Full wwPDB X-ray Structure Validation Report (i)

Jan 16, 2024 – 01:07 am GMT

PDB ID	:	6RKC
Title	:	Inter-dimeric interface controls function and stability of S-methionine adenosyltransferase from U. urealiticum
Authors	:	Shahar, A.; Zarivach, R.; Bershtein, S.; Kleiner, D.; Shmulevich, F.
Deposited on	:	2019-04-30
Resolution	:	2.56 Å(reported)

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

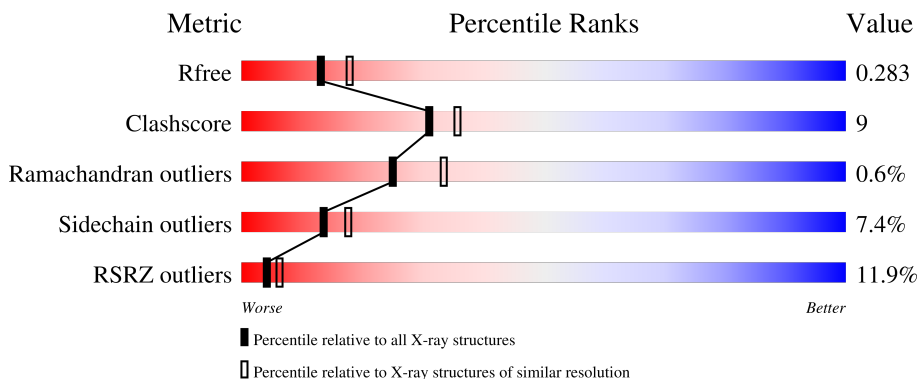|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.56 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		0.283
Clashscore		9
Ramachandran outliers		0.6%
Sidechain outliers		7.4%
RSRZ outliers		11.9%

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	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

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	382	4% / 81% / 14% · ·
1	B	382	3% / 80% / 16% · · ·
1	C	382	5% / 80% / 15% · ·
1	D	382	5% / 79% / 16% · · ·
1	E	382	16% / 71% / 21% · · ·

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Mol	Chain	Length	Quality of chain
1	F	382	15% ... 73% ... 19% ... 5%
1	G	382	23% ... 72% ... 20%
1	H	382	22% ... 70% ... 22% ... 5%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	E	403	-	-	-	X
3	MG	G	402	-	-	-	X
5	PPK	A	405	-	-	X	-
5	PPK	C	405	-	X	-	-
5	PPK	C	408	-	-	X	-

2   Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 24088 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 Methionine adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	372	Total 2917	C 1851	N 490	O 565	S 11	0	0	0
1	B	374	Total 2944	C 1871	N 495	O 567	S 11	0	1	0
1	C	373	Total 2929	C 1860	N 491	O 567	S 11	0	0	0
1	D	372	Total 2917	C 1851	N 490	O 565	S 11	0	0	0
1	E	372	Total 2917	C 1851	N 490	O 565	S 11	0	0	0
1	F	374	Total 2936	C 1863	N 495	O 567	S 11	0	0	0
1	G	373	Total 2929	C 1860	N 491	O 567	S 11	0	0	0
1	H	372	Total 2917	C 1851	N 490	O 565	S 11	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	377	HIS	-	expression tag	UNP B2NE58
A	378	HIS	-	expression tag	UNP B2NE58
A	379	HIS	-	expression tag	UNP B2NE58
A	380	HIS	-	expression tag	UNP B2NE58
A	381	HIS	-	expression tag	UNP B2NE58
A	382	HIS	-	expression tag	UNP B2NE58
B	377	HIS	-	expression tag	UNP B2NE58
B	378	HIS	-	expression tag	UNP B2NE58
B	379	HIS	-	expression tag	UNP B2NE58
B	380	HIS	-	expression tag	UNP B2NE58
B	381	HIS	-	expression tag	UNP B2NE58
B	382	HIS	-	expression tag	UNP B2NE58
C	377	HIS	-	expression tag	UNP B2NE58

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Chain	Residue	Modelled	Actual	Comment	Reference
C	378	HIS	-	expression tag	UNP B2NE58
C	379	HIS	-	expression tag	UNP B2NE58
C	380	HIS	-	expression tag	UNP B2NE58
C	381	HIS	-	expression tag	UNP B2NE58
C	382	HIS	-	expression tag	UNP B2NE58
D	377	HIS	-	expression tag	UNP B2NE58
D	378	HIS	-	expression tag	UNP B2NE58
D	379	HIS	-	expression tag	UNP B2NE58
D	380	HIS	-	expression tag	UNP B2NE58
D	381	HIS	-	expression tag	UNP B2NE58
D	382	HIS	-	expression tag	UNP B2NE58
E	377	HIS	-	expression tag	UNP B2NE58
E	378	HIS	-	expression tag	UNP B2NE58
E	379	HIS	-	expression tag	UNP B2NE58
E	380	HIS	-	expression tag	UNP B2NE58
E	381	HIS	-	expression tag	UNP B2NE58
E	382	HIS	-	expression tag	UNP B2NE58
F	377	HIS	-	expression tag	UNP B2NE58
F	378	HIS	-	expression tag	UNP B2NE58
F	379	HIS	-	expression tag	UNP B2NE58
F	380	HIS	-	expression tag	UNP B2NE58
F	381	HIS	-	expression tag	UNP B2NE58
F	382	HIS	-	expression tag	UNP B2NE58
G	377	HIS	-	expression tag	UNP B2NE58
G	378	HIS	-	expression tag	UNP B2NE58
G	379	HIS	-	expression tag	UNP B2NE58
G	380	HIS	-	expression tag	UNP B2NE58
G	381	HIS	-	expression tag	UNP B2NE58
G	382	HIS	-	expression tag	UNP B2NE58
H	377	HIS	-	expression tag	UNP B2NE58
H	378	HIS	-	expression tag	UNP B2NE58
H	379	HIS	-	expression tag	UNP B2NE58
H	380	HIS	-	expression tag	UNP B2NE58
H	381	HIS	-	expression tag	UNP B2NE58
H	382	HIS	-	expression tag	UNP B2NE58

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	K 2	0	0
2	C	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total 2	K 2	0	0
2	G	2	Total 2	K 2	0	0

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

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

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).
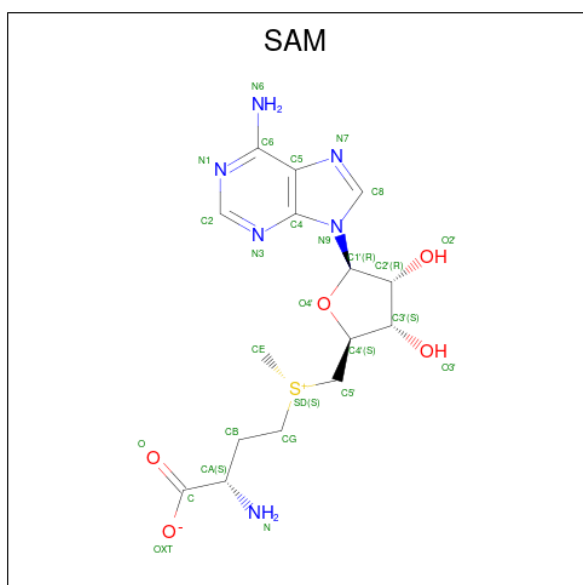
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	D	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	E	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	F	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	G	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
4	H	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 5 is (DIPHOSPHONO)AMINOPHOSPHONIC ACID (three-letter code: PPK) (formula: $H_6NO_9P_3$).

PPK

O2A O2B O1G

OH O OH

PA

O4A O——P——O——P——N——P——O O3G

O3A PB(S) PG

OH OH OH

O1A O1B O2G

N3B

H
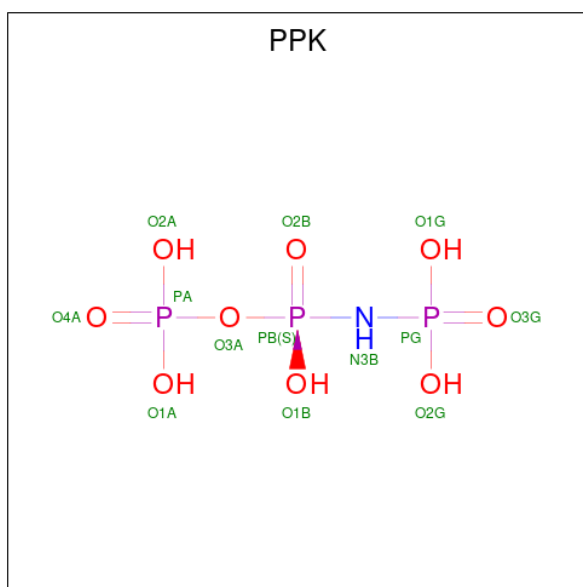
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 13	N 1	O 9	P 3	0	0
5	A	1	Total 13	N 1	O 9	P 3	0	0
5	C	1	Total 13	N 1	O 9	P 3	0	0
5	C	1	Total 13	N 1	O 9	P 3	0	0
5	E	1	Total 13	N 1	O 9	P 3	0	0
5	E	1	Total 13	N 1	O 9	P 3	0	0
5	G	1	Total 13	N 1	O 9	P 3	0	0
5	G	1	Total 13	N 1	O 9	P 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	21	Total 21	O 21	0	0
6	C	16	Total 16	O 16	0	0
6	D	18	Total 18	O 18	0	0

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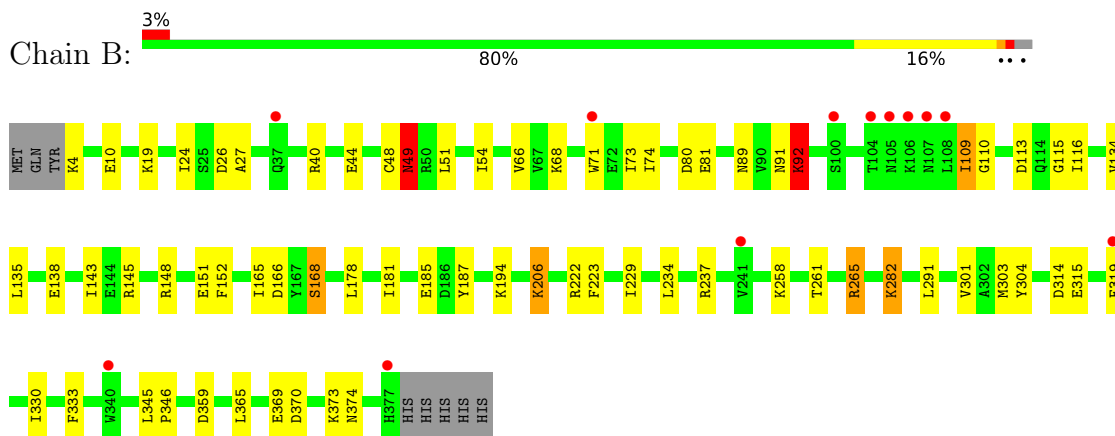| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	15	Total 15	O 15	0	0
6	F	12	Total 12	O 12	0	0
6	G	10	Total 10	O 10	0	0
6	H	6	Total 6	O 6	0	0

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.
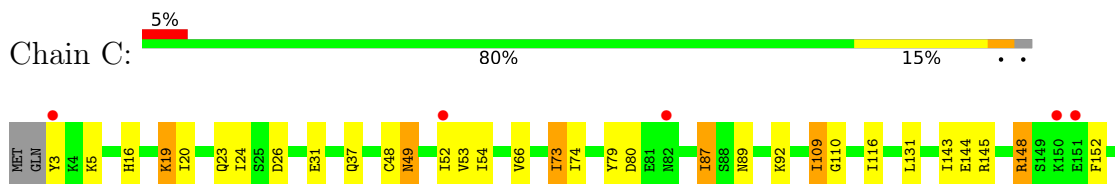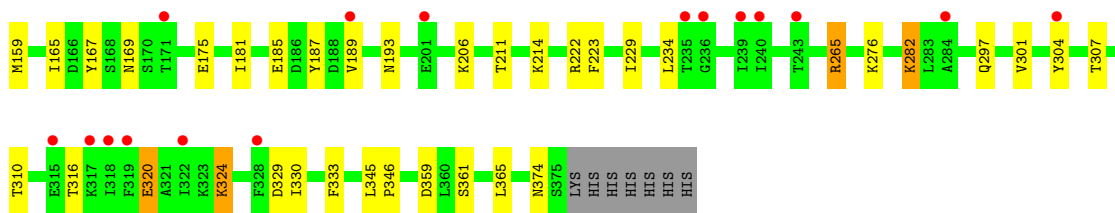
- Molecule 1: Methionine adenosyltransferase
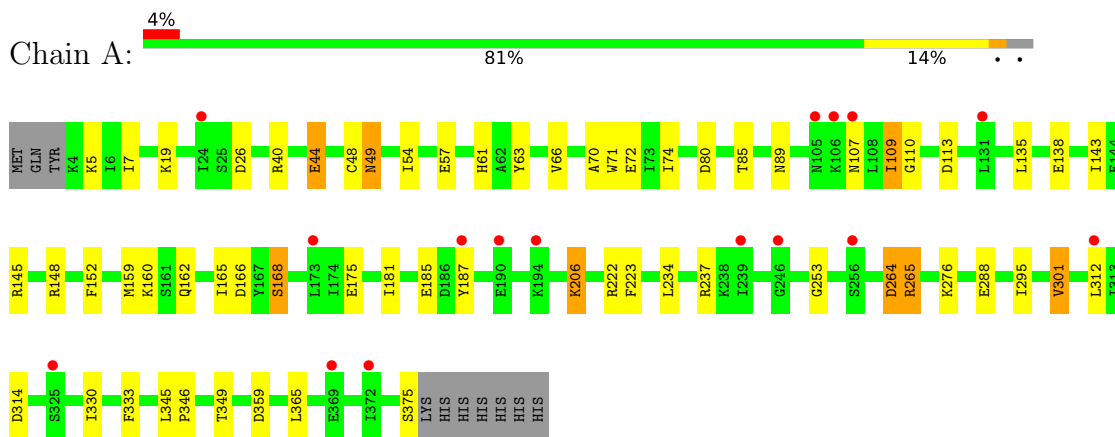
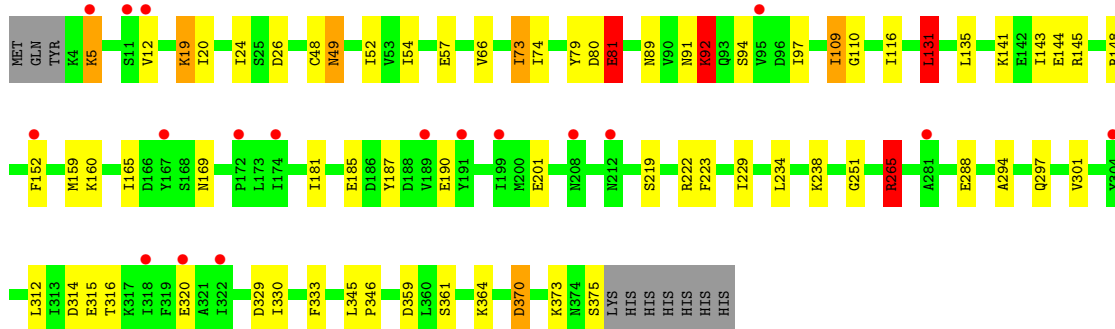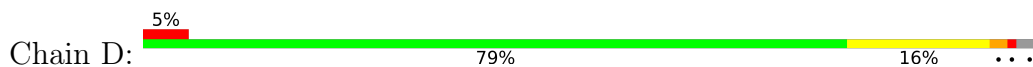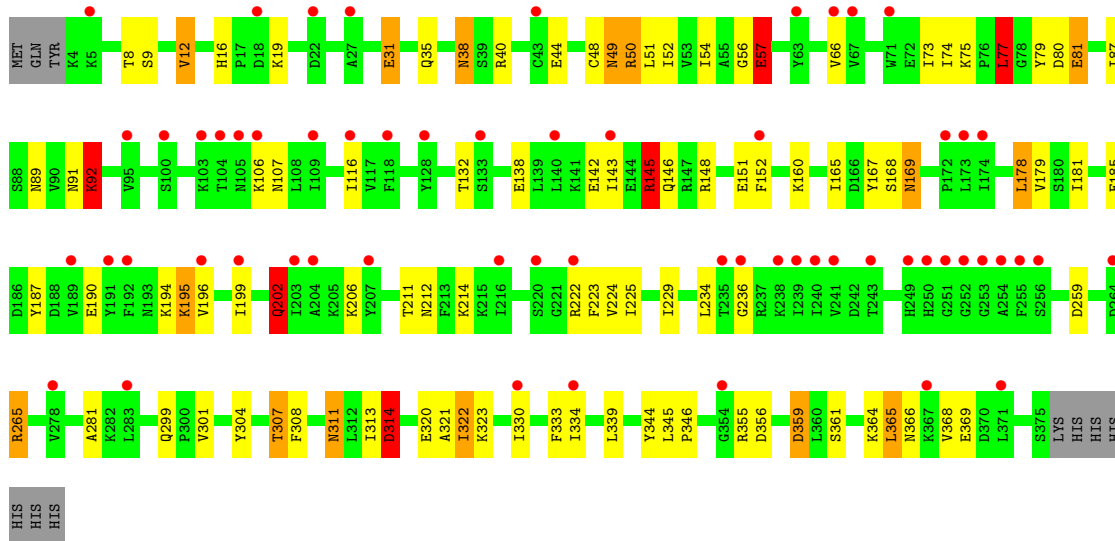- Molecule 1: Methionine adenosyltransferase

- Molecule 1: Methionine adenosyltransferase

• Molecule 1: Methionine adenosyltransferase

Chain D:

• Molecule 1: Methionine adenosyltransferase

Chain E:

• Molecule 1: Methionine adenosyltransferase

Chain F:

• Molecule 1: Methionine adenosyltransferase

Chain G:

• Molecule 1: Methionine adenosyltransferase

Chain H:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	142.37Å　79.47Å　143.79Å 90.00°　105.11°　90.00°	Depositor
Resolution (Å)	47.78　–　2.56 47.78　–　2.56	Depositor EDS
% Data completeness (in resolution range)	99.2 (47.78-2.56) 99.3 (47.78-2.56)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.260　,　0.284 0.260　,　0.283	Depositor DCC
R_{free} test set	4982 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	46.1	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 23.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	24088	wwPDB-VP
Average B, all atoms (Å^2)	66.0	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 38.47 % 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 3.6706e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, PPK, SAM, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z|>5$	RMSZ	$\#|Z|>5$
1	A	0.92	3/2969 (0.1%)	1.06	13/4016 (0.3%)
1	B	0.92	5/3001 (0.2%)	0.99	12/4058 (0.3%)
1	C	0.86	4/2982 (0.1%)	0.98	11/4034 (0.3%)
1	D	0.94	5/2969 (0.2%)	1.03	16/4016 (0.4%)
1	E	0.83	3/2969 (0.1%)	1.12	34/4016 (0.8%)
1	F	0.83	4/2989 (0.1%)	1.11	24/4042 (0.6%)
1	G	0.78	1/2982 (0.0%)	1.07	26/4034 (0.6%)
1	H	0.82	3/2969 (0.1%)	1.11	26/4016 (0.6%)
All	All	0.86	28/23830 (0.1%)	1.06	162/32232 (0.5%)

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	E	0	2
1	F	0	1
1	G	0	1
All	All	0	4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	123	ASP	CB-CG	-8.35	1.34	1.51
1	F	138	GLU	CD-OE2	-7.63	1.17	1.25
1	F	138	GLU	CG-CD	7.04	1.62	1.51
1	D	81	GLU	CG-CD	6.88	1.62	1.51
1	D	320	GLU	CD-OE2	6.65	1.32	1.25
1	B	315	GLU	CD-OE2	6.48	1.32	1.25
1	B	10	GLU	CD-OE2	5.96	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	37	GLN	CG-CD	5.87	1.64	1.51
1	D	57	GLU	CD-OE2	5.85	1.32	1.25
1	E	185	GLU	CD-OE2	-5.82	1.19	1.25
1	E	81	GLU	CD-OE2	-5.57	1.19	1.25
1	C	361	SER	CB-OG	-5.57	1.35	1.42
1	B	151	GLU	CD-OE1	5.56	1.31	1.25
1	C	31	GLU	CD-OE2	-5.54	1.19	1.25
1	B	369	GLU	CG-CD	5.51	1.60	1.51
1	F	168	SER	CB-OG	-5.39	1.35	1.42
1	D	361	SER	CB-OG	-5.35	1.35	1.42
1	A	175	GLU	CD-OE2	5.31	1.31	1.25
1	H	363	GLU	CD-OE2	-5.30	1.19	1.25
1	B	4	LYS	N-CA	5.26	1.56	1.46
1	G	264	ASP	CA-CB	5.16	1.65	1.53
1	A	72	GLU	CD-OE2	5.15	1.31	1.25
1	A	57	GLU	CD-OE1	5.15	1.31	1.25
1	H	251	GLY	C-O	5.12	1.31	1.23
1	E	345	LEU	CA-C	5.10	1.66	1.52
1	C	175	GLU	CG-CD	5.08	1.59	1.51
1	F	57	GLU	CD-OE2	-5.08	1.20	1.25
1	D	92	LYS	N-CA	5.08	1.56	1.46

