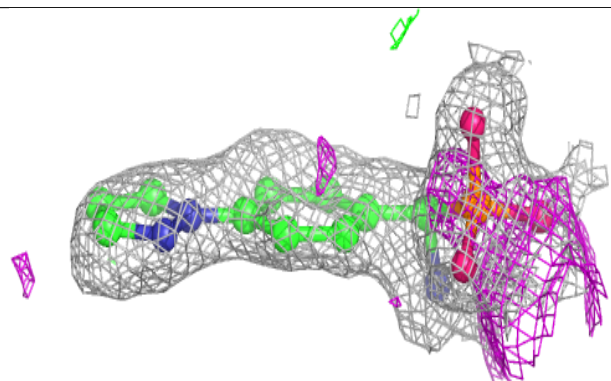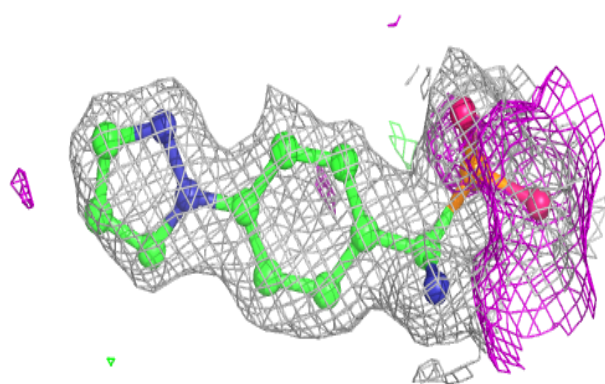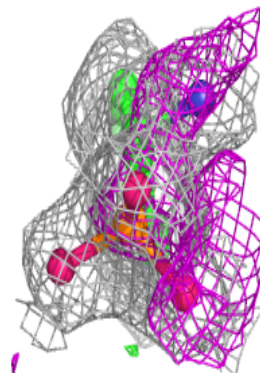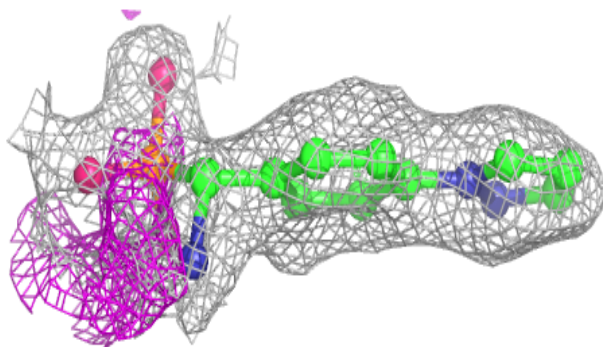$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 2PE I 1010:

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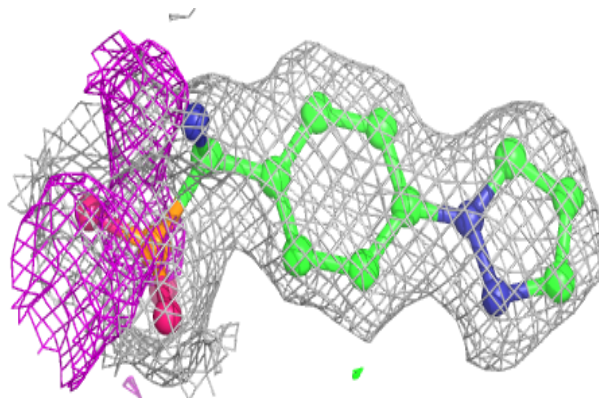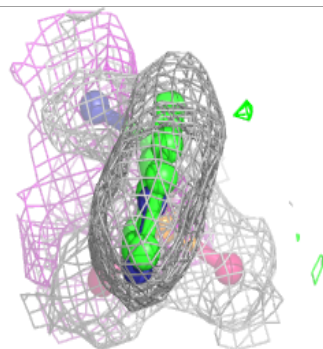$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
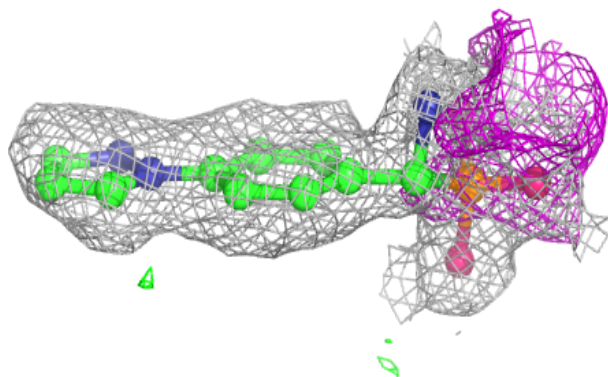and green (positive)

Electron density around 2PE E 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
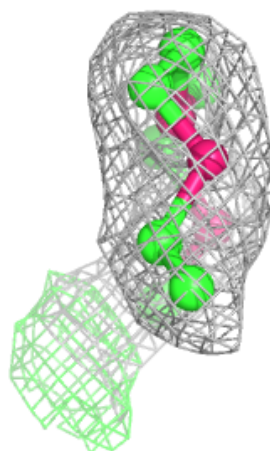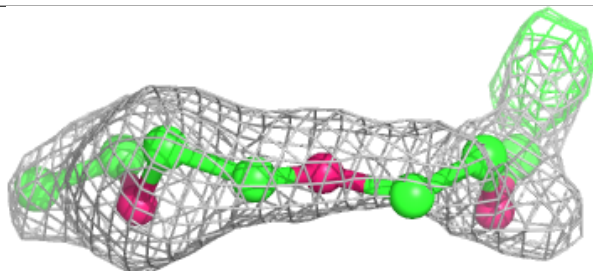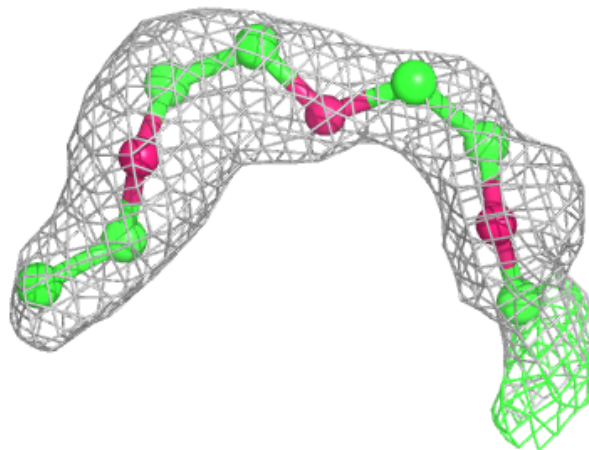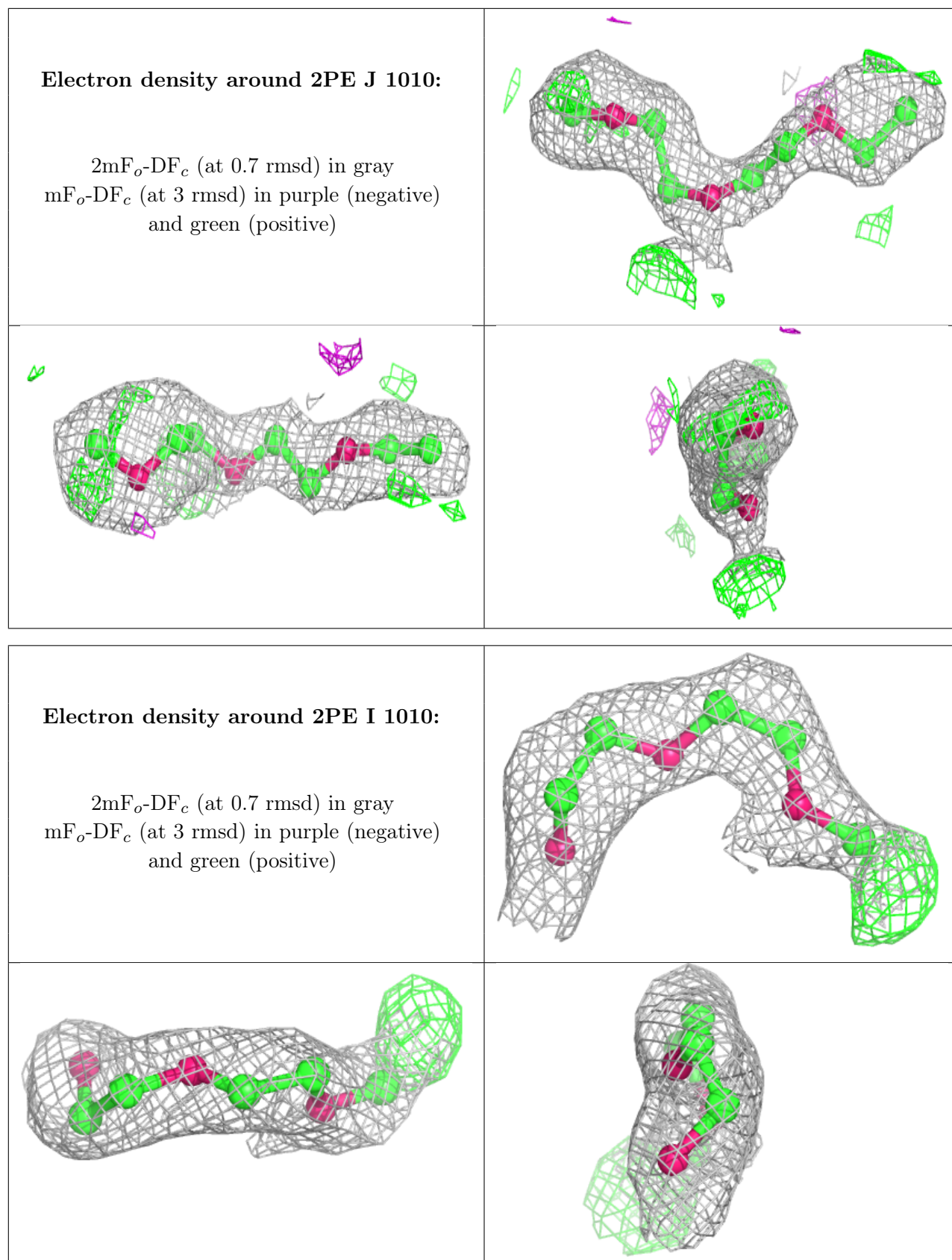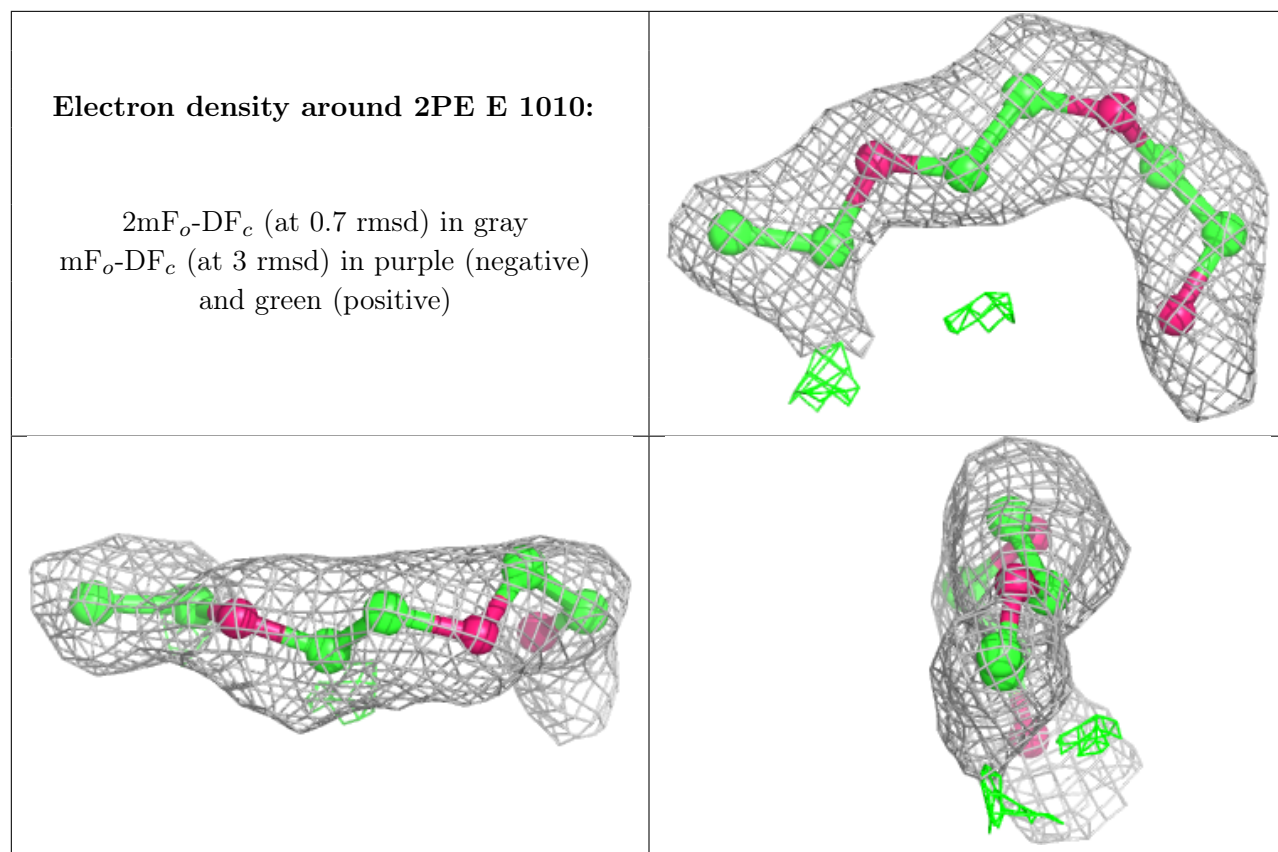
Electron density around 2PE D 1010:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
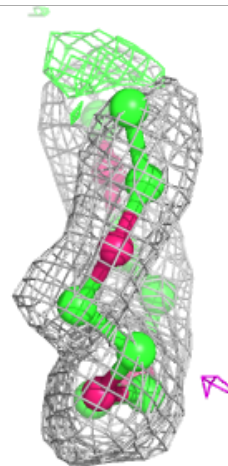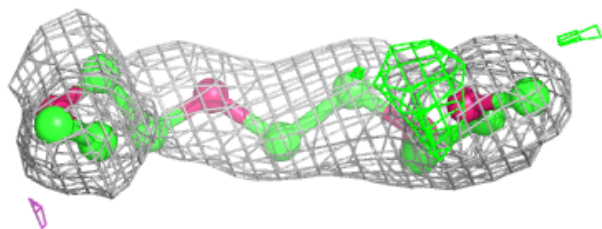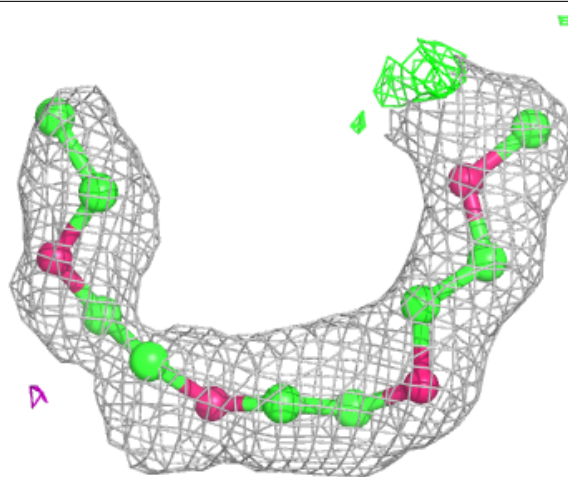
Electron density around 2PE H 1006:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
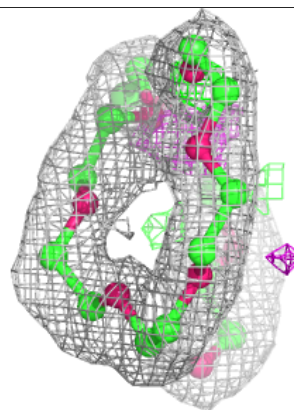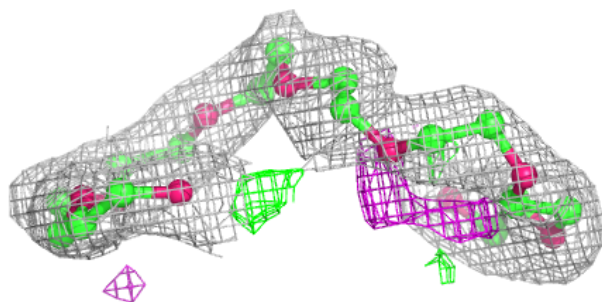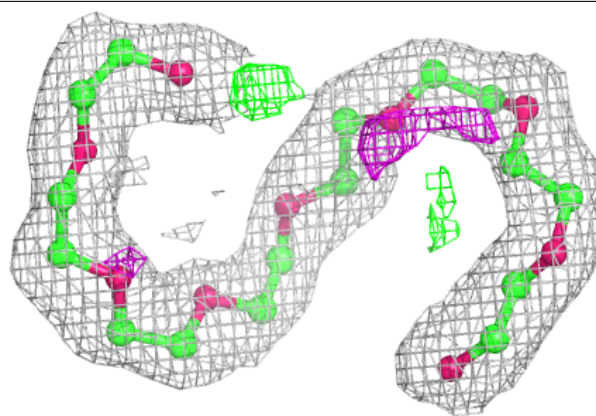