All (162) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	ASP	CB-CG-OD1	-18.40	101.74	118.30
1	E	178	LEU	CB-CG-CD1	11.88	131.19	111.00
1	E	57	GLU	OE1-CD-OE2	-11.47	109.54	123.30
1	G	142	GLU	OE1-CD-OE2	-11.29	109.75	123.30
1	F	102	ASP	CB-CG-OD1	-10.98	108.42	118.30
1	A	314	ASP	CB-CG-OD2	10.87	128.08	118.30
1	G	51	LEU	CA-CB-CG	10.24	138.86	115.30
1	D	80	ASP	CB-CG-OD2	-10.03	109.28	118.30
1	H	273	TRP	CA-CB-CG	9.94	132.58	113.70
1	F	40	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	H	80	ASP	CB-CG-OD1	9.75	127.08	118.30
1	D	145	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	H	145	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	B	80	ASP	CB-CG-OD2	-8.99	110.21	118.30
1	H	123	ASP	CB-CA-C	-8.92	92.55	110.40
1	C	282	LYS	CD-CE-NZ	8.87	132.10	111.70
1	A	264	ASP	CB-CG-OD2	8.85	126.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	265	ARG	NE-CZ-NH2	8.71	124.66	120.30
1	F	117	VAL	CA-CB-CG2	8.69	123.94	110.90
1	C	145	ARG	NE-CZ-NH2	8.45	124.52	120.30
1	A	44	GLU	OE1-CD-OE2	-8.32	113.32	123.30
1	H	187	TYR	N-CA-C	8.26	133.31	111.00
1	C	214	LYS	CD-CE-NZ	8.24	130.64	111.70
1	F	145	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	F	265	ARG	NE-CZ-NH2	8.21	124.41	120.30
1	A	288	GLU	OE1-CD-OE2	-8.20	113.46	123.30
1	D	288	GLU	OE1-CD-OE2	8.13	133.05	123.30
1	G	265	ARG	NE-CZ-NH2	8.03	124.32	120.30
1	G	312	LEU	N-CA-C	-8.03	89.33	111.00
1	B	282	LYS	CD-CE-NZ	7.98	130.05	111.70
1	H	159	MET	CA-CB-CG	7.97	126.85	113.30
1	G	159	MET	CA-CB-CG	7.75	126.48	113.30
1	F	319	PHE	CB-CG-CD1	7.74	126.22	120.80
1	H	250	HIS	N-CA-C	7.54	131.35	111.00
1	E	77	LEU	CB-CG-CD2	7.47	123.70	111.00
1	F	319	PHE	CB-CG-CD2	-7.46	115.58	120.80
1	G	358	LEU	CB-CG-CD1	7.45	123.66	111.00
1	E	145	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	G	51	LEU	CB-CG-CD1	7.27	123.36	111.00
1	F	195	LYS	N-CA-C	-7.26	91.41	111.00
1	D	92	LYS	N-CA-CB	7.18	123.53	110.60
1	E	366	ASN	N-CA-CB	-7.17	97.70	110.60
1	E	356	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	H	370	ASP	CB-CG-OD2	7.14	124.73	118.30
1	B	314	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	E	57	GLU	CG-CD-OE1	7.08	132.46	118.30
1	G	106	LYS	CD-CE-NZ	7.03	127.86	111.70
1	E	314	ASP	CB-CG-OD1	7.00	124.60	118.30
1	H	123	ASP	N-CA-CB	-6.93	98.13	110.60
1	G	142	GLU	CG-CD-OE2	6.85	132.00	118.30
1	C	159	MET	CG-SD-CE	6.85	111.16	100.20
1	E	355	ARG	NE-CZ-NH2	6.85	123.72	120.30
1	G	10	GLU	CA-CB-CG	6.80	128.37	113.40
1	C	175	GLU	OE1-CD-OE2	-6.76	115.18	123.30
1	E	308	PHE	CB-CG-CD1	6.74	125.52	120.80
1	E	202	GLN	CA-CB-CG	6.71	128.17	113.40
1	F	308	PHE	CB-CG-CD1	6.71	125.50	120.80
1	G	185	GLU	OE1-CD-OE2	-6.65	115.31	123.30
1	H	243	THR	CA-CB-CG2	6.65	121.71	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	VAL	CG1-CB-CG2	6.63	121.51	110.90
1	F	222	ARG	NE-CZ-NH1	-6.61	116.99	120.30
1	B	145	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	F	152	PHE	CB-CA-C	6.59	123.58	110.40
1	H	80	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	G	92	LYS	CB-CG-CD	6.55	128.64	111.60
1	B	40	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	H	203	ILE	CG1-CB-CG2	-6.51	97.07	111.40
1	A	359	ASP	CB-CG-OD2	-6.51	112.44	118.30
1	A	145	ARG	NE-CZ-NH2	6.49	123.55	120.30
1	E	322	ILE	N-CA-C	-6.46	93.55	111.00
1	D	80	ASP	CB-CG-OD1	6.46	124.11	118.30
1	E	40	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	F	195	LYS	CD-CE-NZ	6.40	126.43	111.70
1	G	124	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	F	237	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	F	203	ILE	CG1-CB-CG2	-6.34	97.45	111.40
1	D	159	MET	CG-SD-CE	6.32	110.31	100.20
1	H	123	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	370	ASP	CB-CG-OD2	6.26	123.94	118.30
1	D	329	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	C	80	ASP	CB-CG-OD1	6.22	123.89	118.30
1	A	145	ARG	NE-CZ-NH1	-6.21	117.19	120.30
1	D	141	LYS	CD-CE-NZ	6.16	125.87	111.70
1	B	369	GLU	OE1-CD-OE2	-6.10	115.97	123.30
1	F	307	THR	N-CA-C	-6.04	94.68	111.00
1	C	131	LEU	CB-CG-CD1	6.03	121.24	111.00
1	E	359	ASP	CB-CG-OD1	6.01	123.71	118.30
1	E	366	ASN	CB-CA-C	-5.99	98.42	110.40
1	E	307	THR	N-CA-C	-5.98	94.86	111.00
1	F	80	ASP	CB-CG-OD1	5.97	123.67	118.30
1	H	123	ASP	OD1-CG-OD2	-5.96	111.99	123.30
1	H	188	ASP	N-CA-CB	5.95	121.31	110.60
1	D	265	ARG	CG-CD-NE	5.94	124.28	111.80
1	B	80	ASP	CB-CG-OD1	5.94	123.64	118.30
1	G	159	MET	CG-SD-CE	-5.93	90.71	100.20
1	D	145	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	D	314	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	80	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	40	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	H	145	ARG	CG-CD-NE	-5.89	99.42	111.80
1	E	320	GLU	CA-CB-CG	5.85	126.27	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	345	LEU	N-CA-C	-5.85	95.21	111.00
1	B	92	LYS	N-CA-CB	5.83	121.10	110.60
1	H	159	MET	CG-SD-CE	-5.83	90.87	100.20
1	F	148	ARG	NE-CZ-NH1	5.82	123.21	120.30
1	G	80	ASP	CB-CG-OD1	5.81	123.53	118.30
1	D	201	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	A	159	MET	CG-SD-CE	-5.79	90.94	100.20
1	B	206	LYS	CB-CG-CD	5.76	126.59	111.60
1	E	50	ARG	CG-CD-NE	5.75	123.87	111.80
1	G	10	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	D	131	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	40	ARG	NE-CZ-NH2	-5.71	117.45	120.30
1	E	345	LEU	CA-C-N	5.69	133.04	117.10
1	F	308	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	H	264	ASP	CB-CG-OD1	5.65	123.39	118.30
1	E	323	LYS	N-CA-CB	5.62	120.72	110.60
1	F	222	ARG	CA-CB-CG	5.61	125.75	113.40
1	F	301	VAL	CG1-CB-CG2	5.60	119.86	110.90
1	F	308	PHE	N-CA-CB	-5.60	100.52	110.60
1	E	355	ARG	NH1-CZ-NH2	-5.60	113.24	119.40
1	G	314	ASP	CB-CG-OD1	5.56	123.30	118.30
1	H	123	ASP	N-CA-C	5.56	126.01	111.00
1	C	359	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	H	367	LYS	CG-CD-CE	-5.49	95.43	111.90
1	E	80	ASP	CB-CG-OD1	5.47	123.22	118.30
1	E	355	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	G	31	GLU	OE1-CD-OE2	-5.44	116.78	123.30
1	E	365	LEU	C-N-CA	5.41	135.23	121.70
1	C	116	ILE	CG1-CB-CG2	-5.40	99.51	111.40
1	G	312	LEU	CB-CG-CD2	5.38	120.15	111.00
1	H	145	ARG	NH1-CZ-NH2	5.33	125.27	119.40
1	E	308	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	G	243	THR	CA-CB-CG2	5.32	119.85	112.40
1	G	222	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	B	319[A]	PHE	CB-CG-CD1	5.30	124.51	120.80
1	B	319[B]	PHE	CB-CG-CD1	5.30	124.51	120.80
1	F	288	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	G	19	LYS	CB-CG-CD	5.29	125.36	111.60
1	E	92	LYS	N-CA-CB	5.28	120.10	110.60
1	G	103	LYS	CB-CG-CD	5.25	125.24	111.60
1	E	148	ARG	CG-CD-NE	-5.22	100.83	111.80
1	C	148	ARG	CB-CG-CD	5.22	125.16	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	212	ASN	CB-CG-OD1	-5.20	111.19	121.60
1	G	265	ARG	CG-CD-NE	-5.20	100.89	111.80
1	E	346	PRO	CB-CA-C	-5.18	99.04	112.00
1	F	153	ILE	N-CA-CB	5.18	122.70	110.80
1	C	329	ASP	CB-CG-OD1	-5.17	113.65	118.30
1	E	265	ARG	CG-CD-NE	-5.15	100.99	111.80
1	G	259	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	113	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	E	307	THR	CA-C-O	-5.13	109.34	120.10
1	E	308	PHE	N-CA-CB	-5.09	101.44	110.60
1	H	265	ARG	NH1-CZ-NH2	-5.08	113.81	119.40
1	G	81	GLU	CG-CD-OE1	5.08	128.45	118.30
1	H	31	GLU	CG-CD-OE1	5.07	128.44	118.30
1	H	265	ARG	CG-CD-NE	-5.07	101.15	111.80
1	F	151	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	D	315	GLU	CA-CB-CG	5.02	124.44	113.40
1	E	50	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	H	145	ARG	CD-NE-CZ	5.01	130.62	123.60
1	D	5	LYS	CD-CE-NZ	5.01	123.21	111.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	344	TYR	Peptide
1	E	359	ASP	Mainchain
1	F	212	ASN	Sidechain
1	G	50	ARG	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	2917	0	2915	32	0
1	B	2944	0	2944	39	1
1	C	2929	0	2924	36	0
1	D	2917	0	2915	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2917	0	2915	73	1
1	F	2936	0	2935	78	0
1	G	2929	0	2924	67	0
1	H	2917	0	2915	93	0
2	A	2	0	0	0	0
2	C	1	0	0	0	0
2	E	2	0	0	0	0
2	G	2	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
3	G	3	0	0	0	0
3	H	1	0	0	0	0
4	A	54	0	44	8	0
4	B	54	0	44	0	0
4	C	54	0	44	2	0
4	D	54	0	44	2	0
4	E	54	0	44	1	0
4	F	54	0	44	4	0
4	G	54	0	44	8	0
4	H	54	0	44	7	0
5	A	26	0	2	9	0
5	C	26	0	2	7	0
5	E	26	0	2	3	0
5	G	26	0	2	2	0
6	A	25	0	0	2	0
6	B	21	0	0	0	0
6	C	16	0	0	0	0
6	D	18	0	0	1	0
6	E	15	0	0	1	0
6	F	12	0	0	1	0
6	G	10	0	0	1	0
6	H	6	0	0	0	0
All	All	24088	0	23747	436	1

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 9.