Electron density around 2PE D 1012:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
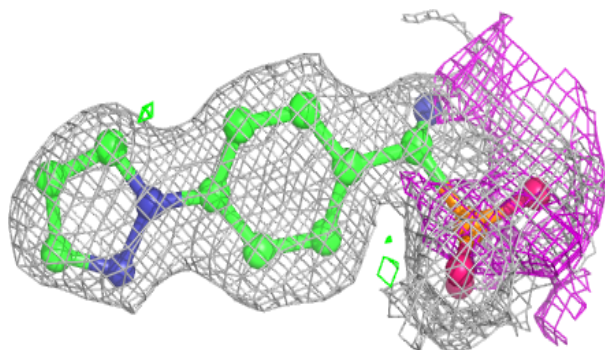$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
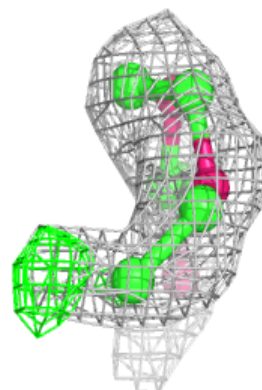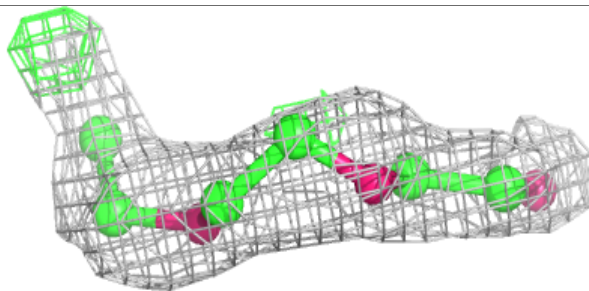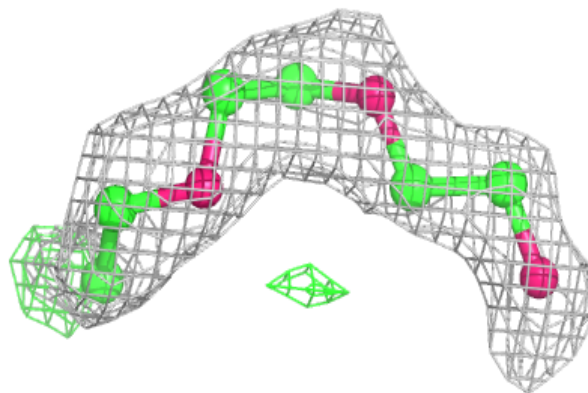
Electron density around 2PE B 1006:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
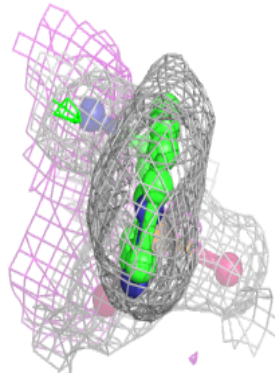mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
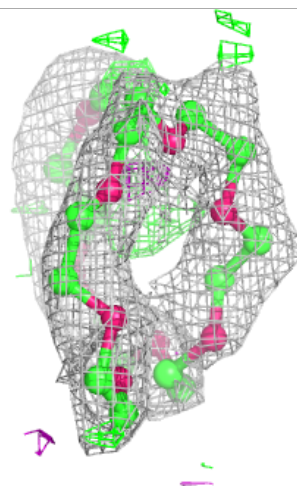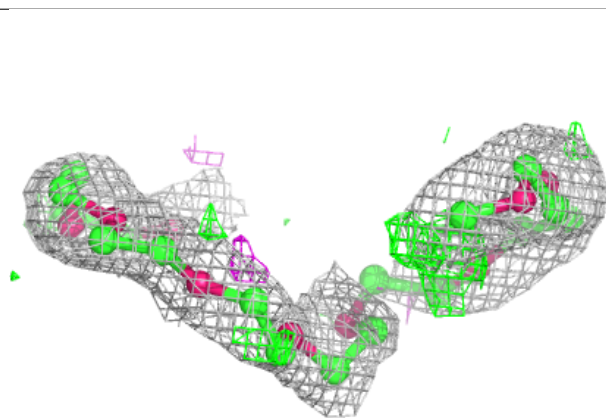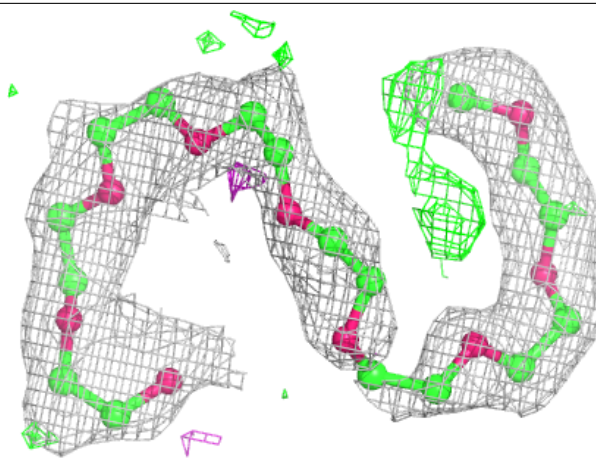
Electron density around 2PE B 1007:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
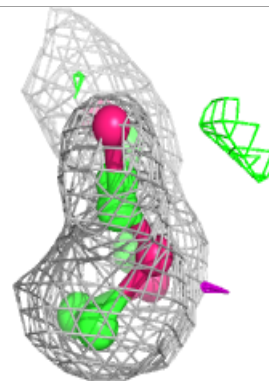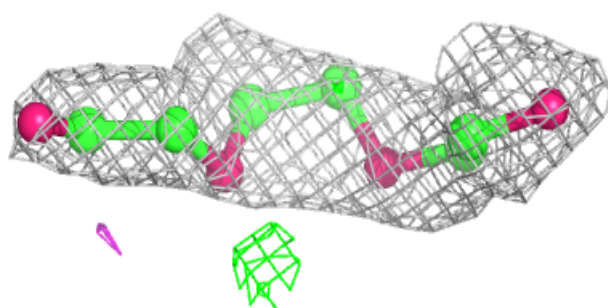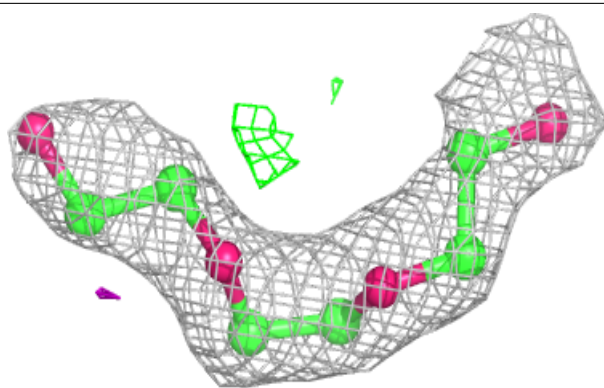
Electron density around 2PE C 1009:

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

Electron density around 2PE F 1010:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
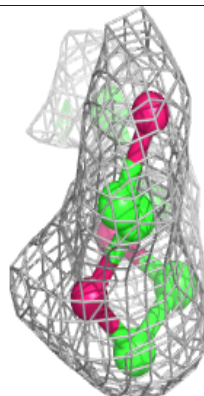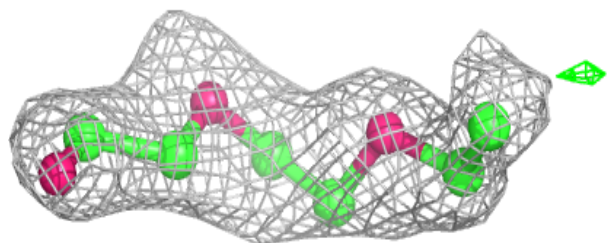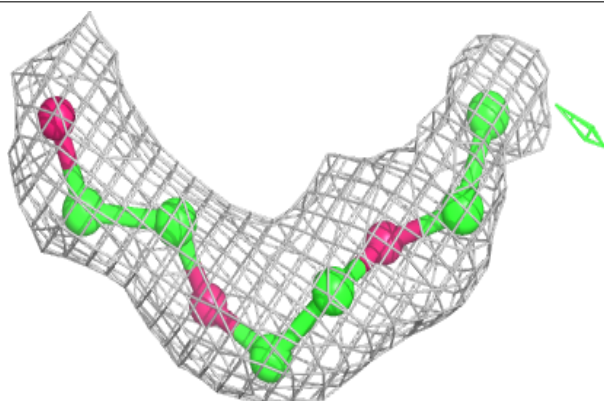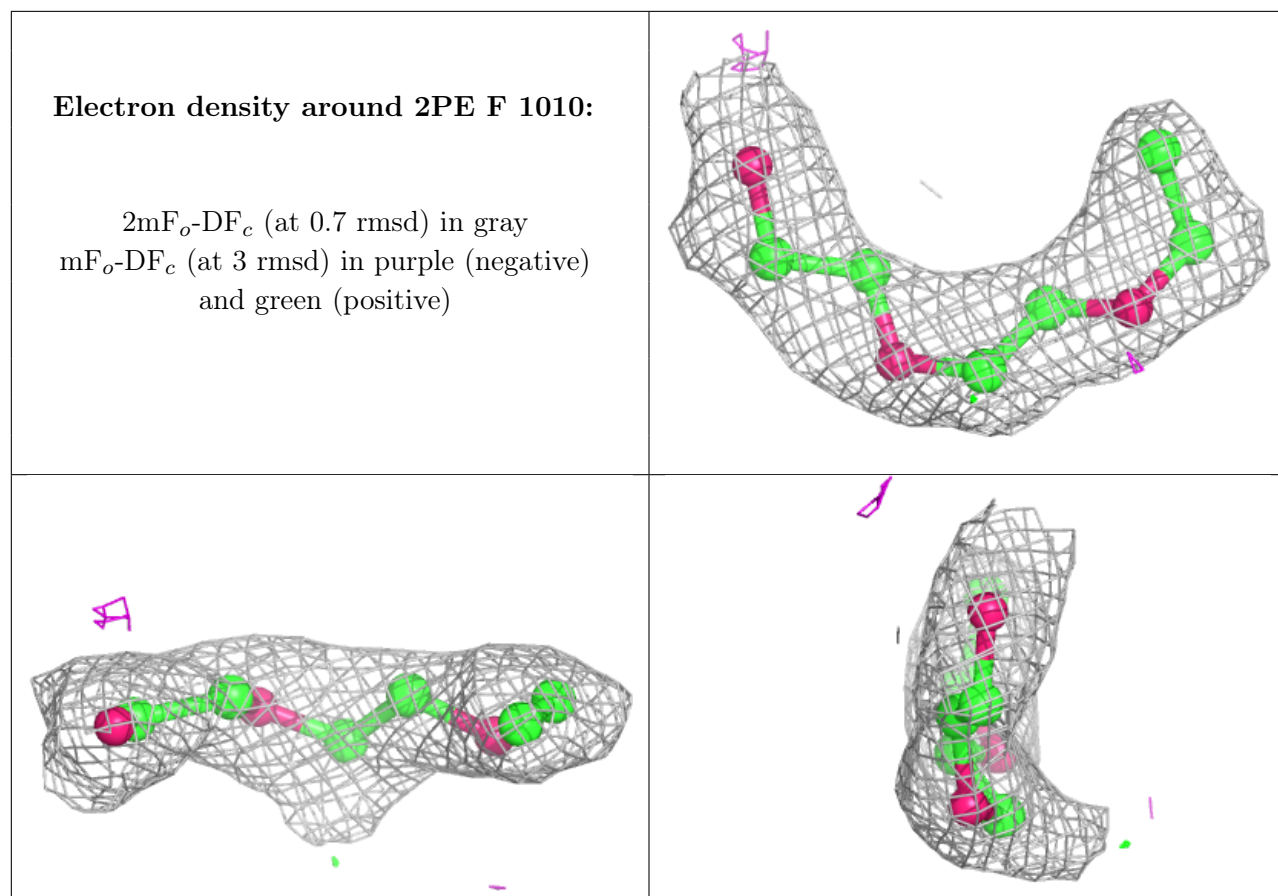