All (436) 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:E:146:GLN:OE1	1:E:195:LYS:NZ	1.76	1.17
1:E:57:GLU:OE2	4:F:402:SAM:N	1.86	1.08
1:F:145:ARG:NH1	1:F:151:GLU:OE1	1.93	1.00
1:H:130:PRO:HG3	1:H:247:VAL:HG11	1.44	0.99
1:H:74:ILE:HG23	1:H:79:TYR:HB2	1.43	0.98
1:D:94:SER:HB3	1:D:97:ILE:HD12	1.43	0.97
1:C:89:ASN:ND2	1:D:48:CYS:SG	2.37	0.97
1:C:74:ILE:HG23	1:C:79:TYR:HB2	1.44	0.97
1:F:152:PHE:O	1:F:191:TYR:OH	1.80	0.96
1:H:90:VAL:HG21	4:H:403:SAM:N7	1.80	0.96
1:H:130:PRO:CG	1:H:247:VAL:HG11	1.96	0.95
1:E:73:ILE:O	1:E:77:LEU:HD22	1.66	0.95
1:D:74:ILE:HG23	1:D:79:TYR:HB2	1.46	0.94
1:G:74:ILE:HG23	1:G:79:TYR:HB2	1.50	0.92
1:G:243:THR:HG22	1:G:244:TYR:CD2	2.05	0.92
1:D:294:ALA:HB3	1:D:297:GLN:HG3	1.53	0.90
1:F:54:ILE:HD13	1:F:66:VAL:HG13	1.54	0.90
1:F:94:SER:O	1:F:97:ILE:HG22	1.72	0.89
1:H:243:THR:HG22	1:H:244:TYR:CD2	2.08	0.89
1:F:74:ILE:HG23	1:F:79:TYR:HB2	1.53	0.89
1:B:91:ASN:O	1:B:91:ASN:ND2	2.06	0.89
1:G:138:GLU:OE2	1:G:207:TYR:OH	1.90	0.88
1:E:31:GLU:OE1	1:E:35:GLN:NE2	2.05	0.88
1:B:54:ILE:HD13	1:B:66:VAL:HG13	1.54	0.87
1:E:73:ILE:O	1:E:77:LEU:CD2	2.25	0.84
1:G:226:GLY:O	1:G:229:ILE:HG22	1.78	0.83
1:G:60:THR:O	4:G:405:SAM:HG1	1.78	0.83
1:G:56:GLY:HA2	1:H:232:THR:HG21	1.62	0.82
1:E:74:ILE:HG23	1:E:79:TYR:HB2	1.61	0.82
1:A:61:HIS:CD2	1:F:373:LYS:HG3	2.16	0.81
1:F:277:ASN:HD21	1:F:365:LEU:HA	1.44	0.81
1:A:54:ILE:HD13	1:A:66:VAL:HG13	1.63	0.81
1:H:54:ILE:HD13	1:H:66:VAL:HG13	1.63	0.81
1:A:312:LEU:HD12	1:A:312:LEU:O	1.81	0.81
1:D:54:ILE:HD13	1:D:66:VAL:HG13	1.63	0.81
1:H:12:VAL:HG23	1:H:19:LYS:HG3	1.62	0.80
4:D:403:SAM:HE3	4:D:403:SAM:N3	1.98	0.79
4:G:403:SAM:HG2	1:H:97:ILE:HD13	1.63	0.79
1:G:258:LYS:NZ	1:G:264:ASP:OD2	2.15	0.79
1:E:12:VAL:HG21	1:E:16:HIS:CD2	2.19	0.78
5:A:405:PPK:O4A	5:A:405:PPK:O3G	2.01	0.77
1:H:90:VAL:CG2	4:H:403:SAM:N7	2.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:HIS:O	1:H:240:ILE:HD13	1.85	0.76
1:F:313:ILE:HG12	1:F:314:ASP:N	1.99	0.76
1:F:334:ILE:HA	1:F:339:LEU:HD12	1.67	0.76
1:E:165:ILE:HG23	1:E:167:TYR:CE2	2.20	0.76
1:H:263:VAL:HG22	1:H:267:ALA:HB2	1.67	0.75
1:F:319:PHE:O	1:F:322:ILE:HG22	1.87	0.74
1:E:12:VAL:HG23	1:E:160:LYS:HG2	1.67	0.74
5:G:409:PPK:O2G	5:G:409:PPK:O2B	2.05	0.74
5:A:409:PPK:O1B	5:A:409:PPK:O3G	2.04	0.74
1:H:153:ILE:HD12	1:H:154:LYS:HG3	1.69	0.74
1:E:146:GLN:HG2	1:E:151:GLU:HB2	1.70	0.74
4:A:406:SAM:HE3	4:A:406:SAM:C4	2.18	0.73
1:F:277:ASN:ND2	1:F:365:LEU:HA	2.03	0.73
1:G:260:PRO:O	1:G:266:SER:OG	2.07	0.72
1:F:225:ILE:HD12	1:F:229:ILE:HG22	1.69	0.72
1:H:91:ASN:O	1:H:92:LYS:HG2	1.90	0.72
1:H:217:ILE:O	1:H:217:ILE:HD12	1.90	0.72
1:E:54:ILE:HD13	1:E:66:VAL:HG13	1.71	0.71
1:G:51:LEU:CD1	1:G:53:VAL:HG23	2.19	0.71
1:G:51:LEU:HD12	1:G:53:VAL:HG23	1.73	0.71
1:H:48:CYS:SG	1:H:232:THR:HG22	2.31	0.70
1:H:27:ALA:HB2	1:H:73:ILE:HD11	1.74	0.70
1:D:131:LEU:HD13	1:D:165:ILE:HD13	1.71	0.70
1:E:321:ALA:C	1:E:322:ILE:O	2.24	0.70
1:C:276:LYS:HE2	1:C:365:LEU:HD11	1.72	0.70
1:C:54:ILE:HD13	1:C:66:VAL:HG13	1.74	0.70
1:A:276:LYS:HE2	1:A:365:LEU:HD11	1.74	0.69
1:F:74:ILE:CG2	1:F:79:TYR:HB2	2.21	0.69
1:H:273:TRP:CH2	1:H:366:ASN:OD1	2.45	0.69
1:G:74:ILE:CG2	1:G:79:TYR:HB2	2.22	0.69
1:C:234:LEU:HD23	1:D:234:LEU:HD23	1.75	0.69
4:D:403:SAM:N3	4:D:403:SAM:CE	2.55	0.68
1:F:260:PRO:O	1:F:266:SER:OG	2.12	0.68
1:G:56:GLY:HA2	1:H:232:THR:CG2	2.23	0.68
1:G:189:VAL:HG22	1:G:193:ASN:ND2	2.07	0.68
1:H:105:ASN:C	1:H:105:ASN:HD22	1.96	0.68
1:E:75:LYS:CE	1:E:81:GLU:OE2	2.42	0.67
1:A:63:TYR:HB2	4:A:406:SAM:HB1	1.75	0.67
1:E:74:ILE:CG2	1:E:79:TYR:HB2	2.23	0.67
1:E:165:ILE:CG2	1:E:167:TYR:CE2	2.78	0.67
1:E:12:VAL:CG2	1:E:16:HIS:CD2	2.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:130:PRO:HG2	1:H:247:VAL:HG11	1.75	0.67
5:C:405:PPK:O1G	5:C:405:PPK:O4A	2.13	0.66
1:A:54:ILE:HD13	1:A:66:VAL:CG1	2.24	0.66
1:B:109:ILE:HD13	1:B:261:THR:HG22	1.76	0.66
1:F:54:ILE:HD13	1:F:66:VAL:CG1	2.25	0.66
1:H:74:ILE:CG2	1:H:79:TYR:HB2	2.21	0.66
1:E:12:VAL:CG1	1:E:19:LYS:HG3	2.26	0.66
1:F:319:PHE:O	1:F:322:ILE:CG2	2.44	0.65
4:A:404:SAM:OXT	6:A:501:HOH:O	2.15	0.65
1:E:54:ILE:HD13	1:E:66:VAL:CG1	2.26	0.65
1:H:131:LEU:HD23	1:H:165:ILE:HD13	1.78	0.65
1:H:90:VAL:HG21	4:H:403:SAM:C5	2.27	0.64
1:D:54:ILE:HD13	1:D:66:VAL:CG1	2.26	0.64
1:D:74:ILE:CG2	1:D:79:TYR:HB2	2.23	0.64
1:G:125:THR:HG22	1:G:129:MET:H	1.64	0.63
1:H:217:ILE:O	1:H:217:ILE:CD1	2.47	0.63
1:E:75:LYS:NZ	1:E:81:GLU:OE2	2.32	0.62
1:H:54:ILE:HD13	1:H:66:VAL:CG1	2.29	0.62
1:G:229:ILE:O	1:H:91:ASN:ND2	2.33	0.62
1:H:263:VAL:HG22	1:H:267:ALA:CB	2.29	0.62
1:A:234:LEU:HD23	1:B:234:LEU:HD23	1.82	0.62
1:F:94:SER:O	1:F:97:ILE:CG2	2.46	0.62
1:H:217:ILE:O	1:H:217:ILE:CG1	2.47	0.62
1:C:74:ILE:CG2	1:C:79:TYR:HB2	2.23	0.62
1:G:374:ASN:O	1:G:375:SER:HB2	1.99	0.61
1:A:253:GLY:HA3	1:A:264:ASP:OD2	2.00	0.61
1:F:75:LYS:NZ	1:F:81:GLU:OE2	2.33	0.61
1:G:58:ILE:O	4:G:405:SAM:O2'	2.14	0.61
1:G:302:ALA:HB1	1:H:6:ILE:HG21	1.81	0.61
1:E:304:TYR:CE1	1:F:5:LYS:HG3	2.36	0.61
1:B:27:ALA:HB2	1:B:73:ILE:HD11	1.83	0.60
1:B:166:ASP:OD1	1:B:168:SER:OG	2.18	0.60
1:B:54:ILE:HD13	1:B:66:VAL:CG1	2.28	0.60
1:G:19:LYS:HD3	1:G:348:ALA:O	2.00	0.60
1:C:53:VAL:HG13	1:C:87:ILE:HG12	1.84	0.60
6:E:513:HOH:O	1:F:42:ALA:HB1	2.01	0.60
1:F:277:ASN:HD21	1:F:365:LEU:CA	2.15	0.60
1:B:71:TRP:HA	1:B:74:ILE:HG12	1.84	0.60
1:G:51:LEU:CD1	1:G:53:VAL:CG2	2.80	0.60
4:A:406:SAM:HE3	4:A:406:SAM:N3	2.16	0.59
1:A:135:LEU:HD12	1:A:165:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ILE:HD13	1:B:181:ILE:HD11	1.85	0.59
1:F:274:ILE:HG21	1:F:322:ILE:CD1	2.33	0.59
1:H:143:ILE:HD13	1:H:181:ILE:HD11	1.84	0.59
1:D:24:ILE:HG13	1:D:73:ILE:HG12	1.84	0.59
1:C:52:ILE:CD1	1:C:74:ILE:HD11	2.32	0.59
1:G:44:GLU:HG3	1:H:232:THR:OG1	2.03	0.59
1:E:222:ARG:NH1	1:E:224:VAL:HG11	2.18	0.58
1:H:260:PRO:HD2	1:H:340:TRP:CZ3	2.37	0.58
5:A:409:PPK:O3G	5:A:409:PPK:O2A	2.20	0.58
1:A:138:GLU:OE1	1:A:206:LYS:NZ	2.35	0.58
1:E:81:GLU:HG2	4:H:403:SAM:HE2	1.85	0.58
1:H:130:PRO:HG2	1:H:247:VAL:CG1	2.33	0.58
1:F:152:PHE:O	1:F:191:TYR:CZ	2.57	0.58
1:A:160:LYS:NZ	1:B:113:ASP:OD1	2.37	0.58
1:C:52:ILE:HD11	1:C:74:ILE:HD11	1.86	0.58
1:E:179:VAL:HG11	1:E:196:VAL:HG11	1.86	0.58
5:E:409:PPK:O2A	1:F:238:LYS:NZ	2.31	0.58
1:H:52:ILE:HD11	1:H:74:ILE:HD11	1.85	0.58
1:G:226:GLY:O	1:G:229:ILE:CG2	2.51	0.58
1:A:166:ASP:OD1	1:A:168:SER:OG	2.21	0.57
1:H:281:ALA:HB3	1:H:283:LEU:HD13	1.84	0.57
1:E:12:VAL:CG2	1:E:160:LYS:HG2	2.34	0.57
1:A:143:ILE:HD13	1:A:181:ILE:HD11	1.86	0.57
1:C:54:ILE:HD13	1:C:66:VAL:CG1	2.34	0.57
1:G:66:VAL:HG21	1:G:88:SER:HB2	1.86	0.57
5:A:405:PPK:O3G	5:A:405:PPK:O2B	2.21	0.57
1:F:64:VAL:HG12	4:F:403:SAM:N1	2.20	0.57
1:F:143:ILE:HD13	1:F:181:ILE:HD11	1.87	0.57
1:H:217:ILE:O	1:H:217:ILE:HG13	2.05	0.57
1:D:135:LEU:HD12	1:D:165:ILE:HD11	1.87	0.56
1:G:179:VAL:HG21	1:G:196:VAL:HG11	1.87	0.56
1:H:27:ALA:CB	1:H:73:ILE:HD11	2.35	0.56
1:E:225:ILE:HD11	1:E:229:ILE:HG22	1.87	0.56
1:E:74:ILE:HA	1:E:77:LEU:HD23	1.86	0.56
1:G:19:LYS:CD	1:G:348:ALA:O	2.53	0.56
1:G:250:HIS:HB3	1:H:240:ILE:CD1	2.35	0.56
1:A:162:GLN:HE22	1:B:115:GLY:N	2.02	0.56
1:F:19:LYS:CD	1:F:348:ALA:O	2.54	0.56
1:G:56:GLY:CA	1:H:232:THR:HG21	2.35	0.56
1:E:143:ILE:HD13	1:E:181:ILE:HD11	1.88	0.56
1:G:135:LEU:HD12	1:G:165:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:259:ASP:OD1	1:G:262:LYS:NZ	2.24	0.56
1:E:51:LEU:HD11	1:E:87:ILE:HD11	1.88	0.56
5:A:405:PPK:H3B	1:B:258:LYS:NZ	2.04	0.55
1:F:194:LYS:C	1:F:195:LYS:O	2.33	0.55
4:G:405:SAM:N6	6:G:501:HOH:O	2.33	0.55
1:F:52:ILE:CD1	1:F:74:ILE:HD11	2.36	0.55
1:G:15:GLY:HA2	1:G:77:LEU:HD13	1.88	0.55
1:E:281:ALA:HB2	1:E:368:VAL:HG23	1.88	0.55
1:H:222:ARG:NH1	1:H:224:VAL:HG11	2.21	0.55
1:C:143:ILE:HD13	1:C:181:ILE:HD11	1.89	0.55
1:H:193:ASN:OD1	1:H:217:ILE:HG12	2.06	0.55
1:D:24:ILE:CG1	1:D:73:ILE:HG12	2.36	0.55
4:E:404:SAM:N	1:F:57:GLU:HG2	2.21	0.55
1:H:250:HIS:O	1:H:250:HIS:ND1	2.40	0.55
1:D:143:ILE:HD13	1:D:181:ILE:HD11	1.88	0.54
5:A:405:PPK:O4A	5:A:405:PPK:O2B	2.26	0.54
1:D:116:ILE:HG13	1:D:251:GLY:HA3	1.89	0.54
1:G:51:LEU:HD11	1:G:53:VAL:CG2	2.37	0.54
1:G:125:THR:CG2	1:G:129:MET:H	2.20	0.54
1:H:58:ILE:O	1:H:92:LYS:HA	2.07	0.54
1:G:302:ALA:HB1	1:H:6:ILE:CG2	2.36	0.54
1:D:20:ILE:HG23	1:D:73:ILE:HD11	1.89	0.54
1:D:185:GLU:OE2	1:D:222:ARG:NH1	2.41	0.54
1:B:359:ASP:OD1	1:B:359:ASP:O	2.25	0.54
1:G:62:ALA:O	4:G:405:SAM:HG2	2.07	0.54
1:B:135:LEU:HD12	1:B:165:ILE:HD11	1.90	0.54
1:H:90:VAL:CG2	4:H:403:SAM:C8	2.86	0.53
1:H:341:THR:O	1:H:341:THR:HG22	2.08	0.53
1:G:143:ILE:HD13	1:G:181:ILE:HD11	1.90	0.53
1:H:158:ASP:OD1	4:H:402:SAM:O2'	2.26	0.53
1:C:20:ILE:HG23	1:C:73:ILE:HD11	1.90	0.53
1:F:322:ILE:HG23	1:F:323:LYS:N	2.24	0.53
1:G:51:LEU:HD11	1:G:53:VAL:HG23	1.91	0.53
1:H:81:GLU:OE2	1:H:81:GLU:N	2.39	0.53
1:E:8:THR:HG22	1:F:116:ILE:HD11	1.91	0.53
1:F:313:ILE:HD11	1:F:317:LYS:HB2	1.90	0.53
1:A:44:GLU:OE2	1:B:237:ARG:NH1	2.37	0.53
1:H:189:VAL:HG12	1:H:193:ASN:ND2	2.24	0.53
1:A:71:TRP:HA	1:A:74:ILE:HG12	1.90	0.52
1:A:162:GLN:HE22	1:B:115:GLY:H	1.57	0.52
1:E:12:VAL:HG12	1:E:19:LYS:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:ILE:CD1	1:F:317:LYS:HB2	2.40	0.52
5:C:405:PPK:O1B	5:C:405:PPK:O2G	2.27	0.52
1:E:52:ILE:CD1	1:E:74:ILE:HD11	2.39	0.52
1:H:90:VAL:HG23	1:H:90:VAL:O	2.09	0.52
1:E:199:ILE:HA	1:E:202:GLN:CG	2.39	0.52
1:E:234:LEU:HD23	1:F:234:LEU:HD23	1.91	0.52
1:E:8:THR:HG22	1:F:116:ILE:CD1	2.39	0.52
1:H:324:LYS:HB3	1:H:374:ASN:ND2	2.25	0.52
1:H:153:ILE:HD12	1:H:154:LYS:CG	2.40	0.52
1:E:165:ILE:CG2	1:E:167:TYR:HE2	2.23	0.51
1:G:5:LYS:HG3	1:H:304:TYR:CE1	2.45	0.51
5:C:408:PPK:O2G	5:C:408:PPK:O2B	2.29	0.51
4:A:406:SAM:N3	4:A:406:SAM:CE	2.74	0.51
1:B:365:LEU:HD12	1:B:365:LEU:N	2.26	0.51
1:G:144:GLU:O	1:G:148:ARG:HG2	2.10	0.51
5:C:405:PPK:O2G	5:C:405:PPK:O2A	2.29	0.51
5:A:405:PPK:H3B	1:B:258:LYS:HZ3	1.57	0.51
1:C:23:GLN:HB2	1:C:73:ILE:HD13	1.92	0.51
1:E:225:ILE:HG22	1:F:96:ASP:OD2	2.11	0.51
1:B:185:GLU:OE2	1:B:222:ARG:NH1	2.44	0.51
1:F:193:ASN:O	1:F:195:LYS:O	2.29	0.51
1:G:179:VAL:HG21	1:G:196:VAL:CG1	2.41	0.51
1:D:52:ILE:HD11	1:D:74:ILE:HD11	1.92	0.51
1:F:274:ILE:HG21	1:F:322:ILE:HD12	1.92	0.51
1:C:189:VAL:HG12	1:C:193:ASN:ND2	2.25	0.50
1:F:19:LYS:HD2	1:F:348:ALA:O	2.11	0.50
1:G:9:SER:OG	1:G:132:THR:HG23	2.11	0.50
1:H:283:LEU:N	1:H:283:LEU:HD12	2.27	0.50
1:E:313:ILE:O	1:E:314:ASP:CB	2.58	0.50
1:B:24:ILE:HA	1:B:73:ILE:HD13	1.93	0.50
1:C:53:VAL:HG13	1:C:87:ILE:CG1	2.42	0.50
1:E:365:LEU:HD12	1:E:365:LEU:N	2.27	0.50
1:G:234:LEU:HD23	1:H:234:LEU:HD23	1.93	0.50
1:C:109:ILE:HD11	1:C:330:ILE:HG21	1.94	0.50
1:E:138:GLU:OE1	1:E:206:LYS:NZ	2.45	0.50
4:G:403:SAM:HG2	1:H:97:ILE:CD1	2.36	0.50
1:A:185:GLU:OE2	1:A:222:ARG:NH1	2.44	0.50
1:F:64:VAL:O	1:F:64:VAL:HG13	2.11	0.50
1:G:159:MET:HG2	1:G:181:ILE:HG23	1.93	0.50
1:F:19:LYS:HD3	1:F:348:ALA:O	2.11	0.49
1:G:31:GLU:OE1	1:G:31:GLU:HA	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:159:MET:HG2	1:H:181:ILE:HG23	1.94	0.49
1:D:330:ILE:HA	1:D:333:PHE:CE2	2.47	0.49
1:E:9:SER:OG	1:E:132:THR:HG23	2.12	0.49
1:E:44:GLU:OE1	1:F:237:ARG:NH1	2.46	0.49
1:E:51:LEU:HD11	1:E:87:ILE:CD1	2.43	0.49
1:F:52:ILE:HD11	1:F:74:ILE:HD11	1.94	0.49
1:F:142:GLU:OE2	1:F:145:ARG:NH2	2.46	0.49
1:H:91:ASN:O	1:H:92:LYS:CG	2.60	0.49
5:C:408:PPK:O2G	5:C:408:PPK:O2A	2.31	0.49
1:D:359:ASP:OD1	1:D:364:LYS:NZ	2.46	0.49
1:F:152:PHE:O	1:F:191:TYR:CE2	2.66	0.49
5:C:408:PPK:O1A	1:D:160:LYS:NZ	2.44	0.49
1:G:49:ASN:HB3	1:H:89:ASN:HD21	1.77	0.49
1:H:330:ILE:HA	1:H:333:PHE:CE2	2.48	0.49
1:C:73:ILE:HG13	1:C:74:ILE:N	2.28	0.48
1:F:313:ILE:HG12	1:F:314:ASP:H	1.76	0.48
1:G:105:ASN:OD1	1:G:107:ASN:HB2	2.13	0.48
1:G:125:THR:HG22	1:G:129:MET:O	2.13	0.48
1:E:51:LEU:HD22	1:F:89:ASN:HD22	1.78	0.48
1:F:330:ILE:HA	1:F:333:PHE:CE2	2.48	0.48
1:G:243:THR:CG2	1:G:244:TYR:CD2	2.90	0.48
1:E:91:ASN:ND2	1:F:229:ILE:O	2.47	0.48
1:B:330:ILE:HA	1:B:333:PHE:CE2	2.49	0.48
1:A:330:ILE:HA	1:A:333:PHE:CE2	2.48	0.48
1:E:330:ILE:HA	1:E:333:PHE:CE2	2.48	0.48
1:G:330:ILE:HA	1:G:333:PHE:CE2	2.48	0.48
1:H:24:ILE:HA	1:H:73:ILE:HD13	1.96	0.48
1:B:27:ALA:CB	1:B:73:ILE:HD11	2.43	0.48
1:H:262:LYS:HD2	1:H:262:LYS:N	2.29	0.48
1:F:313:ILE:HD11	1:F:317:LYS:CB	2.43	0.48
4:G:403:SAM:CG	1:H:97:ILE:HD13	2.40	0.47
1:D:91:ASN:OD1	1:D:91:ASN:O	2.32	0.47
1:E:146:GLN:HG2	1:E:151:GLU:CB	2.41	0.47
1:C:330:ILE:HA	1:C:333:PHE:CE2	2.49	0.47
1:G:147:ARG:HH12	1:G:148:ARG:HD2	1.80	0.47
1:G:189:VAL:HG22	1:G:193:ASN:HD21	1.76	0.47
1:C:297:GLN:HE21	1:D:219:SER:HB2	1.80	0.47
1:E:12:VAL:HG21	1:E:16:HIS:CG	2.49	0.47
1:E:361:SER:HA	1:E:364:LYS:HD2	1.97	0.47
1:G:48:CYS:O	1:G:49:ASN:C	2.53	0.47
1:C:48:CYS:O	1:C:49:ASN:C	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:250:HIS:HD2	1:G:252:GLY:H	1.62	0.47
1:H:74:ILE:HG23	1:H:79:TYR:CB	2.30	0.47
1:C:324:LYS:CB	1:C:374:ASN:ND2	2.78	0.46
1:H:263:VAL:CG2	1:H:267:ALA:HB2	2.40	0.46
5:A:405:PPK:N3B	1:B:258:LYS:NZ	2.64	0.46
1:C:109:ILE:HD11	1:C:330:ILE:CG2	2.45	0.46
1:E:199:ILE:HA	1:E:202:GLN:HG2	1.95	0.46
1:A:89:ASN:HD22	1:B:51:LEU:HD22	1.81	0.46
1:H:193:ASN:OD1	1:H:217:ILE:CD1	2.64	0.46
1:A:109:ILE:HD11	1:A:330:ILE:HG21	1.98	0.46
1:B:370:ASP:O	1:B:374:ASN:ND2	2.48	0.46
1:C:109:ILE:HD12	1:C:110:GLY:O	2.16	0.46
1:E:179:VAL:HG11	1:E:196:VAL:CG1	2.46	0.46
1:A:48:CYS:SG	1:B:89:ASN:ND2	2.78	0.46
1:G:202:GLN:HA	1:G:205:LYS:HG2	1.98	0.46
1:A:5:LYS:HG3	1:B:304:TYR:CE1	2.51	0.46
1:C:74:ILE:HG23	1:C:79:TYR:CB	2.32	0.46
1:F:9:SER:OG	1:F:132:THR:CG2	2.64	0.46
1:F:108:LEU:HD23	1:F:298:PRO:CB	2.46	0.46
1:C:5:LYS:HD3	1:C:167:TYR:HB2	1.98	0.45
1:F:9:SER:OG	1:F:132:THR:HG23	2.16	0.45
1:F:266:SER:HB3	1:F:339:LEU:HD13	1.96	0.45
4:A:406:SAM:HE3	4:A:406:SAM:O4'	2.16	0.45
1:F:211:THR:HG22	1:F:211:THR:O	2.16	0.45
5:C:408:PPK:O2A	1:D:238:LYS:NZ	2.49	0.45
1:G:144:GLU:OE2	1:G:148:ARG:HD3	2.16	0.45
1:H:19:LYS:HE2	1:H:19:LYS:HA	1.97	0.45
1:H:89:ASN:HD22	1:H:89:ASN:C	2.20	0.45
1:C:24:ILE:CG1	1:C:73:ILE:HG12	2.47	0.45
1:E:74:ILE:HA	1:E:77:LEU:CD2	2.46	0.45
1:G:9:SER:OG	1:G:132:THR:CG2	2.65	0.45
1:G:64:VAL:HG13	1:G:64:VAL:O	2.17	0.45
1:F:373:LYS:HD2	1:F:373:LYS:HA	1.83	0.45
1:E:89:ASN:HD22	1:F:51:LEU:CD2	2.29	0.45
1:H:324:LYS:HB3	1:H:374:ASN:HD22	1.81	0.45
1:A:85:THR:OG1	1:D:89:ASN:ND2	2.50	0.45
1:H:12:VAL:HG23	1:H:19:LYS:CG	2.39	0.45
1:H:105:ASN:C	1:H:105:ASN:ND2	2.68	0.45
1:C:144:GLU:O	1:C:148:ARG:HG2	2.17	0.45
1:E:281:ALA:CA	1:E:368:VAL:HG23	2.46	0.45
1:A:109:ILE:HD11	1:A:330:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:LEU:N	1:A:346:PRO:CD	2.80	0.45
4:A:406:SAM:H5'1	1:D:81:GLU:OE2	2.16	0.45
1:B:134:VAL:O	1:B:138:GLU:HG2	2.16	0.45
1:C:19:LYS:HE2	1:C:19:LYS:HA	1.99	0.45
1:G:7:ILE:HD12	1:G:167:TYR:CD2	2.52	0.45
1:G:250:HIS:HB3	1:H:240:ILE:HD11	1.98	0.45
1:E:8:THR:HB	1:F:116:ILE:HD12	1.99	0.44
1:H:324:LYS:CB	1:H:374:ASN:HD22	2.30	0.44
1:A:49:ASN:HB2	1:B:91:ASN:OD1	2.18	0.44
5:A:405:PPK:O1G	5:A:405:PPK:O1A	2.35	0.44
1:A:48:CYS:O	1:A:49:ASN:C	2.53	0.44
1:C:324:LYS:HB3	1:C:374:ASN:ND2	2.32	0.44
1:D:109:ILE:HD12	1:D:110:GLY:O	2.18	0.44
1:F:50:ARG:HD2	1:H:50:ARG:HB2	1.98	0.44
5:G:404:PPK:O2G	5:G:404:PPK:O2A	2.35	0.44
1:D:26:ASP:OD1	1:D:265:ARG:NH1	2.50	0.44
1:E:9:SER:OG	1:E:132:THR:CG2	2.66	0.44
1:F:97:ILE:HG23	1:F:98:ALA:N	2.32	0.44
1:B:26:ASP:OD1	1:B:265:ARG:NH1	2.50	0.44
1:C:26:ASP:OD1	1:C:265:ARG:NH1	2.50	0.44
1:H:149:SER:OG	1:H:151:GLU:HG3	2.18	0.44
1:D:109:ILE:HD11	1:D:330:ILE:CG2	2.47	0.44
1:D:109:ILE:HD11	1:D:330:ILE:HG21	1.98	0.44
1:E:12:VAL:HG22	1:E:16:HIS:CD2	2.53	0.44
5:E:409:PPK:O1A	5:E:409:PPK:O1G	2.36	0.44
1:G:202:GLN:HA	1:G:205:LYS:HE2	1.99	0.44
1:G:345:LEU:N	1:G:346:PRO:CD	2.81	0.44
1:D:345:LEU:N	1:D:346:PRO:CD	2.81	0.44
1:H:285:LYS:HB2	1:H:310:THR:HB	1.99	0.44
1:C:345:LEU:N	1:C:346:PRO:CD	2.81	0.43
1:E:142:GLU:OE2	1:E:145:ARG:NH2	2.50	0.43
1:F:345:LEU:N	1:F:346:PRO:CD	2.80	0.43
1:H:90:VAL:HG21	4:H:403:SAM:C8	2.44	0.43
1:H:345:LEU:N	1:H:346:PRO:CD	2.81	0.43
1:F:48:CYS:O	1:F:49:ASN:C	2.55	0.43
1:G:229:ILE:HG23	1:G:230:GLY:N	2.33	0.43
1:F:291:LEU:CD1	1:F:303:MET:HG3	2.48	0.43
1:E:368:VAL:HG13	1:E:369:GLU:N	2.33	0.43
1:C:229:ILE:O	1:D:91:ASN:ND2	2.51	0.43
1:D:48:CYS:O	1:D:49:ASN:C	2.56	0.43
1:H:82:ASN:O	1:H:82:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:TYR:O	1:H:247:VAL:HG12	2.19	0.43
1:C:320:GLU:OE1	1:C:320:GLU:HA	2.19	0.43
6:A:520:HOH:O	1:B:48:CYS:HB2	2.18	0.43
1:B:48:CYS:O	1:B:49:ASN:C	2.56	0.43
1:A:26:ASP:OD1	1:A:265:ARG:NH1	2.51	0.42
1:E:48:CYS:O	1:E:49:ASN:C	2.55	0.42
1:E:311:ASN:HD22	1:E:311:ASN:H	1.67	0.42
4:F:402:SAM:O4'	4:F:402:SAM:CE	2.66	0.42
1:D:12:VAL:HG23	1:D:19:LYS:HD2	2.00	0.42
1:E:8:THR:CG2	1:F:116:ILE:CD1	2.97	0.42
1:F:40:ARG:HD2	6:F:501:HOH:O	2.20	0.42
1:B:345:LEU:N	1:B:346:PRO:CD	2.81	0.42
1:A:109:ILE:HD12	1:A:110:GLY:O	2.19	0.42
1:E:281:ALA:HA	1:E:368:VAL:CG2	2.50	0.42
1:H:52:ILE:CD1	1:H:74:ILE:HD11	2.49	0.42
1:G:75:LYS:NZ	1:G:81:GLU:OE2	2.38	0.42
1:H:273:TRP:HZ3	1:H:364:LYS:HB2	1.84	0.42
1:H:283:LEU:N	1:H:283:LEU:CD1	2.83	0.42
1:F:225:ILE:HD11	1:F:230:GLY:HA2	2.01	0.42
1:D:74:ILE:HG23	1:D:79:TYR:CB	2.34	0.42
1:F:222:ARG:O	4:F:402:SAM:N6	2.48	0.42
1:G:142:GLU:O	1:G:142:GLU:OE1	2.38	0.42
1:H:291:LEU:CD1	1:H:303:MET:HG3	2.50	0.42
1:H:311:ASN:H	1:H:311:ASN:HD22	1.67	0.42
1:C:304:TYR:CE1	1:D:5:LYS:HG3	2.55	0.41
4:A:406:SAM:O4'	1:D:81:GLU:OE2	2.39	0.41
1:D:144:GLU:HB2	6:D:510:HOH:O	2.19	0.41
1:E:91:ASN:O	1:E:91:ASN:OD1	2.38	0.41
1:F:105:ASN:OD1	1:F:107:ASN:HB2	2.20	0.41
1:F:152:PHE:C	1:F:152:PHE:HD1	2.23	0.41
1:A:237:ARG:NH1	1:B:44:GLU:OE2	2.46	0.41
1:F:319:PHE:C	1:F:322:ILE:HG22	2.40	0.41
1:H:48:CYS:O	1:H:49:ASN:C	2.57	0.41
1:E:38:ASN:N	1:E:38:ASN:HD22	2.18	0.41
1:G:243:THR:OG1	1:G:250:HIS:HE1	2.04	0.41
1:B:109:ILE:HD12	1:B:110:GLY:O	2.20	0.41
1:E:75:LYS:HE3	1:E:81:GLU:OE2	2.18	0.41
1:E:224:VAL:HG12	1:F:96:ASP:OD2	2.21	0.41
1:H:91:ASN:O	1:H:91:ASN:OD1	2.38	0.41
1:H:207:TYR:HB2	1:H:209:LEU:HD12	2.01	0.41
1:E:56:GLY:HA2	1:E:57:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:6:ILE:CG2	1:H:6:ILE:O	2.68	0.41
1:E:281:ALA:CB	1:E:368:VAL:HG23	2.50	0.41
1:E:334:ILE:HG23	1:E:339:LEU:HB2	2.02	0.41
1:F:132:THR:HG23	1:F:133:SER:N	2.36	0.41
1:F:178:LEU:HD23	1:F:178:LEU:C	2.42	0.41
1:F:283:LEU:N	1:F:283:LEU:CD1	2.84	0.41
1:B:109:ILE:O	1:B:109:ILE:HG13	2.21	0.40
1:C:185:GLU:OE1	1:C:222:ARG:NH1	2.54	0.40
1:D:73:ILE:HG13	1:D:74:ILE:N	2.36	0.40
1:H:289:ILE:HD13	1:H:305:VAL:HG13	2.02	0.40
1:B:178:LEU:C	1:B:178:LEU:HD23	2.42	0.40
1:E:313:ILE:O	1:E:314:ASP:HB3	2.21	0.40
1:E:12:VAL:CG2	1:E:16:HIS:CG	3.04	0.40
1:G:179:VAL:CG2	1:G:196:VAL:HG11	2.50	0.40
1:H:9:SER:OG	1:H:132:THR:OG1	2.37	0.40
1:B:81:GLU:HG3	4:C:406:SAM:H5'1	2.03	0.40
1:B:291:LEU:HD23	1:B:303:MET:HG3	2.02	0.40
1:F:189:VAL:HG12	1:F:193:ASN:ND2	2.37	0.40
1:G:169:ASN:OD1	1:G:169:ASN:N	2.54	0.40
1:A:70:ALA:O	1:A:74:ILE:HG12	2.21	0.40
1:C:16:HIS:NE2	4:C:404:SAM:O3'	2.55	0.40
1:E:236:GLY:HA3	1:F:237:ARG:HE	1.87	0.40
5:E:409:PPK:O2G	5:E:409:PPK:O1B	2.40	0.40
1:F:149:SER:OG	1:F:151:GLU:HG3	2.22	0.40
4:G:403:SAM:CG	1:H:97:ILE:CD1	2.99	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:NZ	1:E:35:GLN:O[1_556]	2.16	0.04