Electron density around 2PE D 1011:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
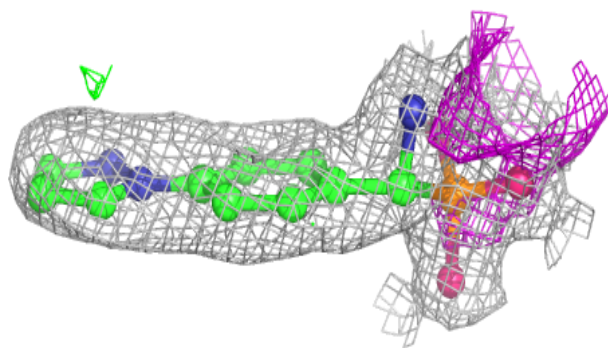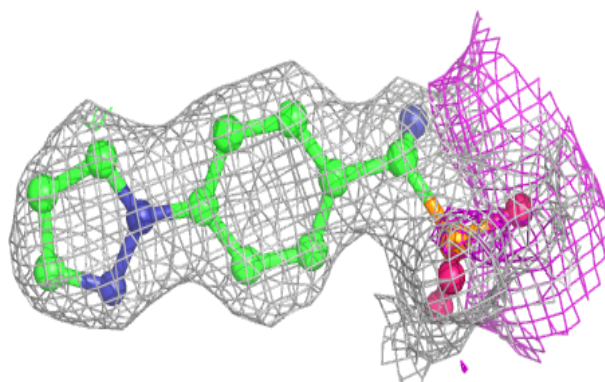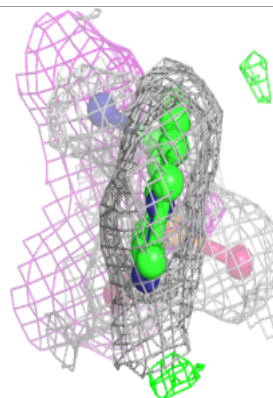and green (positive)
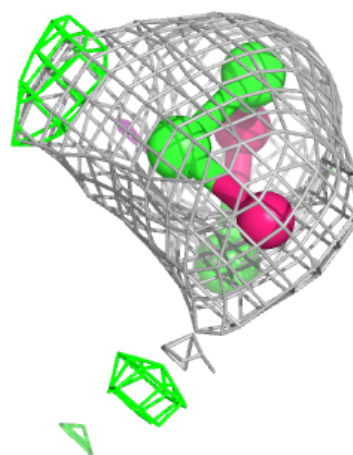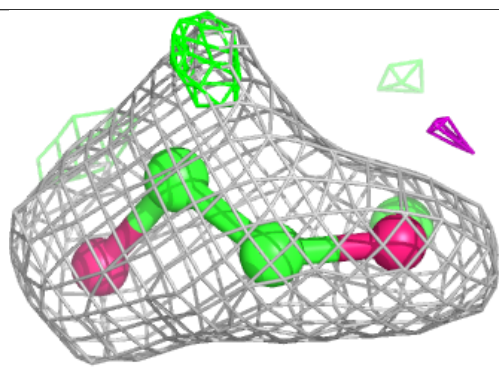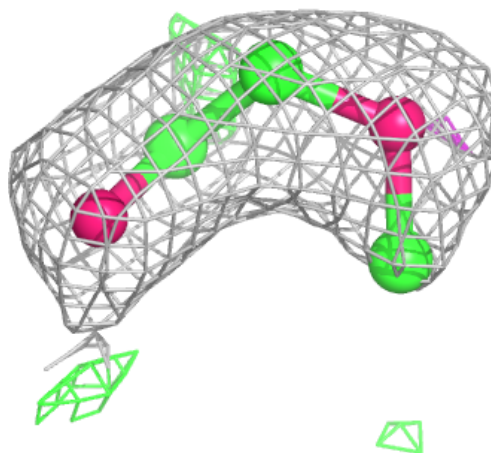
Electron density around 1OT F 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
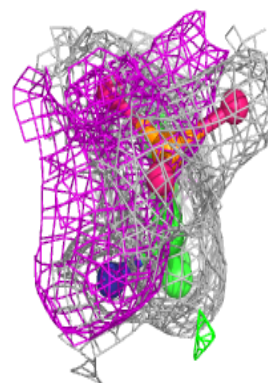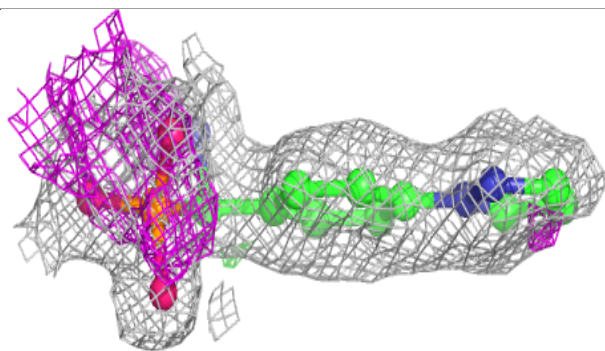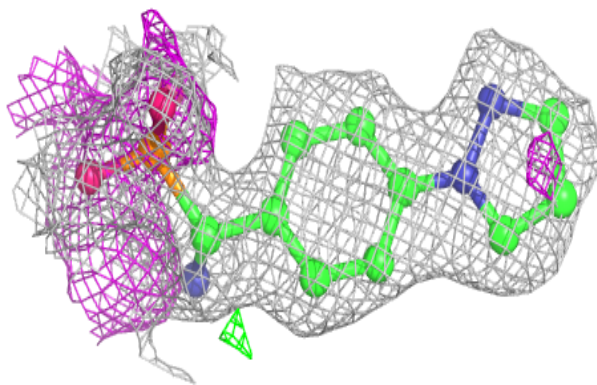
Electron density around 1OT H 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
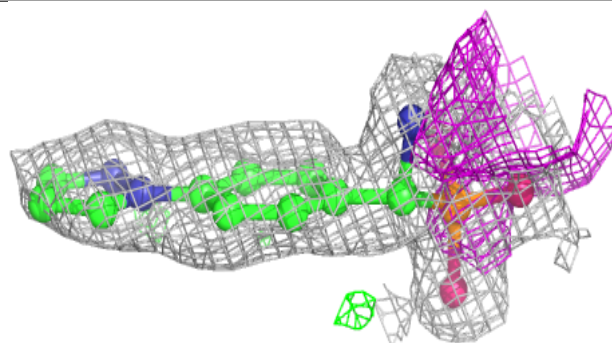and green (positive)
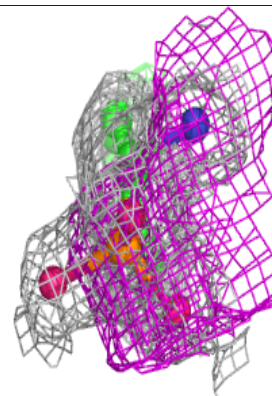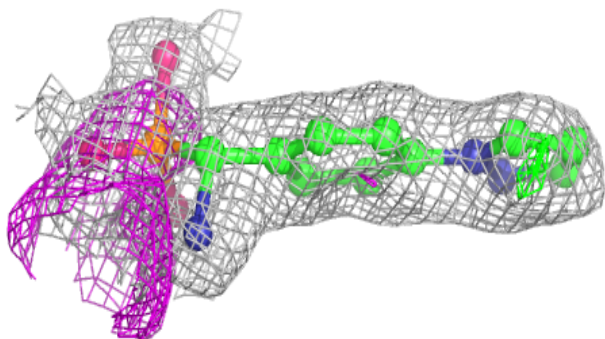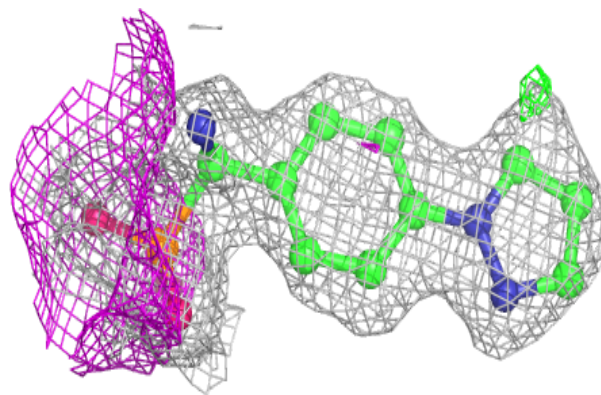
Electron density around 1OT L 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
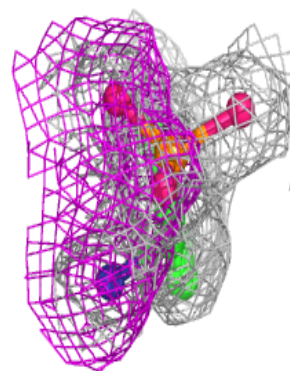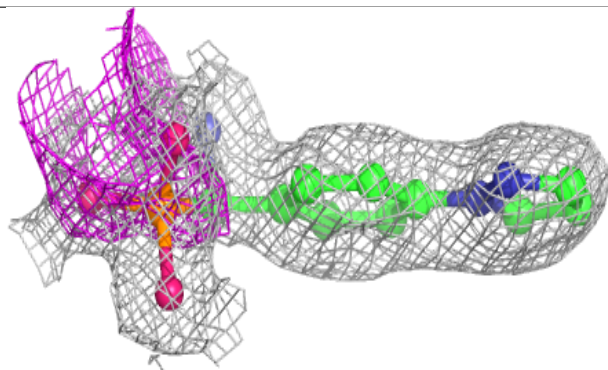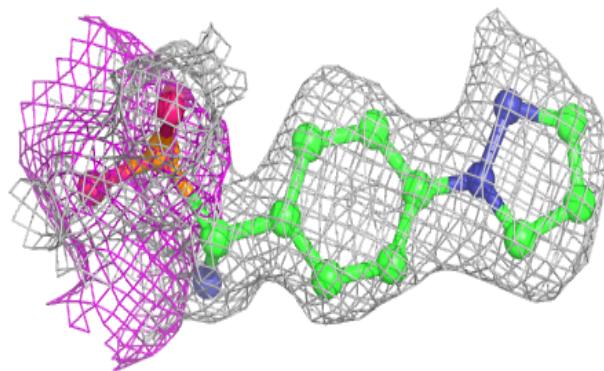
Electron density around 1OT J 1004:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
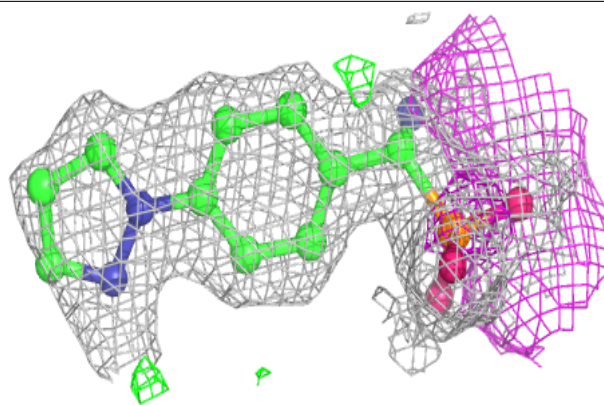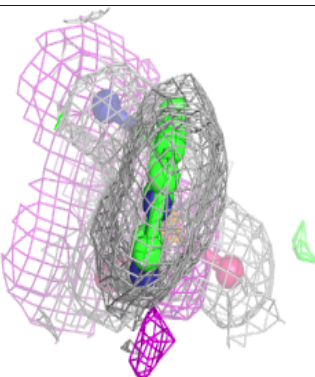and green (positive)