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	370/382 (97%)	358 (97%)	11 (3%)	1 (0%)	41	50
1	B	373/382 (98%)	362 (97%)	9 (2%)	2 (0%)	29	39
1	C	371/382 (97%)	361 (97%)	9 (2%)	1 (0%)	41	50
1	D	370/382 (97%)	357 (96%)	11 (3%)	2 (0%)	29	39
1	E	370/382 (97%)	353 (95%)	13 (4%)	4 (1%)	14	19
1	F	372/382 (97%)	357 (96%)	12 (3%)	3 (1%)	19	27
1	G	371/382 (97%)	358 (96%)	11 (3%)	2 (0%)	29	39
1	H	370/382 (97%)	352 (95%)	15 (4%)	3 (1%)	19	27
All	All	2967/3056 (97%)	2858 (96%)	91 (3%)	18 (1%)	25	33

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	49	ASN
1	G	313	ILE
1	H	188	ASP
1	A	49	ASN
1	B	49	ASN
1	C	49	ASN
1	E	49	ASN
1	E	169	ASN
1	F	153	ILE
1	H	187	TYR
1	D	49	ASN
1	F	49	ASN
1	H	49	ASN
1	E	314	ASP
1	B	92	LYS
1	D	92	LYS
1	E	92	LYS
1	F	196	VAL

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	322/332 (97%)	307 (95%)	15 (5%)	26	35
1	B	325/332 (98%)	308 (95%)	17 (5%)	23	31
1	C	323/332 (97%)	302 (94%)	21 (6%)	17	22
1	D	322/332 (97%)	302 (94%)	20 (6%)	18	23
1	E	322/332 (97%)	293 (91%)	29 (9%)	9	11
1	F	324/332 (98%)	295 (91%)	29 (9%)	9	11
1	G	323/332 (97%)	294 (91%)	29 (9%)	9	11
1	H	322/332 (97%)	290 (90%)	32 (10%)	8	9
All	All	2583/2656 (97%)	2391 (93%)	192 (7%)	13	18

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ILE
1	A	19	LYS
1	A	107	ASN
1	A	109	ILE
1	A	148	ARG
1	A	152	PHE
1	A	168	SER
1	A	187	TYR
1	A	206	LYS
1	A	223	PHE
1	A	265	ARG
1	A	295	ILE
1	A	301	VAL
1	A	349	THR
1	A	375	SER
1	B	19	LYS
1	B	49	ASN
1	B	68	LYS
1	B	92	LYS
1	B	109	ILE
1	B	116	ILE
1	B	148	ARG
1	B	152	PHE
1	B	168	SER

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Mol	Chain	Res	Type
1	B	187	TYR
1	B	194	LYS
1	B	206	LYS
1	B	223	PHE
1	B	229	ILE
1	B	265	ARG
1	B	282	LYS
1	B	301	VAL
1	C	3	TYR
1	C	19	LYS
1	C	73	ILE
1	C	87	ILE
1	C	92	LYS
1	C	109	ILE
1	C	152	PHE
1	C	165	ILE
1	C	169	ASN
1	C	187	TYR
1	C	206	LYS
1	C	211	THR
1	C	223	PHE
1	C	265	ARG
1	C	282	LYS
1	C	301	VAL
1	C	307	THR
1	C	310	THR
1	C	316	THR
1	C	320	GLU
1	C	324	LYS
1	D	19	LYS
1	D	73	ILE
1	D	81	GLU
1	D	92	LYS
1	D	109	ILE
1	D	131	LEU
1	D	148	ARG
1	D	152	PHE
1	D	169	ASN
1	D	187	TYR
1	D	190	GLU
1	D	223	PHE
1	D	229	ILE

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Mol	Chain	Res	Type
1	D	265	ARG
1	D	301	VAL
1	D	312	LEU
1	D	316	THR
1	D	370	ASP
1	D	373	LYS
1	D	375	SER
1	E	12	VAL
1	E	31	GLU
1	E	38	ASN
1	E	50	ARG
1	E	57	GLU
1	E	77	LEU
1	E	92	LYS
1	E	106	LYS
1	E	107	ASN
1	E	116	ILE
1	E	145	ARG
1	E	152	PHE
1	E	168	SER
1	E	169	ASN
1	E	178	LEU
1	E	187	TYR
1	E	190	GLU
1	E	194	LYS
1	E	195	LYS
1	E	202	GLN
1	E	211	THR
1	E	214	LYS
1	E	223	PHE
1	E	259	ASP
1	E	265	ARG
1	E	299	GLN
1	E	301	VAL
1	E	307	THR
1	E	311	ASN
1	F	19	LYS
1	F	50	ARG
1	F	57	GLU
1	F	81	GLU
1	F	99	GLN
1	F	106	LYS

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Mol	Chain	Res	Type
1	F	116	ILE
1	F	131	LEU
1	F	133	SER
1	F	145	ARG
1	F	150	LYS
1	F	152	PHE
1	F	168	SER
1	F	169	ASN
1	F	185	GLU
1	F	187	TYR
1	F	195	LYS
1	F	203	ILE
1	F	222	ARG
1	F	223	PHE
1	F	225	ILE
1	F	237	ARG
1	F	265	ARG
1	F	266	SER
1	F	291	LEU
1	F	313	ILE
1	F	323	LYS
1	F	343	LYS
1	F	373	LYS
1	G	10	GLU
1	G	19	LYS
1	G	50	ARG
1	G	51	LEU
1	G	74	ILE
1	G	92	LYS
1	G	131	LEU
1	G	142	GLU
1	G	149	SER
1	G	152	PHE
1	G	154	LYS
1	G	159	MET
1	G	169	ASN
1	G	187	TYR
1	G	195	LYS
1	G	206	LYS
1	G	211	THR
1	G	223	PHE
1	G	229	ILE

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Mol	Chain	Res	Type
1	G	264	ASP
1	G	265	ARG
1	G	266	SER
1	G	283	LEU
1	G	286	GLN
1	G	307	THR
1	G	324	LYS
1	G	338	ASN
1	G	358	LEU
1	G	375	SER
1	H	4	LYS
1	H	6	ILE
1	H	31	GLU
1	H	68	LYS
1	H	75	LYS
1	H	89	ASN
1	H	99	GLN
1	H	105	ASN
1	H	123	ASP
1	H	133	SER
1	H	152	PHE
1	H	153	ILE
1	H	159	MET
1	H	169	ASN
1	H	176	THR
1	H	187	TYR
1	H	190	GLU
1	H	203	ILE
1	H	223	PHE
1	H	229	ILE
1	H	262	LYS
1	H	265	ARG
1	H	291	LEU
1	H	299	GLN
1	H	301	VAL
1	H	311	ASN
1	H	323	LYS
1	H	349	THR
1	H	363	GLU
1	H	370	ASP
1	H	373	LYS
1	H	375	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	HIS
1	A	89	ASN
1	A	93	GLN
1	A	162	GLN
1	A	193	ASN
1	A	202	GLN
1	A	286	GLN
1	B	93	GLN
1	B	193	ASN
1	B	286	GLN
1	C	38	ASN
1	C	49	ASN
1	C	89	ASN
1	C	286	GLN
1	C	297	GLN
1	C	338	ASN
1	C	374	ASN
1	D	49	ASN
1	D	89	ASN
1	D	193	ASN
1	D	202	GLN
1	D	208	ASN
1	D	249	HIS
1	E	37	GLN
1	E	38	ASN
1	E	89	ASN
1	E	193	ASN
1	E	297	GLN
1	E	311	ASN
1	F	82	ASN
1	F	89	ASN
1	F	93	GLN
1	F	277	ASN
1	F	338	ASN
1	G	38	ASN
1	G	137	HIS
1	G	162	GLN
1	G	250	HIS
1	G	290	GLN
1	G	338	ASN
1	H	37	GLN

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Mol	Chain	Res	Type
1	H	82	ASN
1	H	105	ASN
1	H	107	ASN
1	H	146	GLN
1	H	297	GLN
1	H	311	ASN
1	H	366	ASN
1	H	374	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 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	SAM	E	406	-	24,29,29	1.46	5 (20%)	23,42,42	2.34	9 (39%)
5	PPK	G	409	2,3	11,12,12	3.52	6 (54%)	15,20,20	2.64	6 (40%)
4	SAM	E	404	-	24,29,29	1.37	2 (8%)	23,42,42	1.82	6 (26%)
5	PPK	E	409	2,3	11,12,12	3.29	6 (54%)	15,20,20	3.05	6 (40%)
4	SAM	C	406	-	24,29,29	1.53	4 (16%)	23,42,42	2.35	9 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
5	PPK	C	405	2,3	11,12,12	4.69	7 (63%)	15,20,20	3.19	9 (60%)
4	SAM	D	403	-	24,29,29	1.79	4 (16%)	23,42,42	3.00	8 (34%)
4	SAM	B	402	-	24,29,29	1.66	5 (20%)	23,42,42	1.97	6 (26%)
4	SAM	A	406	-	24,29,29	1.12	2 (8%)	23,42,42	2.09	7 (30%)
5	PPK	C	408	3	11,12,12	4.60	5 (45%)	15,20,20	5.06	7 (46%)
4	SAM	F	403	-	24,29,29	1.16	2 (8%)	23,42,42	2.07	7 (30%)
4	SAM	H	403	-	24,29,29	1.26	4 (16%)	23,42,42	1.96	7 (30%)
4	SAM	A	404	-	24,29,29	1.32	3 (12%)	23,42,42	1.93	7 (30%)
5	PPK	A	405	2,3	11,12,12	5.68	5 (45%)	15,20,20	3.80	9 (60%)
5	PPK	A	409	2,3	11,12,12	5.94	7 (63%)	15,20,20	3.04	7 (46%)
4	SAM	F	402	-	24,29,29	1.11	1 (4%)	23,42,42	2.01	8 (34%)
5	PPK	E	405	2,3	11,12,12	5.07	7 (63%)	15,20,20	2.42	7 (46%)
4	SAM	D	402	-	24,29,29	1.06	1 (4%)	23,42,42	2.42	9 (39%)
4	SAM	G	405	-	24,29,29	1.28	1 (4%)	23,42,42	2.40	8 (34%)
4	SAM	H	402	-	24,29,29	1.12	0	23,42,42	2.06	8 (34%)
4	SAM	G	403	-	24,29,29	1.12	3 (12%)	23,42,42	2.30	9 (39%)
4	SAM	B	403	-	24,29,29	1.27	3 (12%)	23,42,42	1.84	5 (21%)
5	PPK	G	404	2,3	11,12,12	4.96	7 (63%)	15,20,20	3.83	4 (26%)
4	SAM	C	404	-	24,29,29	1.41	4 (16%)	23,42,42	2.07	9 (39%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	E	406	-	-	9/12/33/33	0/3/3/3
5	PPK	G	409	2,3	-	1/8/12/12	-
4	SAM	E	404	-	-	6/12/33/33	0/3/3/3
5	PPK	E	409	2,3	-	3/8/12/12	-
4	SAM	C	406	-	-	7/12/33/33	0/3/3/3
5	PPK	C	405	2,3	-	2/8/12/12	-
4	SAM	D	403	-	-	4/12/33/33	0/3/3/3
4	SAM	B	402	-	-	7/12/33/33	0/3/3/3
4	SAM	A	406	-	-	4/12/33/33	0/3/3/3
5	PPK	C	408	3	-	2/8/12/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SAM	F	403	-	-	3/12/33/33	0/3/3/3
4	SAM	H	403	-	-	4/12/33/33	0/3/3/3
4	SAM	A	404	-	-	4/12/33/33	0/3/3/3
5	PPK	A	405	2,3	-	2/8/12/12	-
5	PPK	A	409	2,3	-	2/8/12/12	-
4	SAM	F	402	-	-	7/12/33/33	0/3/3/3
5	PPK	E	405	2,3	-	1/8/12/12	-
4	SAM	D	402	-	-	4/12/33/33	0/3/3/3
4	SAM	G	405	-	-	5/12/33/33	0/3/3/3
4	SAM	H	402	-	-	5/12/33/33	0/3/3/3
4	SAM	G	403	-	-	6/12/33/33	0/3/3/3
4	SAM	B	403	-	-	3/12/33/33	0/3/3/3
5	PPK	G	404	2,3	-	2/8/12/12	-
4	SAM	C	404	-	-	11/12/33/33	0/3/3/3

All (94) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	405	PPK	PG-O3G	17.47	1.73	1.46
5	A	409	PPK	PG-O3G	15.35	1.70	1.46
5	E	405	PPK	PG-O3G	13.30	1.67	1.46
5	C	405	PPK	PB-O2B	12.98	1.66	1.46
5	C	408	PPK	PG-O3G	12.73	1.66	1.46
5	G	404	PPK	PG-O3G	12.13	1.65	1.46
5	G	409	PPK	PG-O3G	9.45	1.61	1.46
5	A	409	PPK	PB-O2B	8.62	1.59	1.46
5	E	409	PPK	PB-O2B	7.60	1.58	1.46
5	G	404	PPK	PB-O2B	6.08	1.55	1.46
5	G	404	PPK	PG-N3B	5.46	1.77	1.63
5	E	405	PPK	PB-O3A	5.20	1.65	1.59
5	C	408	PPK	PG-N3B	5.10	1.76	1.63
4	D	403	SAM	CG-CB	4.94	1.67	1.51
5	G	404	PPK	PB-O1B	-4.92	1.43	1.56
5	E	405	PPK	PB-N3B	4.84	1.76	1.63
5	C	408	PPK	PB-O2B	-4.74	1.38	1.46
5	C	405	PPK	PB-N3B	4.59	1.75	1.63
5	A	409	PPK	PG-O1G	4.54	1.69	1.56
5	E	405	PPK	PG-N3B	4.45	1.75	1.63
5	A	405	PPK	PG-O2G	-4.07	1.45	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	409	PPK	PG-N3B	4.05	1.73	1.63
5	A	409	PPK	PG-N3B	3.89	1.73	1.63
4	C	406	SAM	C4-N3	-3.78	1.30	1.35
4	B	402	SAM	C4-N3	-3.69	1.30	1.35
5	E	405	PPK	PG-O1G	3.66	1.66	1.56
5	C	405	PPK	PG-O3G	3.65	1.52	1.46
5	E	409	PPK	PB-O1B	-3.64	1.46	1.56
5	G	404	PPK	PB-N3B	3.61	1.72	1.63
4	D	403	SAM	C4-N3	-3.59	1.30	1.35
5	A	409	PPK	PB-O3A	3.56	1.63	1.59
5	A	409	PPK	PB-O1B	-3.52	1.47	1.56
5	E	409	PPK	PB-N3B	3.40	1.72	1.63
5	C	405	PPK	PB-O1B	-3.39	1.47	1.56
5	A	405	PPK	PG-N3B	3.36	1.72	1.63
4	C	404	SAM	O-C	3.31	1.32	1.22
5	G	409	PPK	PB-O2B	3.29	1.51	1.46
5	A	409	PPK	PB-N3B	3.28	1.71	1.63
5	G	409	PPK	PG-N3B	3.15	1.71	1.63
4	C	404	SAM	C4-N3	-3.09	1.31	1.35
5	G	409	PPK	PG-O1G	-3.07	1.48	1.56
4	B	402	SAM	C5-N7	-3.04	1.28	1.39
5	E	405	PPK	PG-O2G	-2.99	1.48	1.56
4	C	404	SAM	C5-N7	-2.96	1.29	1.39
5	E	409	PPK	PB-O3A	2.95	1.62	1.59
4	E	404	SAM	O-C	2.92	1.31	1.22
5	G	409	PPK	PB-N3B	2.92	1.71	1.63
4	D	403	SAM	CE-SD	-2.90	1.60	1.78
4	E	404	SAM	OXT-C	2.83	1.39	1.30
4	D	403	SAM	C2-N1	-2.83	1.28	1.33
4	C	406	SAM	C2'-C1'	-2.83	1.49	1.53
5	A	405	PPK	PB-N3B	2.82	1.70	1.63
4	G	405	SAM	C5-C4	2.81	1.48	1.40
4	E	406	SAM	C5-C4	2.78	1.48	1.40
5	C	405	PPK	PG-N3B	2.78	1.70	1.63
4	C	404	SAM	O4'-C4'	-2.73	1.38	1.45
5	E	405	PPK	PA-O2A	-2.73	1.44	1.54
4	A	404	SAM	C5-C4	2.72	1.48	1.40
5	G	404	PPK	PG-O2G	2.69	1.64	1.56
4	E	406	SAM	C2-N3	2.64	1.36	1.32
4	G	403	SAM	C5-C4	2.61	1.47	1.40
5	C	405	PPK	PG-O2G	2.60	1.63	1.56
4	B	402	SAM	C2-N3	2.58	1.36	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	404	SAM	OXT-C	2.58	1.39	1.30
5	A	405	PPK	PG-O1G	2.55	1.63	1.56
4	G	403	SAM	C4-N3	2.54	1.39	1.35
4	B	403	SAM	C5-C4	2.53	1.47	1.40
4	C	406	SAM	C5-C4	2.47	1.47	1.40
4	C	406	SAM	C2-N3	2.43	1.36	1.32
4	H	403	SAM	C5-N7	-2.41	1.31	1.39
5	C	408	PPK	PB-N3B	2.40	1.69	1.63
5	G	404	PPK	PG-O1G	-2.37	1.50	1.56
4	B	403	SAM	O4'-C4'	-2.35	1.39	1.45
4	F	402	SAM	C2'-C1'	-2.31	1.50	1.53
4	A	406	SAM	C2-N3	2.30	1.35	1.32
4	B	402	SAM	C2'-C1'	-2.27	1.50	1.53
5	C	405	PPK	PB-O3A	2.24	1.61	1.59
4	B	403	SAM	OXT-C	-2.23	1.23	1.30
4	H	403	SAM	CE-SD	-2.22	1.64	1.78
5	G	409	PPK	PG-O2G	2.20	1.62	1.56
4	H	403	SAM	C2-N3	2.19	1.35	1.32
4	A	404	SAM	C2-N3	2.19	1.35	1.32
4	F	403	SAM	C5-C4	2.17	1.46	1.40
4	D	402	SAM	C5-N7	-2.16	1.31	1.39
4	F	403	SAM	OXT-C	-2.14	1.23	1.30
4	E	406	SAM	C5'-C4'	2.13	1.59	1.53
5	E	409	PPK	PG-O2G	2.12	1.62	1.56
4	A	406	SAM	C5-C4	2.12	1.46	1.40
4	B	402	SAM	O4'-C1'	-2.11	1.38	1.41
5	C	408	PPK	PG-O2G	2.11	1.62	1.56
4	G	403	SAM	C5-N7	-2.07	1.32	1.39
4	H	403	SAM	C2'-C1'	-2.05	1.50	1.53
4	E	406	SAM	C3'-C4'	2.04	1.58	1.53
4	E	406	SAM	OXT-C	-2.04	1.23	1.30