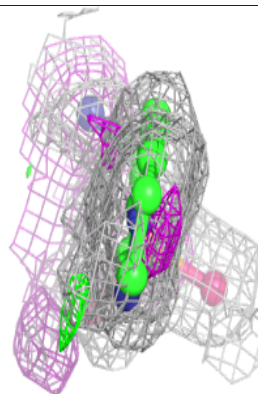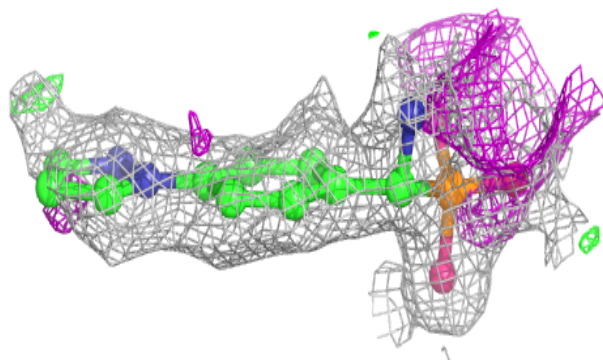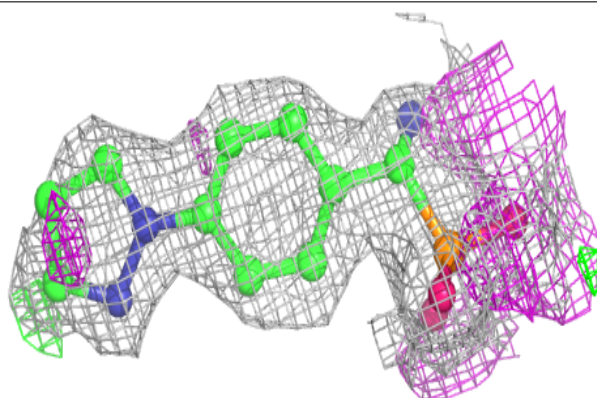
Electron density around 1OT I 1004:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
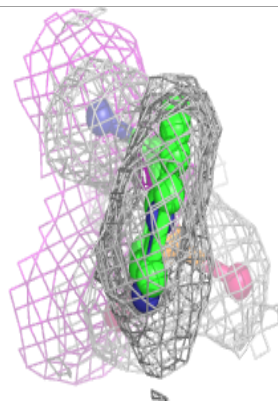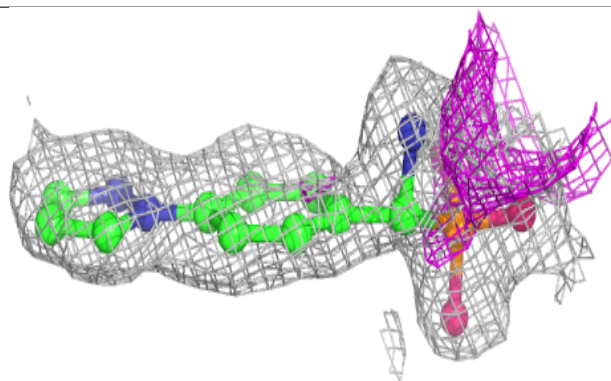
Electron density around 1OT K 1004:

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 1OT E 1004:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
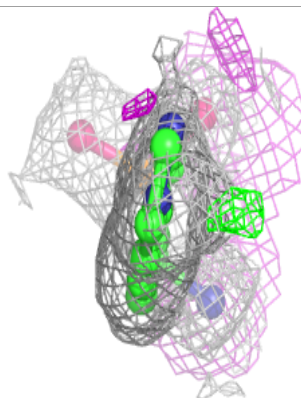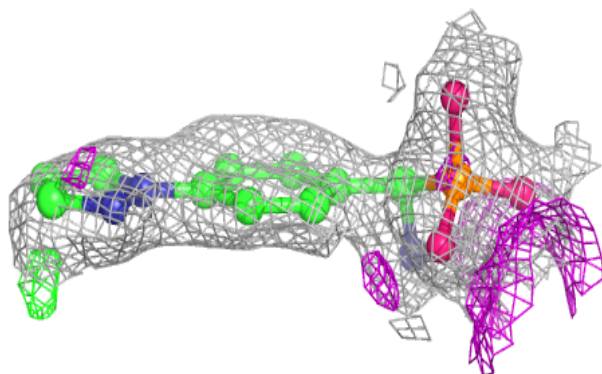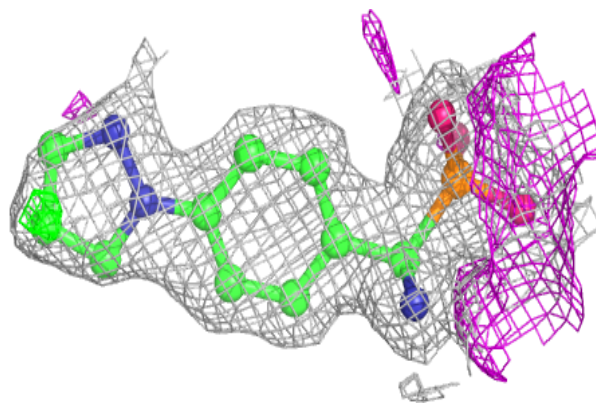