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	408	PPK	O3G-PG-N3B	-15.17	89.43	111.77
5	G	404	PPK	O3G-PG-N3B	-12.61	93.20	111.77
5	A	405	PPK	O1B-PB-O2B	10.05	131.00	109.92
5	C	408	PPK	O2B-PB-N3B	-9.59	97.65	111.77
4	D	403	SAM	CB-CA-C	8.65	130.89	110.30
5	A	409	PPK	O1B-PB-O2B	8.16	127.02	109.92
5	E	409	PPK	O2B-PB-N3B	7.99	123.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	409	PPK	O3G-PG-N3B	-6.72	101.87	111.77
4	E	406	SAM	CG-SD-C5'	6.23	119.30	103.40
5	C	405	PPK	O1B-PB-O2B	6.11	122.73	109.92
4	G	403	SAM	N3-C2-N1	-6.08	119.18	128.68
5	A	405	PPK	O3G-PG-N3B	-5.71	103.37	111.77
5	C	405	PPK	O3G-PG-N3B	-5.60	103.53	111.77
4	G	405	SAM	CB-CA-N	-5.58	95.55	110.17
4	C	406	SAM	CB-CA-N	-5.39	96.03	110.17
4	A	406	SAM	C3'-C2'-C1'	5.12	108.69	100.98
4	F	403	SAM	N3-C2-N1	-5.08	120.75	128.68
4	C	406	SAM	C3'-C2'-C1'	5.05	108.58	100.98
4	F	402	SAM	CB-CA-N	-5.00	97.07	110.17
4	D	402	SAM	N3-C2-N1	-4.92	120.98	128.68
5	C	408	PPK	O1B-PB-O3A	4.86	120.87	104.64
5	E	409	PPK	O1G-PG-O2G	4.85	120.57	107.64
5	C	405	PPK	PB-O3A-PA	-4.83	115.61	132.62
4	D	403	SAM	C1'-N9-C4	4.82	135.11	126.64
4	H	402	SAM	N3-C2-N1	-4.77	121.22	128.68
4	D	403	SAM	OXT-C-CA	4.67	129.28	113.38
5	G	404	PPK	PB-O3A-PA	-4.64	116.29	132.62
4	B	403	SAM	N3-C2-N1	-4.61	121.47	128.68
4	D	403	SAM	OXT-C-O	-4.57	113.72	124.09
4	D	403	SAM	C4-C5-N7	-4.55	104.66	109.40
4	B	402	SAM	C4-C5-N7	-4.39	104.82	109.40
4	D	402	SAM	C3'-C2'-C1'	4.36	107.54	100.98
4	F	403	SAM	C3'-C2'-C1'	4.36	107.54	100.98
5	C	405	PPK	O1G-PG-O3G	4.24	124.12	113.45
4	G	405	SAM	CB-CA-C	4.21	120.33	110.30
5	E	405	PPK	O2B-PB-N3B	-4.14	105.68	111.77
4	G	403	SAM	CB-CA-N	-4.07	99.49	110.17
4	D	403	SAM	C3'-C2'-C1'	4.07	107.10	100.98
4	H	403	SAM	C4-C5-N7	-4.06	105.17	109.40
4	A	406	SAM	C4-C5-N7	-4.04	105.19	109.40
4	H	403	SAM	N3-C2-N1	-3.97	122.47	128.68
4	A	404	SAM	N3-C2-N1	-3.96	122.49	128.68
4	G	405	SAM	C3'-C2'-C1'	3.89	106.84	100.98
5	A	409	PPK	PB-O3A-PA	-3.86	119.01	132.62
4	G	405	SAM	N3-C2-N1	-3.83	122.69	128.68
4	B	402	SAM	C3'-C2'-C1'	3.83	106.74	100.98
4	G	405	SAM	O3'-C3'-C4'	-3.79	100.10	111.05
5	G	404	PPK	O2B-PB-N3B	-3.78	106.20	111.77
5	A	405	PPK	O2A-PA-O4A	3.76	125.42	110.68

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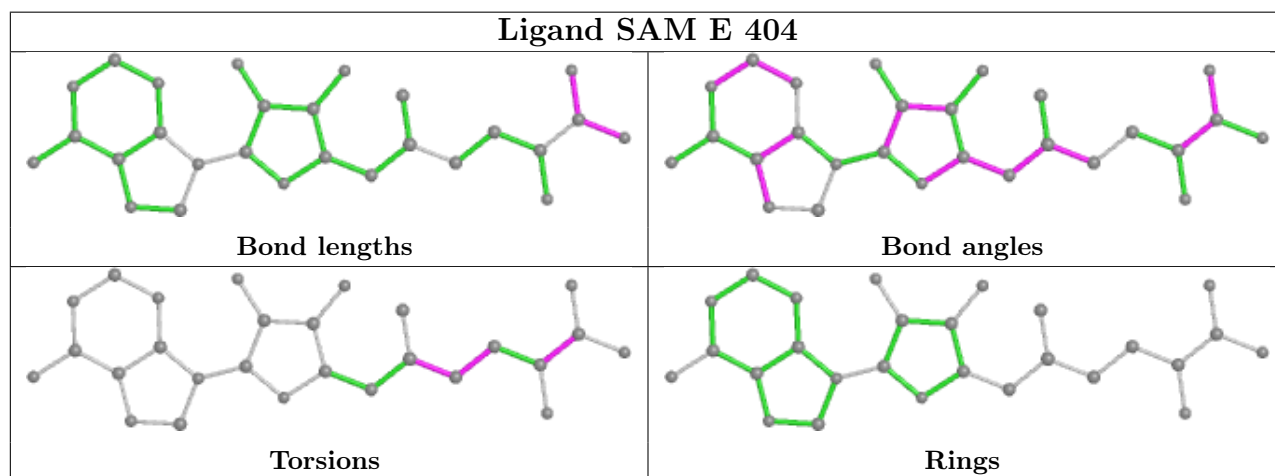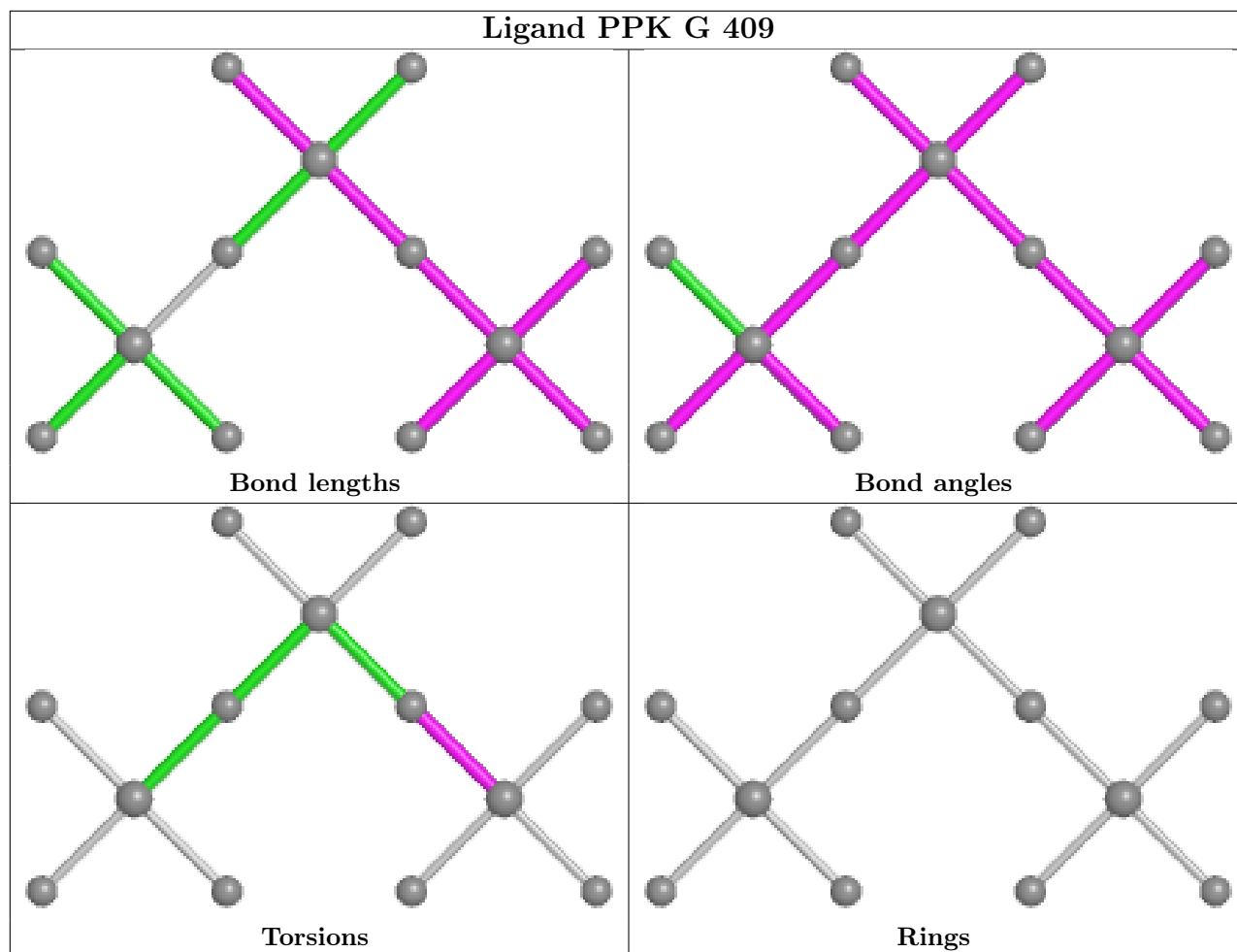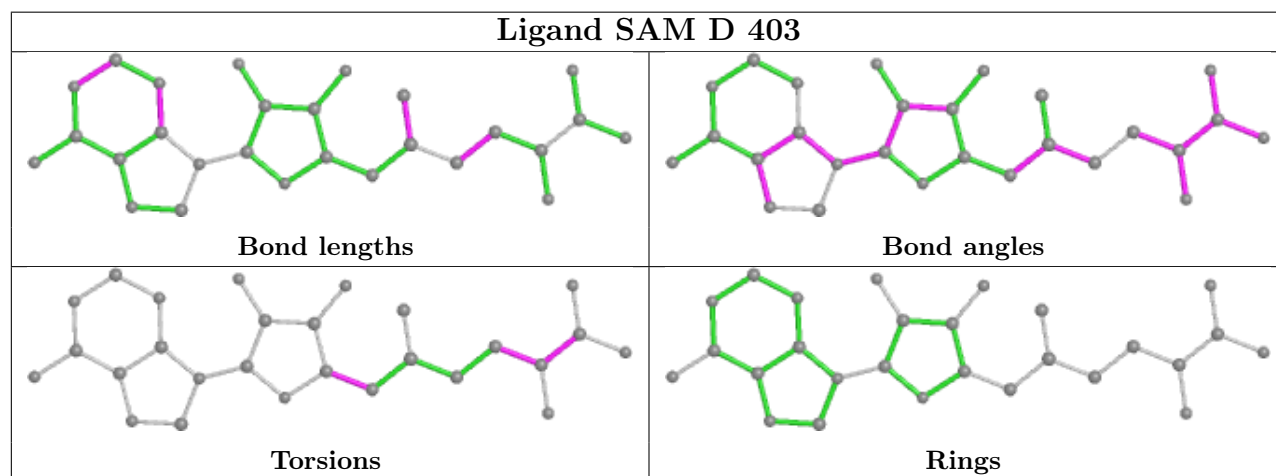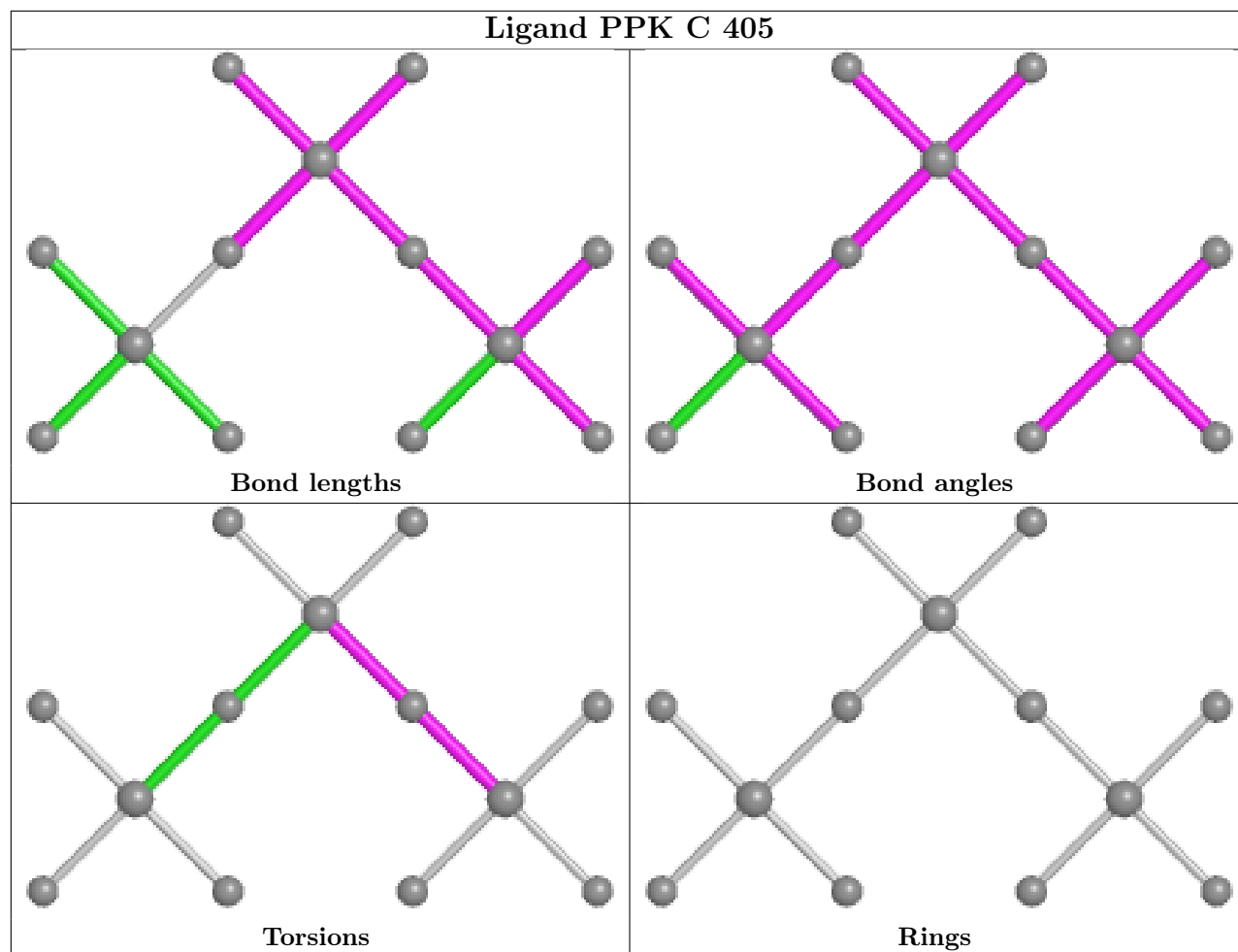| Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	404	SAM	CB-CA-N	-3.75	100.34	110.17
4	D	402	SAM	N6-C6-N1	3.74	126.33	118.57
5	E	405	PPK	O2G-PG-O3G	-3.73	104.07	113.45
4	G	403	SAM	C2-N1-C6	3.73	125.13	118.75
4	A	404	SAM	C3'-C2'-C1'	3.71	106.57	100.98
4	F	402	SAM	CB-CA-C	3.69	119.09	110.30
4	E	406	SAM	N6-C6-N1	3.67	126.20	118.57
4	C	404	SAM	N3-C2-N1	-3.64	122.98	128.68
5	G	409	PPK	O1B-PB-O2B	3.63	117.53	109.92
4	D	402	SAM	O4'-C4'-C3'	3.62	112.27	105.11
5	C	408	PPK	PB-O3A-PA	-3.62	119.88	132.62
4	B	402	SAM	OXT-C-O	-3.59	115.94	124.09
4	F	403	SAM	C2-N1-C6	3.58	124.88	118.75
5	E	405	PPK	O1G-PG-O2G	3.57	117.16	107.64
5	E	409	PPK	O3A-PB-N3B	-3.57	96.70	106.59
4	D	402	SAM	C2'-C3'-C4'	-3.57	95.71	102.64
5	A	405	PPK	PB-O3A-PA	-3.55	120.11	132.62
5	C	405	PPK	O2B-PB-N3B	-3.50	106.62	111.77
5	E	409	PPK	O2G-PG-O3G	-3.49	104.67	113.45
4	A	406	SAM	N3-C2-N1	-3.49	123.23	128.68
4	E	404	SAM	C4-C5-N7	-3.47	105.78	109.40
4	D	402	SAM	C2-N1-C6	3.46	124.67	118.75
4	H	402	SAM	C2-N1-C6	3.46	124.67	118.75
5	A	409	PPK	O3G-PG-N3B	-3.44	106.71	111.77
4	C	406	SAM	OXT-C-O	-3.43	116.30	124.09
4	E	406	SAM	CB-CA-C	3.40	118.41	110.30
4	C	404	SAM	O3'-C3'-C4'	-3.39	101.25	111.05
5	G	409	PPK	O2B-PB-N3B	-3.38	106.80	111.77
4	B	403	SAM	C3'-C2'-C1'	3.36	106.04	100.98
5	G	409	PPK	PB-O3A-PA	-3.35	120.81	132.62
4	E	404	SAM	C3'-C2'-C1'	3.34	106.01	100.98
5	E	409	PPK	O1G-PG-O3G	-3.32	105.10	113.45
4	C	406	SAM	C4-C5-N7	-3.30	105.96	109.40
4	H	403	SAM	CB-CA-C	3.29	118.15	110.30
5	E	405	PPK	O1A-PA-O3A	3.28	115.65	104.64
5	A	409	PPK	O2A-PA-O1A	3.15	119.68	107.64
4	H	402	SAM	O3'-C3'-C4'	3.15	120.16	111.05
4	D	403	SAM	CB-CA-N	-3.14	101.93	110.17
4	C	406	SAM	O4'-C1'-C2'	-3.13	102.35	106.93
4	G	405	SAM	OXT-C-O	-3.12	117.00	124.09
5	C	405	PPK	O1A-PA-O3A	-3.10	94.23	104.64
4	C	404	SAM	O4'-C4'-C5'	3.10	116.70	108.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	406	SAM	O4'-C4'-C5'	3.07	116.64	108.88
4	D	402	SAM	OXT-C-O	-3.07	117.12	124.09
5	A	405	PPK	O2G-PG-O3G	-3.07	105.74	113.45
4	A	404	SAM	O4'-C1'-C2'	-3.07	102.44	106.93
4	C	404	SAM	N6-C6-N1	3.05	124.91	118.57
4	A	406	SAM	C5-C6-N6	3.05	124.98	120.35
4	G	405	SAM	O4'-C4'-C5'	3.03	116.55	108.88
4	E	406	SAM	C5-C6-N6	-3.01	115.78	120.35
5	A	405	PPK	O1B-PB-O3A	-3.00	94.64	104.64
5	A	405	PPK	O3A-PB-N3B	2.97	114.83	106.59
4	H	403	SAM	OXT-C-CA	2.97	123.49	113.38
5	G	404	PPK	O2G-PG-O3G	2.94	120.83	113.45
4	A	404	SAM	C5-C6-N6	-2.93	115.90	120.35
5	A	405	PPK	O1G-PG-O2G	2.90	115.37	107.64
4	E	404	SAM	OXT-C-CA	2.89	123.24	113.38
4	F	402	SAM	N3-C2-N1	-2.83	124.25	128.68
5	C	408	PPK	O1G-PG-O2G	2.82	115.15	107.64
4	G	403	SAM	C3'-C2'-C1'	2.82	105.22	100.98
5	A	409	PPK	O3A-PA-O4A	-2.81	95.59	111.19
4	G	403	SAM	CG-SD-C5'	2.80	110.55	103.40
4	E	404	SAM	N3-C2-N1	-2.80	124.30	128.68
4	E	406	SAM	N3-C2-N1	-2.79	124.31	128.68
5	E	405	PPK	O1B-PB-O3A	2.78	113.91	104.64
4	A	404	SAM	N6-C6-N1	2.72	124.22	118.57
4	C	406	SAM	CB-CA-C	2.72	116.77	110.30
4	D	402	SAM	OXT-C-CA	2.69	122.56	113.38
4	B	402	SAM	O2'-C2'-C3'	-2.69	103.12	111.82
4	E	404	SAM	CG-SD-C5'	2.69	110.25	103.40
5	A	405	PPK	O2B-PB-N3B	2.68	115.71	111.77
4	H	402	SAM	C1'-N9-C4	-2.66	121.96	126.64
4	G	403	SAM	OXT-C-CA	2.59	122.19	113.38
4	F	402	SAM	CG-SD-C5'	2.57	109.95	103.40
4	C	406	SAM	O2'-C2'-C1'	-2.56	101.39	110.85
4	E	404	SAM	O4'-C4'-C5'	2.53	115.28	108.88
5	C	405	PPK	O1B-PB-O3A	2.51	113.03	104.64
5	A	409	PPK	O1A-PA-O3A	2.49	112.99	104.64
5	E	405	PPK	PB-O3A-PA	-2.48	123.89	132.62
4	G	403	SAM	OXT-C-O	-2.48	118.47	124.09
4	B	403	SAM	OXT-C-CA	2.47	121.80	113.38
4	B	403	SAM	O4'-C1'-C2'	-2.45	103.34	106.93
5	A	409	PPK	O1G-PG-O3G	2.44	119.59	113.45
4	F	402	SAM	C4-C5-N7	-2.44	106.85	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	402	SAM	O4'-C4'-C5'	2.44	115.04	108.88
4	H	402	SAM	N6-C6-N1	2.44	123.63	118.57
5	E	405	PPK	O1A-PA-O4A	2.43	120.21	110.68
4	B	403	SAM	C2-N1-C6	2.43	122.91	118.75
4	B	402	SAM	C5-C6-N6	2.42	124.02	120.35
4	C	404	SAM	C5-C6-N1	-2.41	114.88	120.35
4	H	403	SAM	O4'-C4'-C5'	2.41	114.96	108.88
4	C	404	SAM	C4-C5-N7	-2.39	106.91	109.40
5	C	405	PPK	O2G-PG-O3G	2.38	119.45	113.45
4	F	402	SAM	C2'-C3'-C4'	-2.36	98.06	102.64
4	H	403	SAM	CB-CA-N	-2.35	104.01	110.17
5	C	405	PPK	O1A-PA-O4A	2.34	119.85	110.68
4	F	403	SAM	CB-CA-N	-2.34	104.04	110.17
4	E	406	SAM	C2'-C3'-C4'	2.34	107.18	102.64
4	E	406	SAM	OXT-C-CA	2.34	121.34	113.38
5	C	408	PPK	O2A-PA-O1A	2.33	116.55	107.64
4	H	402	SAM	CG-SD-C5'	2.33	109.34	103.40
4	G	405	SAM	C2-N1-C6	2.30	122.68	118.75
4	A	404	SAM	OXT-C-CA	2.30	121.21	113.38
4	F	403	SAM	C4-C5-N7	-2.28	107.02	109.40
4	C	406	SAM	CE-SD-C5'	2.27	118.41	100.54
4	A	404	SAM	C2'-C3'-C4'	-2.27	98.24	102.64
4	D	403	SAM	CG-SD-C5'	2.27	109.18	103.40
4	H	402	SAM	C5-C6-N1	-2.26	115.23	120.35
4	G	403	SAM	O4'-C4'-C3'	2.25	109.58	105.11
4	E	406	SAM	O2'-C2'-C3'	2.23	119.05	111.82
5	G	409	PPK	O2A-PA-O4A	2.23	119.42	110.68
5	C	408	PPK	O1G-PG-O3G	2.22	119.02	113.45
4	F	403	SAM	OXT-C-CA	2.21	120.90	113.38
4	E	406	SAM	OXT-C-O	-2.19	119.12	124.09
4	F	403	SAM	OXT-C-O	-2.19	119.12	124.09
4	G	403	SAM	N6-C6-N1	2.19	123.11	118.57
4	H	402	SAM	C4-C5-N7	-2.18	107.12	109.40
4	H	403	SAM	C2'-C3'-C4'	2.15	106.82	102.64
4	C	404	SAM	C2-N1-C6	2.15	122.43	118.75
4	C	406	SAM	O3'-C3'-C2'	2.15	118.78	111.82
4	A	406	SAM	OXT-C-CA	2.13	120.64	113.38
4	F	402	SAM	C1'-N9-C4	-2.11	122.94	126.64
5	G	409	PPK	O1G-PG-O2G	2.10	113.22	107.64
4	F	402	SAM	C2-N1-C6	2.05	122.26	118.75
4	B	402	SAM	O4'-C4'-C5'	2.05	114.06	108.88
5	E	409	PPK	O1B-PB-O3A	2.05	111.47	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	406	SAM	CG-SD-C5'	2.03	108.57	103.40
4	C	404	SAM	C3'-C2'-C1'	2.02	104.01	100.98