Electron density around 1OT G 1004:

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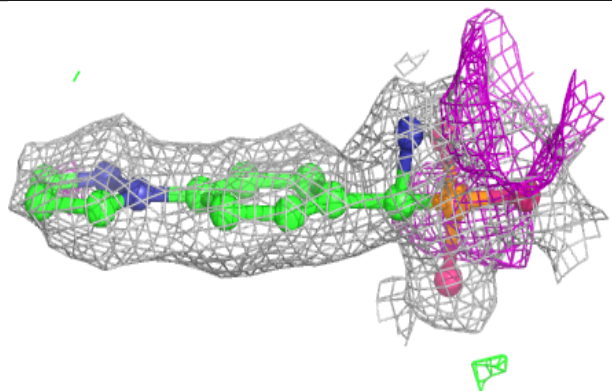and green (positive)

Electron density around 1OT A 1004:

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

Electron density around 1OT B 1004:

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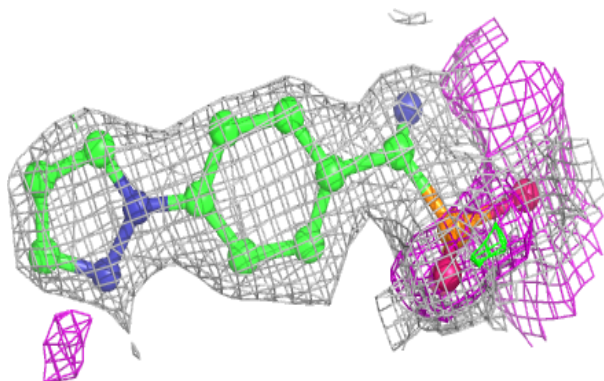mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around 1OT C 1004:

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

Electron density around 1OT D 1004:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.