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	406	SAM	CB-CG-SD-CE
4	B	402	SAM	N-CA-CB-CG
4	B	402	SAM	C-CA-CB-CG
4	B	402	SAM	CA-CB-CG-SD
4	B	402	SAM	CB-CG-SD-CE
4	B	402	SAM	CB-CG-SD-C5'
4	B	403	SAM	CA-CB-CG-SD
4	B	403	SAM	CB-CG-SD-CE
4	B	403	SAM	CB-CG-SD-C5'
4	C	404	SAM	CA-CB-CG-SD
4	C	404	SAM	CB-CG-SD-CE
4	C	404	SAM	O4'-C4'-C5'-SD
4	C	406	SAM	N-CA-CB-CG
4	C	406	SAM	C-CA-CB-CG
4	C	406	SAM	CB-CG-SD-CE
4	C	406	SAM	CB-CG-SD-C5'
4	D	402	SAM	C3'-C4'-C5'-SD
4	E	406	SAM	N-CA-CB-CG
4	E	406	SAM	C-CA-CB-CG
4	E	406	SAM	CA-CB-CG-SD
4	E	406	SAM	CB-CG-SD-C5'
4	G	403	SAM	O-C-CA-N
4	G	403	SAM	O4'-C4'-C5'-SD
4	G	403	SAM	C3'-C4'-C5'-SD
4	G	405	SAM	O-C-CA-N
4	H	403	SAM	O4'-C4'-C5'-SD
4	H	403	SAM	C3'-C4'-C5'-SD
5	C	405	PPK	PB-N3B-PG-O3G
5	C	405	PPK	PG-N3B-PB-O2B
5	C	408	PPK	PB-N3B-PG-O3G
5	E	409	PPK	PB-N3B-PG-O3G
5	E	409	PPK	PG-N3B-PB-O2B
5	G	404	PPK	PB-N3B-PG-O3G
5	G	404	PPK	PG-N3B-PB-O2B
5	G	409	PPK	PB-N3B-PG-O3G

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Mol	Chain	Res	Type	Atoms
4	G	405	SAM	OXT-C-CA-N
4	G	403	SAM	OXT-C-CA-N
4	D	403	SAM	OXT-C-CA-N
4	E	406	SAM	OXT-C-CA-N
4	E	404	SAM	CB-CG-SD-CE
4	C	404	SAM	C-CA-CB-CG
4	F	402	SAM	OXT-C-CA-N
4	A	406	SAM	O-C-CA-CB
4	A	406	SAM	OXT-C-CA-CB
4	E	406	SAM	CB-CG-SD-CE
4	F	402	SAM	CB-CG-SD-CE
4	H	402	SAM	CB-CG-SD-CE
4	C	404	SAM	OXT-C-CA-N
4	H	402	SAM	OXT-C-CA-N
4	C	404	SAM	O-C-CA-N
4	D	403	SAM	O-C-CA-N
4	E	406	SAM	O-C-CA-N
4	F	402	SAM	O-C-CA-N
4	H	402	SAM	O-C-CA-N
4	G	405	SAM	OXT-C-CA-CB
4	C	404	SAM	N-CA-CB-CG
4	B	402	SAM	O-C-CA-CB
4	D	402	SAM	OXT-C-CA-CB
5	A	405	PPK	PG-N3B-PB-O3A
5	A	409	PPK	PG-N3B-PB-O3A
5	E	405	PPK	PG-N3B-PB-O3A
4	C	404	SAM	CB-CG-SD-C5'
4	D	402	SAM	O4'-C4'-C5'-SD
4	F	402	SAM	O4'-C4'-C5'-SD
4	A	404	SAM	CA-CB-CG-SD
4	C	404	SAM	C3'-C4'-C5'-SD
4	E	404	SAM	CA-CB-CG-SD
4	E	406	SAM	C3'-C4'-C5'-SD
4	F	403	SAM	C3'-C4'-C5'-SD
4	G	405	SAM	CA-CB-CG-SD
4	H	403	SAM	CA-CB-CG-SD
4	D	402	SAM	O-C-CA-CB
4	E	404	SAM	O-C-CA-CB
4	G	403	SAM	O-C-CA-CB
4	G	403	SAM	OXT-C-CA-CB
4	G	405	SAM	O-C-CA-CB
4	B	402	SAM	OXT-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	C	406	SAM	O-C-CA-CB
4	C	406	SAM	OXT-C-CA-CB
4	C	404	SAM	O-C-CA-CB
4	F	402	SAM	O-C-CA-CB
4	A	404	SAM	O-C-CA-CB
4	E	404	SAM	OXT-C-CA-CB
4	H	402	SAM	O-C-CA-CB
4	C	404	SAM	OXT-C-CA-CB
4	F	402	SAM	OXT-C-CA-CB
5	A	405	PPK	PG-N3B-PB-O2B
5	A	409	PPK	PG-N3B-PB-O2B
4	D	403	SAM	C-CA-CB-CG
4	H	403	SAM	C-CA-CB-CG
4	A	404	SAM	OXT-C-CA-CB
4	A	404	SAM	OXT-C-CA-N
4	F	403	SAM	CB-CG-SD-CE
4	C	406	SAM	OXT-C-CA-N
4	H	402	SAM	OXT-C-CA-CB
4	E	404	SAM	OXT-C-CA-N
5	C	408	PPK	PG-N3B-PB-O3A
5	E	409	PPK	PG-N3B-PB-O3A
4	A	406	SAM	CB-CG-SD-C5'
4	D	403	SAM	O4'-C4'-C5'-SD
4	E	404	SAM	CB-CG-SD-C5'
4	E	406	SAM	O4'-C4'-C5'-SD
4	F	402	SAM	CB-CG-SD-C5'
4	F	403	SAM	CB-CG-SD-C5'

There are no ring outliers.

19 monomers are involved in 53 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	409	PPK	1	0
4	E	404	SAM	1	0
5	E	409	PPK	3	0
4	C	406	SAM	1	0
5	C	405	PPK	3	0
4	D	403	SAM	2	0
4	A	406	SAM	7	0
5	C	408	PPK	4	0
4	F	403	SAM	1	0
4	H	403	SAM	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	SAM	1	0
5	A	405	PPK	7	0
5	A	409	PPK	2	0
4	F	402	SAM	3	0
4	G	405	SAM	4	0
4	H	402	SAM	1	0
4	G	403	SAM	4	0
5	G	404	PPK	1	0
4	C	404	SAM	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 SAM E 406

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK G 409

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM E 404

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK E 409

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM C 406

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK C 405

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM D 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM B 402

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM A 406

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK C 408

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM F 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM H 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM A 404

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK A 405

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK A 409

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM F 402

Bond lengths

Bond angles

Torsions

Rings

Ligand PPK E 405	
Bond lengths	Bond angles
Torsions	Rings

Ligand SAM D 402	
Bond lengths	Bond angles
Torsions	Rings

Ligand SAM G 405

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM H 402

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM G 403

Bond lengths

Bond angles

Torsions

Rings

Ligand SAM B 403	
Bond lengths
Bond angles
Torsions |
Rings |

Ligand PPK G 404	
Bond lengths
Bond angles
Torsions |
Rings |

Ligand SAM C 404	
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   ⓘ

6.1   Protein, DNA and RNA chains   ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	372/382 (97%)	0.57	16 (4%)	35	44	36, 47, 66, 89	0
1	B	374/382 (97%)	0.52	12 (3%)	47	57	34, 46, 65, 96	0
1	C	373/382 (97%)	0.62	21 (5%)	24	31	44, 57, 84, 106	0
1	D	372/382 (97%)	0.54	18 (4%)	30	39	44, 58, 81, 94	0
1	E	372/382 (97%)	1.11	60 (16%)	1	2	58, 75, 89, 109	0
1	F	374/382 (97%)	1.05	58 (15%)	2	3	60, 74, 95, 131	0
1	G	373/382 (97%)	1.35	87 (23%)	0	0	62, 80, 98, 125	0
1	H	372/382 (97%)	1.26	84 (22%)	0	0	63, 80, 99, 120	0
All	All	2982/3056 (97%)	0.88	356 (11%)	4	6	34, 68, 92, 131	0

All (356) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	322	ILE	7.1
1	G	149	SER	7.1
1	H	108	LEU	6.1
1	G	313	ILE	5.9
1	G	14	ALA	5.8
1	B	377	HIS	5.8
1	E	189	VAL	5.7
1	H	368	VAL	5.3
1	E	104	THR	5.2
1	G	294	ALA	5.1
1	G	170	SER	5.1
1	H	371	LEU	4.7
1	G	336	ASP	4.7
1	F	15	GLY	4.7
1	H	39	SER	4.7
1	G	289	ILE	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	281	ALA	4.5
1	F	293	PHE	4.5
1	H	326	PHE	4.5
1	B	319[A]	PHE	4.5
1	H	77	LEU	4.4
1	H	168	SER	4.4
1	E	199	ILE	4.2
1	E	371	LEU	4.2
1	G	373	LYS	4.1
1	G	191	TYR	4.1
1	F	319	PHE	4.1
1	H	230	GLY	4.0
1	B	108	LEU	4.0
1	H	279	VAL	4.0
1	F	104	THR	4.0
1	G	192	PHE	3.9
1	E	253	GLY	3.9
1	G	366	ASN	3.9
1	G	213	PHE	3.9
1	F	239	ILE	3.9
1	H	204	ALA	3.9
1	H	208	ASN	3.8
1	G	305	VAL	3.8
1	H	372	ILE	3.8
1	G	235	THR	3.8
1	H	76	PRO	3.7
1	E	106	LYS	3.7
1	H	152	PHE	3.6
1	H	135	LEU	3.6
1	E	203	ILE	3.6
1	F	252	GLY	3.6
1	H	33	LEU	3.6
1	G	281	ALA	3.6
1	C	236	GLY	3.6
1	A	312	LEU	3.6
1	G	151	GLU	3.6
1	G	212	ASN	3.6
1	F	240	ILE	3.6
1	G	274	ILE	3.6
1	H	143	ILE	3.6
1	F	353	PHE	3.5
1	E	118	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	G	266	SER	3.5
1	C	3	TYR	3.5
1	A	106	LYS	3.5
1	E	204	ALA	3.5
1	F	298	PRO	3.5
1	G	239	ILE	3.4
1	G	240	ILE	3.4
1	G	365	LEU	3.4
1	F	20	ILE	3.4
1	G	253	GLY	3.4
1	F	312	LEU	3.4
1	G	148	ARG	3.4
1	H	74	ILE	3.4
1	A	131	LEU	3.3
1	D	174	ILE	3.3
1	H	155	ILE	3.3
1	G	244	TYR	3.3
1	F	251	GLY	3.3
1	G	327	ASN	3.3
1	G	195	LYS	3.3
1	G	122	CYS	3.3
1	G	303	MET	3.3
1	F	48	CYS	3.3
1	E	63	TYR	3.3
1	G	233	GLY	3.3
1	H	344	TYR	3.3
1	G	291	LEU	3.2
1	E	207	TYR	3.2
1	G	237	ARG	3.2
1	F	280	ALA	3.2
1	H	62	ALA	3.2
1	D	212	ASN	3.2
1	E	236	GLY	3.1
1	C	235	THR	3.1
1	G	277	ASN	3.1
1	H	170	SER	3.1
1	F	295	ILE	3.1
1	G	317	LYS	3.1
1	F	356	ASP	3.1
1	H	139	LEU	3.1
1	H	253	GLY	3.1
1	G	254	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	241	VAL	3.1
1	H	304	TYR	3.1
1	H	336	ASP	3.1
1	E	278	VAL	3.1
1	H	375	SER	3.1
1	G	273	TRP	3.0
1	F	47	ALA	3.0
1	E	239	ILE	3.0
1	D	281	ALA	3.0
1	H	212	ASN	3.0
1	G	320	GLU	3.0
1	H	136	ALA	3.0
1	E	241	VAL	2.9
1	G	250	HIS	2.9
1	F	153	ILE	2.9
1	D	95	VAL	2.9
1	H	45	VAL	2.9
1	E	27	ALA	2.9
1	H	364	LYS	2.9
1	C	150	LYS	2.9
1	H	251	GLY	2.9
1	E	128	TYR	2.9
1	E	71	TRP	2.9
1	G	234	LEU	2.9
1	H	235	THR	2.9
1	F	253	GLY	2.9
1	G	246	GLY	2.9
1	E	192	PHE	2.9
1	E	216	ILE	2.9
1	F	185	GLU	2.8
1	F	248	GLY	2.8
1	H	282	LYS	2.8
1	F	322	ILE	2.8
1	G	372	ILE	2.8
1	H	333	PHE	2.8
1	H	21	CYS	2.8
1	G	312	LEU	2.8
1	A	105	ASN	2.8
1	F	120	TYR	2.8
1	C	319	PHE	2.8
1	G	243	THR	2.8
1	H	340	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	207	TYR	2.8
1	H	181	ILE	2.8
1	G	256	SER	2.8
1	C	328	PHE	2.8
1	D	152	PHE	2.8
1	E	252	GLY	2.8
1	G	199	ILE	2.8
1	D	5	LYS	2.8
1	F	291	LEU	2.7
1	G	252	GLY	2.7
1	H	248	GLY	2.7
1	C	284	ALA	2.7
1	H	339	LEU	2.7
1	D	12	VAL	2.7
1	E	66	VAL	2.7
1	E	95	VAL	2.7
1	G	279	VAL	2.7
1	H	252	GLY	2.7
1	E	334	ILE	2.7
1	E	67	VAL	2.7
1	A	325	SER	2.7
1	E	152	PHE	2.7
1	C	151	GLU	2.7
1	G	236	GLY	2.7
1	G	184	ASP	2.7
1	B	100	SER	2.7
1	G	232	THR	2.7
1	D	199	ILE	2.7
1	G	155	ILE	2.7
1	F	237	ARG	2.7
1	F	235	THR	2.7
1	E	354	GLY	2.7
1	F	300	PRO	2.7
1	B	104	THR	2.6
1	G	328	PHE	2.6
1	F	303	MET	2.6
1	F	377	HIS	2.6
1	G	45	VAL	2.6
1	H	6	ILE	2.6
1	H	177	MET	2.6
1	F	106	LYS	2.6
1	E	283	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	318	ILE	2.6
1	E	330	ILE	2.6
1	F	328	PHE	2.6
1	F	71	TRP	2.6
1	E	22	ASP	2.6
1	G	201	GLU	2.6
1	F	224	VAL	2.5
1	C	317	LYS	2.5
1	F	4	LYS	2.5
1	F	35	GLN	2.5
1	E	255	PHE	2.5
1	G	118	PHE	2.5
1	H	169	ASN	2.5
1	H	250	HIS	2.5
1	E	256	SER	2.5
1	H	67	VAL	2.5
1	H	32	CYS	2.5
1	D	318	ILE	2.5
1	G	329	ASP	2.5
1	E	222	ARG	2.5
1	G	283	LEU	2.5
1	F	250	HIS	2.5
1	C	171	THR	2.5
1	D	167	TYR	2.5
1	G	304	TYR	2.5
1	H	238	LYS	2.5
1	F	236	GLY	2.5
1	G	13	GLY	2.5
1	G	296	GLY	2.5
1	F	109	ILE	2.5
1	H	270	PHE	2.5
1	G	190	GLU	2.5
1	G	46	LEU	2.5
1	C	240	ILE	2.5
1	E	240	ILE	2.5
1	F	313	ILE	2.5
1	G	375	SER	2.5
1	H	239	ILE	2.5
1	H	147	ARG	2.5
1	E	43	CYS	2.5
1	F	188	ASP	2.5
1	H	243	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	239	ILE	2.5
1	F	213	PHE	2.5
1	E	18	ASP	2.5
1	E	251	GLY	2.5
1	E	367	LYS	2.4
1	E	264	ASP	2.4
1	H	320	GLU	2.4
1	E	172	PRO	2.4
1	A	173	LEU	2.4
1	G	255	PHE	2.4
1	B	37	GLN	2.4
1	E	196	VAL	2.4
1	A	194	LYS	2.4
1	G	152	PHE	2.4
1	H	236	GLY	2.4
1	H	273	TRP	2.4
1	H	232	THR	2.4
1	H	369	GLU	2.4
1	G	218	ASN	2.4
1	C	243	THR	2.4
1	E	243	THR	2.4
1	F	150	LYS	2.4
1	G	197	SER	2.4
1	G	335	ASN	2.4
1	D	320	GLU	2.4
1	H	322	ILE	2.4
1	F	14	ALA	2.4
1	B	107	ASN	2.4
1	A	372	ILE	2.4
1	B	71	TRP	2.4
1	C	201	GLU	2.4
1	D	11	SER	2.4
1	H	283	LEU	2.4
1	D	172	PRO	2.3
1	G	249	HIS	2.3
1	E	174	ILE	2.3
1	H	55	ALA	2.3
1	E	220	SER	2.3
1	F	25	SER	2.3
1	H	211	THR	2.3
1	F	318	ILE	2.3
1	E	235	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	249	HIS	2.3
1	E	116	ILE	2.3
1	A	187	TYR	2.3
1	E	191	TYR	2.3
1	G	208	ASN	2.3
1	E	173	LEU	2.3
1	H	189	VAL	2.3
1	A	256	SER	2.3
1	C	82	ASN	2.3
1	E	100	SER	2.3
1	C	304	TYR	2.3
1	G	3	TYR	2.3
1	E	140	LEU	2.3
1	G	139	LEU	2.3
1	D	208	ASN	2.3
1	G	153	ILE	2.3
1	H	187	TYR	2.3
1	G	12	VAL	2.3
1	G	163	VAL	2.3
1	F	192	PHE	2.3
1	F	8	THR	2.3
1	B	105	ASN	2.2
1	H	159	MET	2.2
1	H	342	THR	2.2
1	F	19	LYS	2.2
1	H	172	PRO	2.2
1	H	249	HIS	2.2
1	H	362	TRP	2.2
1	G	300	PRO	2.2
1	E	5	LYS	2.2
1	F	95	VAL	2.2
1	C	52	ILE	2.2
1	G	337	LEU	2.2
1	B	106	LYS	2.2
1	D	304	TYR	2.2
1	F	301	VAL	2.2
1	H	64	VAL	2.2
1	G	116	ILE	2.2
1	E	133	SER	2.2
1	E	254	ALA	2.2
1	H	289	ILE	2.2
1	G	172	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	103	LYS	2.2
1	G	146	GLN	2.2
1	A	369	GLU	2.2
1	F	256	SER	2.2
1	F	249	HIS	2.1
1	H	263	VAL	2.1
1	E	105	ASN	2.1
1	H	221	GLY	2.1
1	F	126	PRO	2.1
1	H	117	VAL	2.1
1	E	143	ILE	2.1
1	E	238	LYS	2.1
1	F	123	ASP	2.1
1	G	145	ARG	2.1
1	D	191	TYR	2.1
1	A	24	ILE	2.1
1	H	234	LEU	2.1
1	H	365	LEU	2.1
1	B	241	VAL	2.1
1	H	18	ASP	2.1
1	F	128	TYR	2.1
1	A	107	ASN	2.1
1	F	369	GLU	2.1
1	H	129	MET	2.1
1	F	302	ALA	2.1
1	H	154	LYS	2.1
1	H	205	LYS	2.1
1	D	189	VAL	2.1
1	F	247	VAL	2.1
1	D	322	ILE	2.1
1	H	29	LEU	2.1
1	G	251	GLY	2.1
1	C	189	VAL	2.0
1	A	190	GLU	2.0
1	C	239	ILE	2.0
1	E	109	ILE	2.0
1	A	246	GLY	2.0
1	E	250	HIS	2.0
1	G	347	VAL	2.0
1	G	202	GLN	2.0
1	H	128	TYR	2.0
1	B	340	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	G	222	ARG	2.0
1	G	173	LEU	2.0
1	C	315	GLU	2.0
1	H	175	GLU	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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
3	MG	G	402	1/1	0.76	0.54	72,72,72,72	0
3	MG	E	403	1/1	0.77	0.45	68,68,68,68	0
2	K	G	408	1/1	0.77	0.27	121,121,121,121	0
4	SAM	G	403	27/27	0.81	0.22	78,81,86,86	0
4	SAM	F	403	27/27	0.83	0.22	76,78,96,97	0
4	SAM	G	405	27/27	0.86	0.27	77,87,94,95	0
2	K	E	408	1/1	0.88	0.29	75,75,75,75	0
4	SAM	H	403	27/27	0.88	0.23	76,81,85,87	0
4	SAM	H	402	27/27	0.89	0.26	76,81,97,101	0
3	MG	A	407	1/1	0.90	0.48	39,39,39,39	0
4	SAM	A	406	27/27	0.90	0.22	60,62,101,104	0
4	SAM	E	406	27/27	0.90	0.18	71,75,81,83	0
3	MG	A	403	1/1	0.90	0.52	37,37,37,37	0
4	SAM	E	404	27/27	0.92	0.18	69,71,81,82	0
4	SAM	A	404	27/27	0.92	0.19	44,45,54,54	0
4	SAM	F	402	27/27	0.92	0.17	61,63,70,71	0
4	SAM	C	404	27/27	0.92	0.19	54,56,58,58	0
3	MG	C	402	1/1	0.93	0.34	40,40,40,40	0
3	MG	C	403	1/1	0.93	0.51	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	SAM	B	403	27/27	0.93	0.14	48,52,67,69	0
3	MG	A	402	1/1	0.93	0.47	66,66,66,66	0
3	MG	B	401	1/1	0.93	0.54	60,60,60,60	0
3	MG	G	406	1/1	0.93	0.50	67,67,67,67	0
3	MG	E	407	1/1	0.94	0.34	49,49,49,49	0
4	SAM	C	406	27/27	0.94	0.19	53,55,68,71	0
4	SAM	D	402	27/27	0.94	0.18	53,55,59,60	0
4	SAM	D	403	27/27	0.94	0.16	49,52,61,61	0
3	MG	F	401	1/1	0.94	0.31	77,77,77,77	0
3	MG	G	407	1/1	0.94	0.62	60,60,60,60	0
5	PPK	E	409	13/13	0.94	0.22	60,63,69,71	0
2	K	C	401	1/1	0.95	0.19	67,67,67,67	0
2	K	A	401	1/1	0.95	0.12	50,50,50,50	0
2	K	A	408	1/1	0.95	0.16	57,57,57,57	0
4	SAM	B	402	27/27	0.95	0.17	37,39,46,46	0
3	MG	C	407	1/1	0.95	0.56	53,53,53,53	0
5	PPK	E	405	13/13	0.95	0.19	59,60,61,62	0
3	MG	D	401	1/1	0.95	0.30	39,39,39,39	0
5	PPK	G	409	13/13	0.95	0.17	70,72,73,74	0
2	K	E	401	1/1	0.96	0.18	73,73,73,73	0
5	PPK	A	405	13/13	0.96	0.24	41,42,43,43	0
5	PPK	C	405	13/13	0.96	0.21	41,42,43,43	0
5	PPK	C	408	13/13	0.97	0.20	42,42,43,43	0
5	PPK	G	404	13/13	0.97	0.26	61,62,64,66	0
2	K	G	401	1/1	0.97	0.21	67,67,67,67	0
3	MG	H	401	1/1	0.98	0.29	60,60,60,60	0
5	PPK	A	409	13/13	0.98	0.21	36,36,38,38	0
3	MG	E	402	1/1	0.99	0.35	73,73,73,73	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 SAM G 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
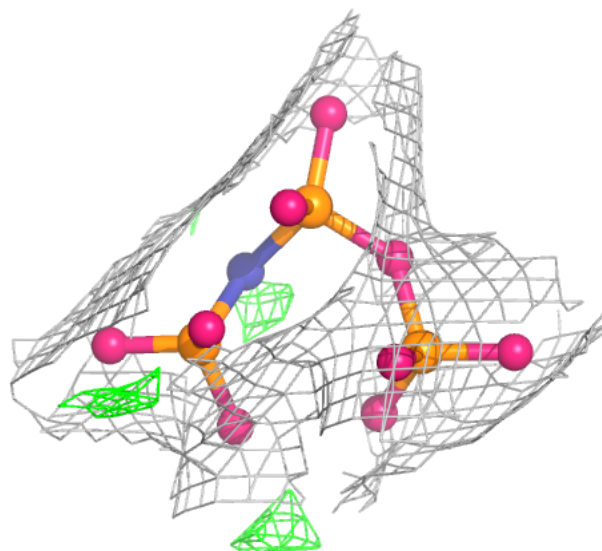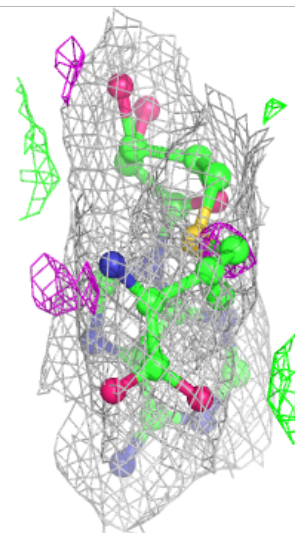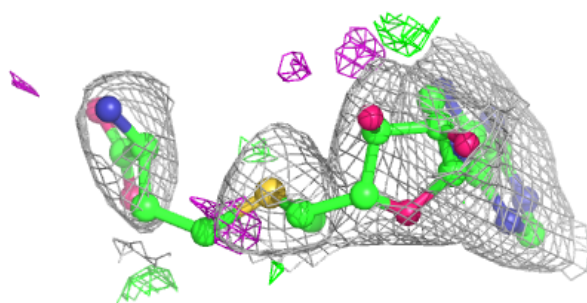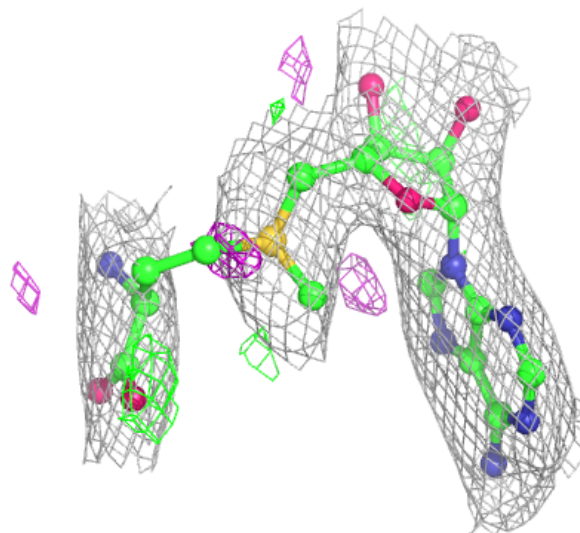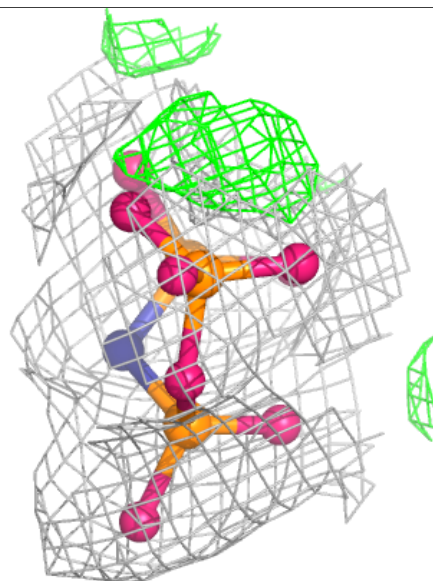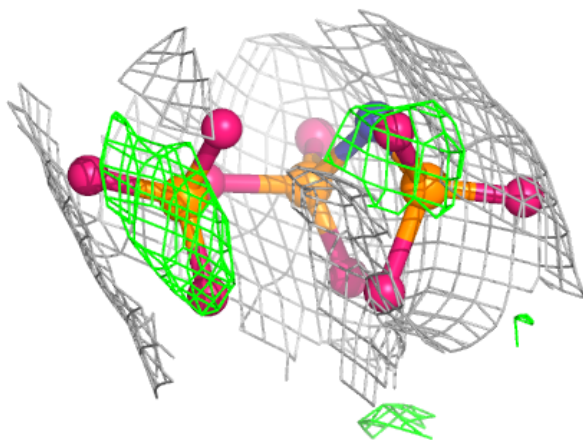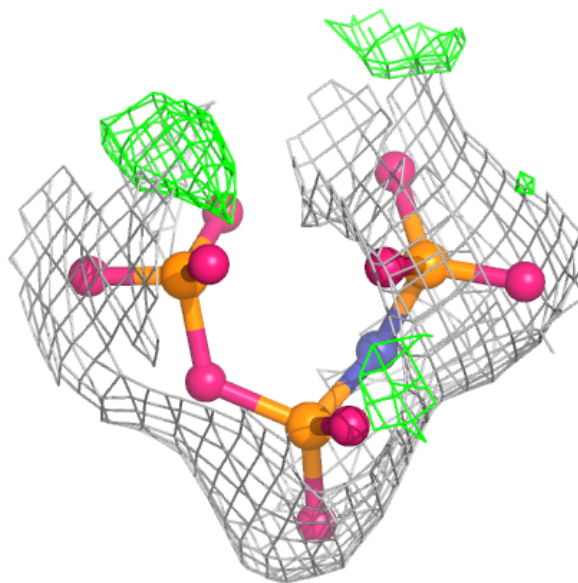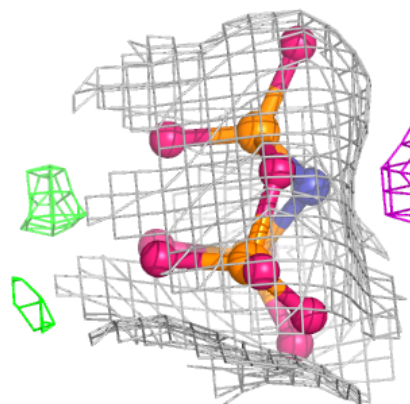and green (positive)
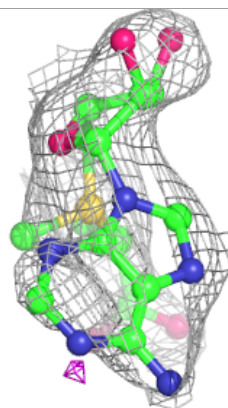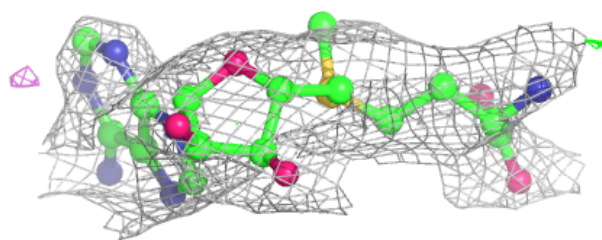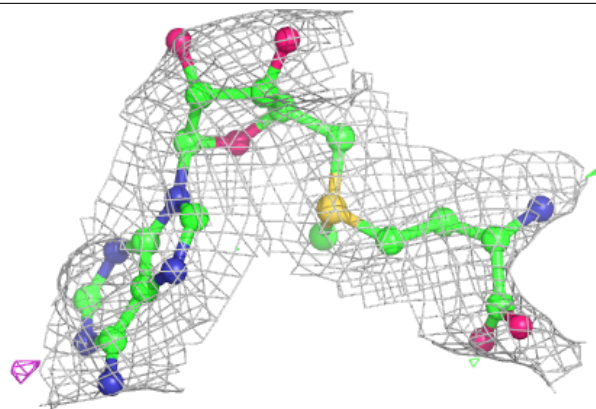
Electron density around SAM F 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
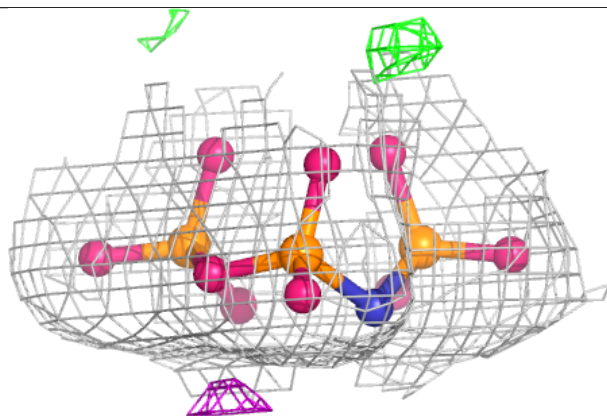$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
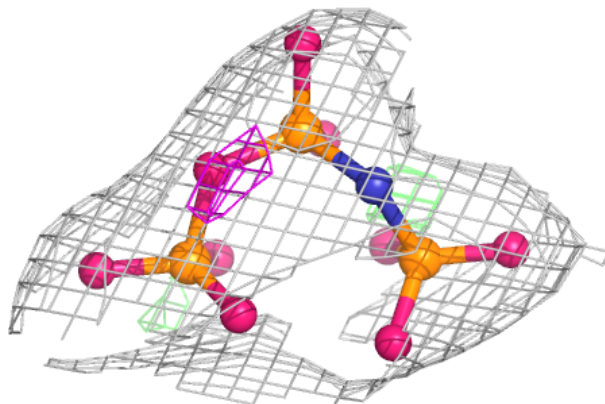and green (positive)
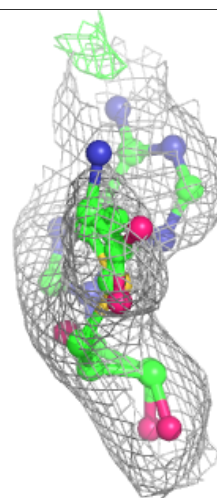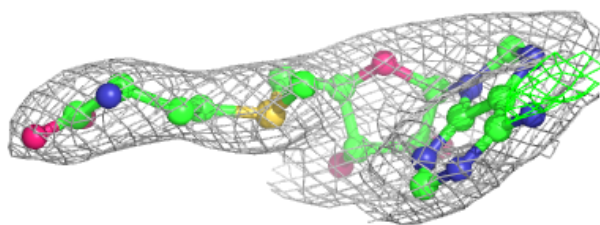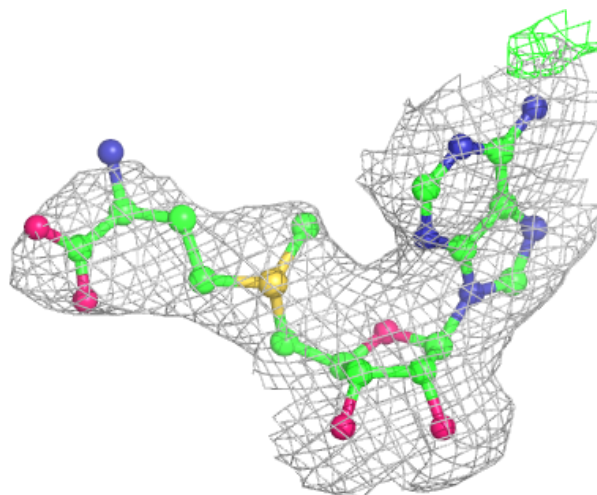
Electron density around SAM G 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
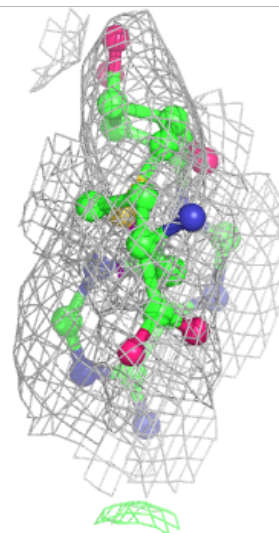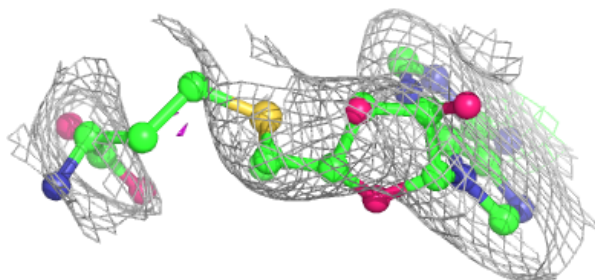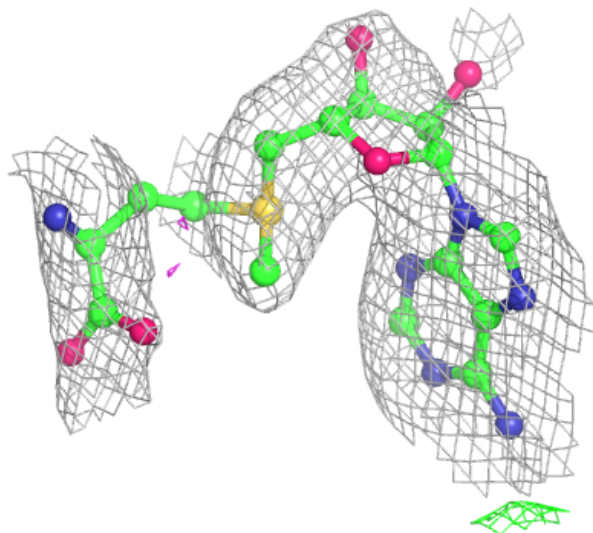
Electron density around SAM H 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
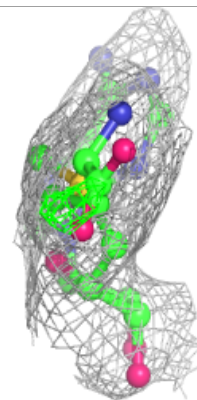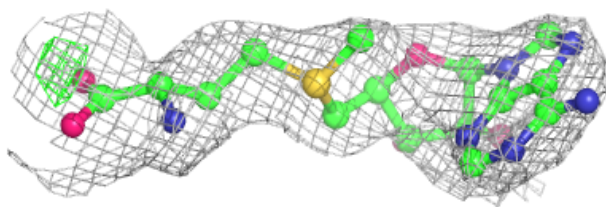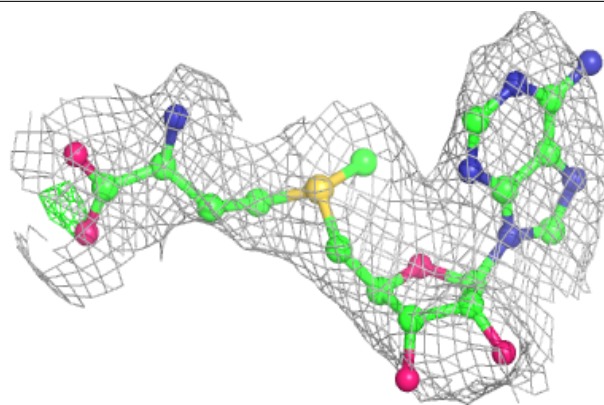
Electron density around SAM H 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
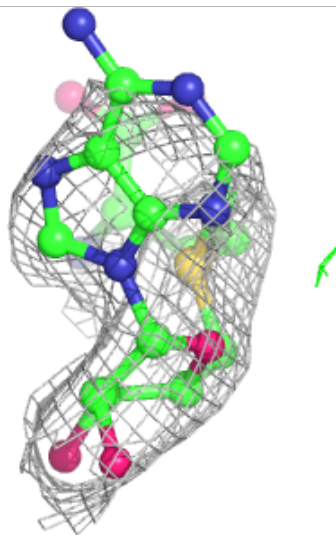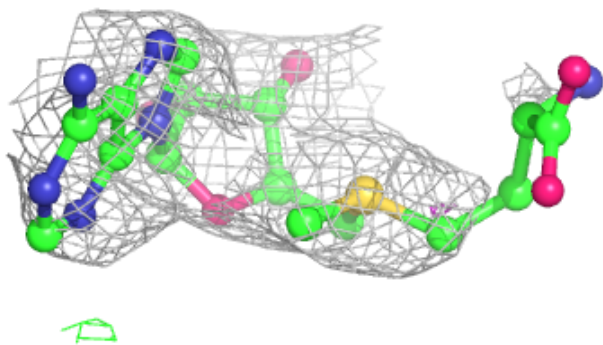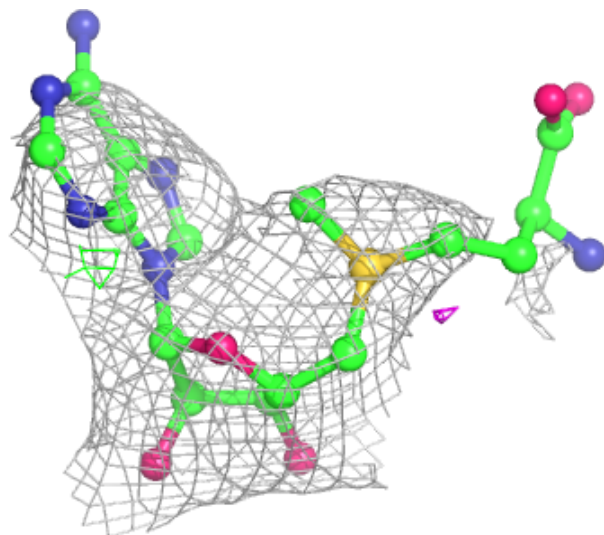
Electron density around SAM A 406:

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

Electron density around SAM E 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
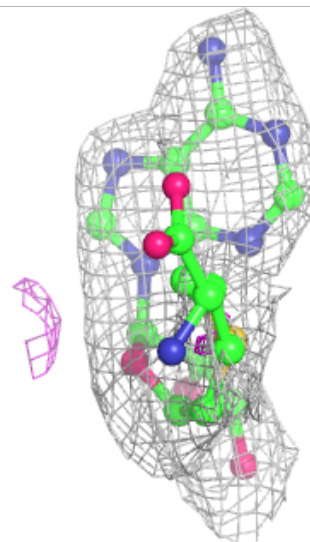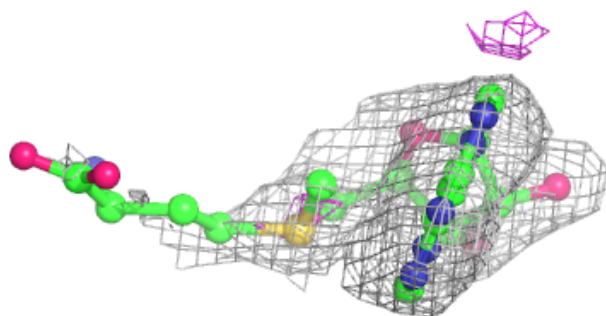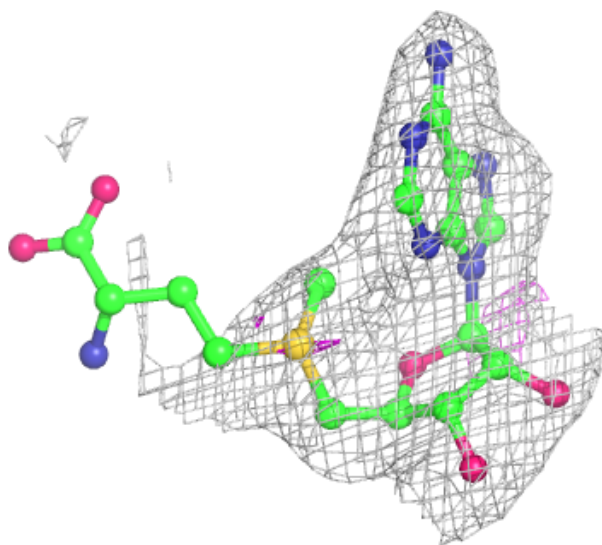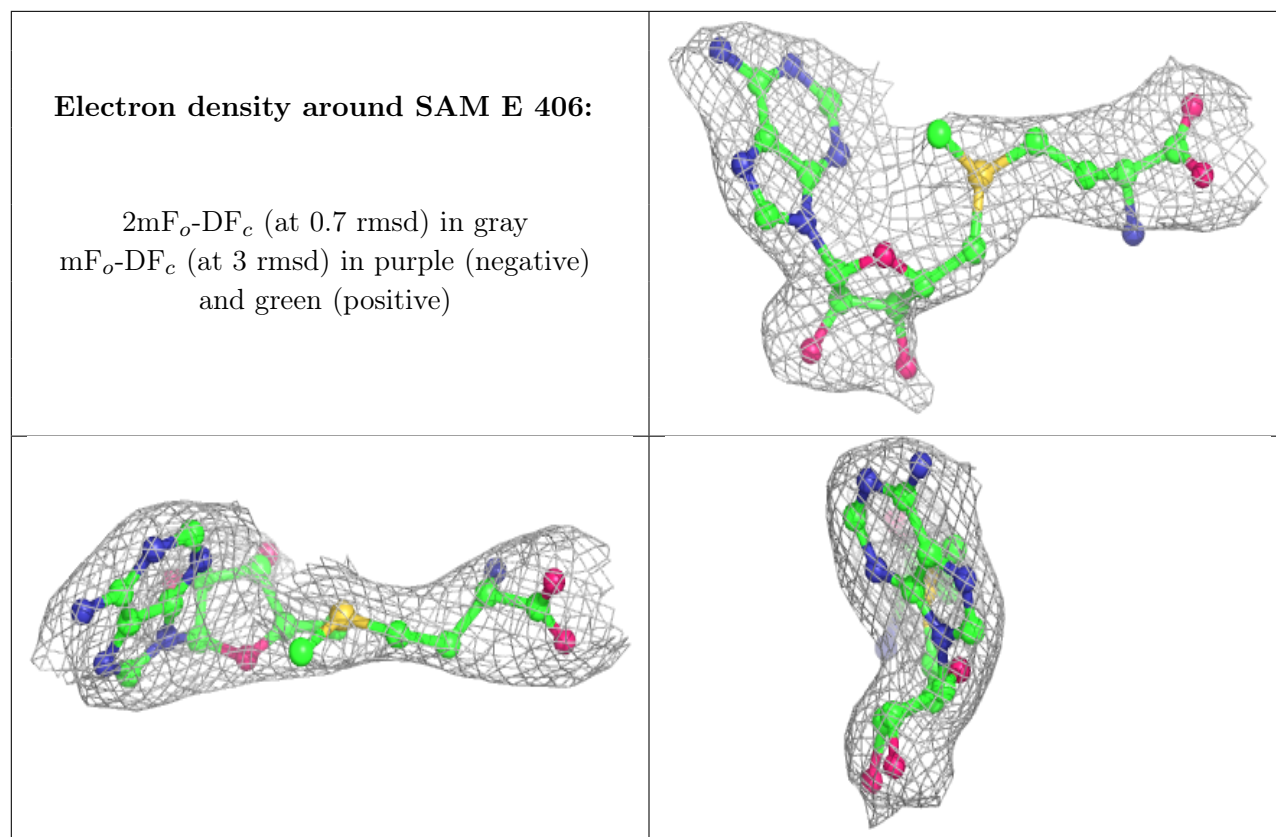
Electron density around SAM E 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
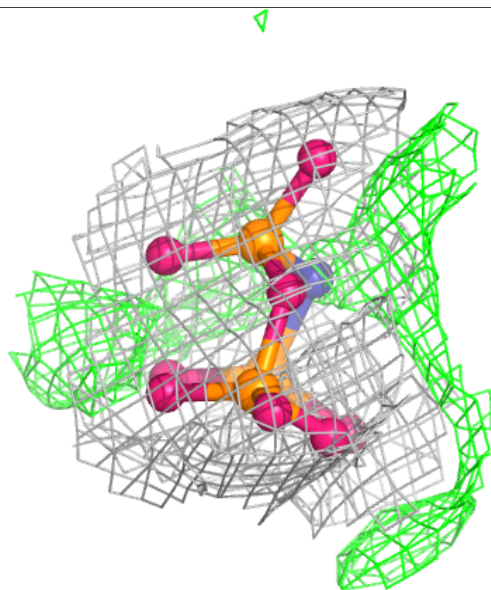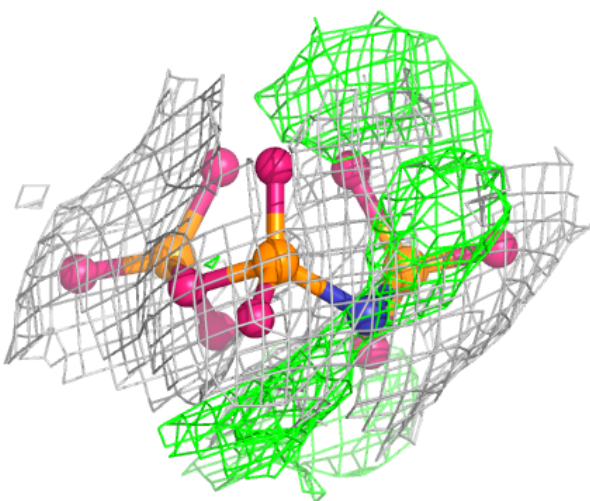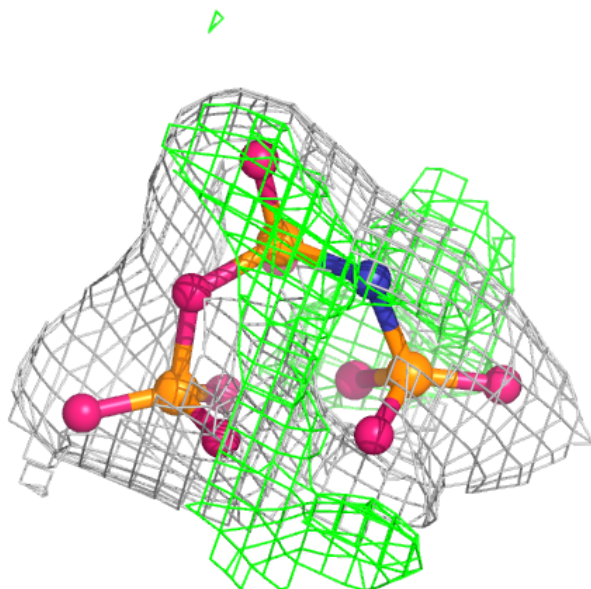mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
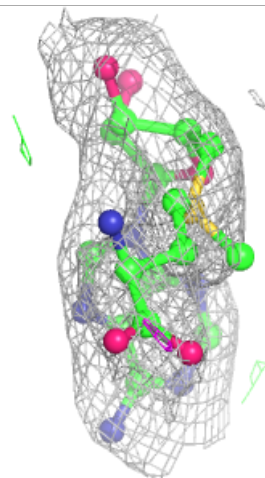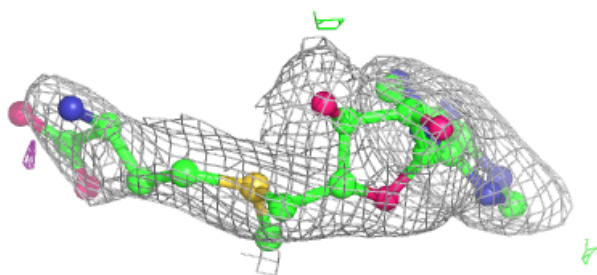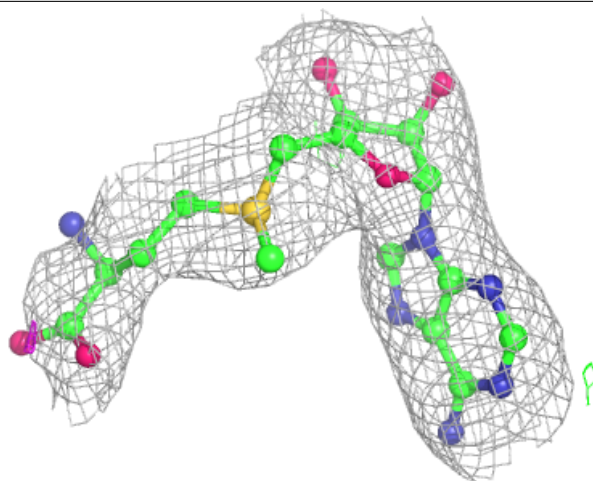
Electron density around SAM A 404:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
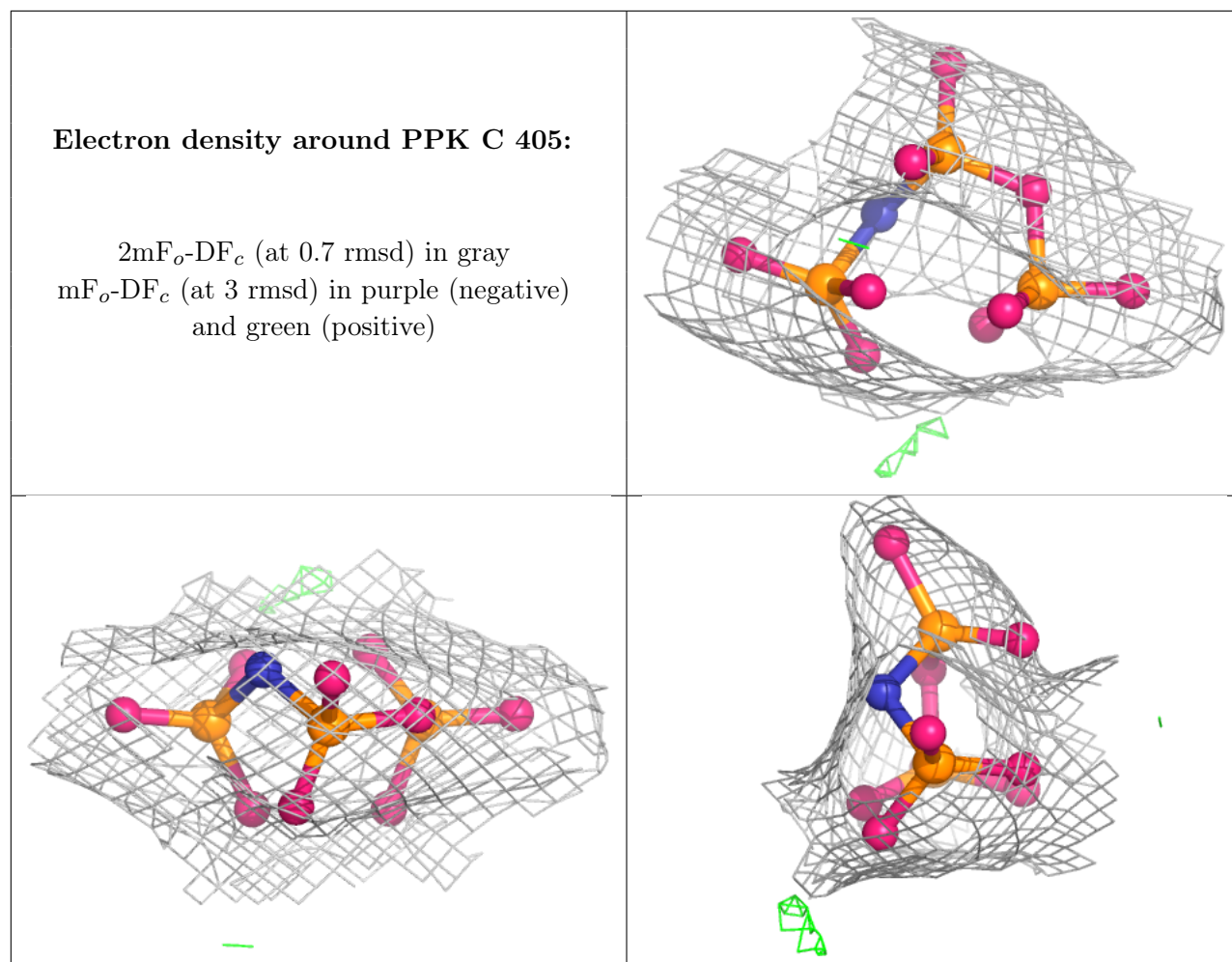and green (positive)
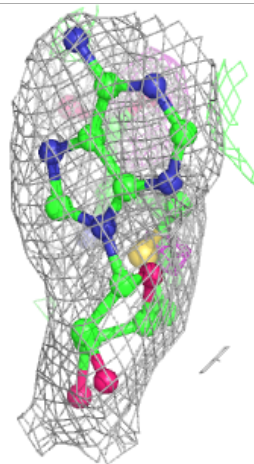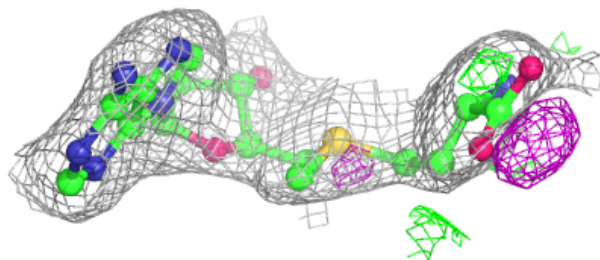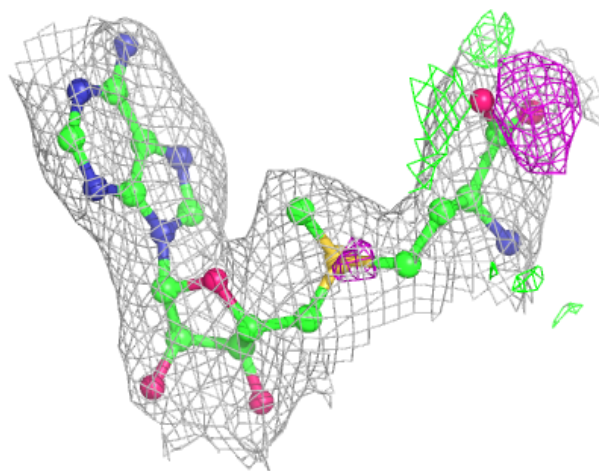
Electron density around SAM F 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
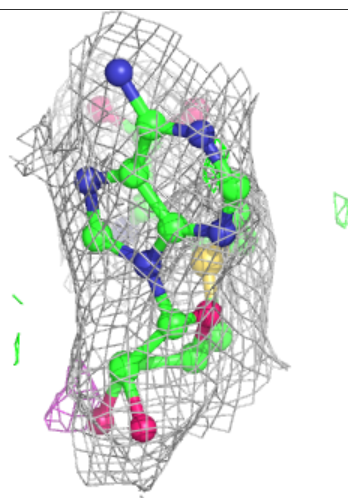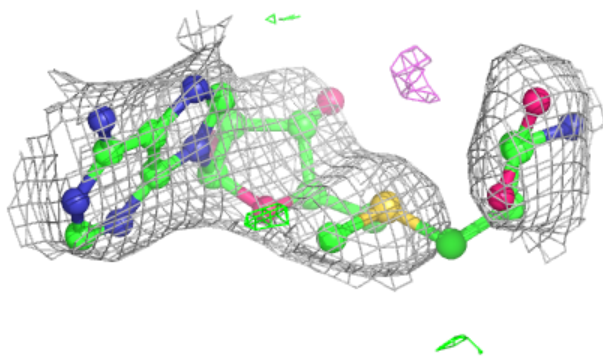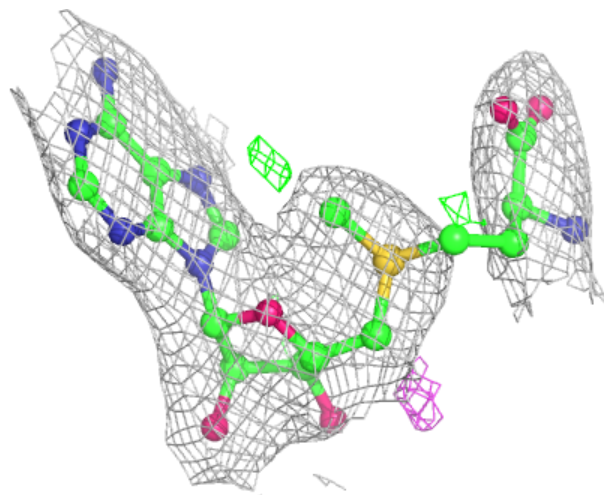
Electron density around SAM C 404:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
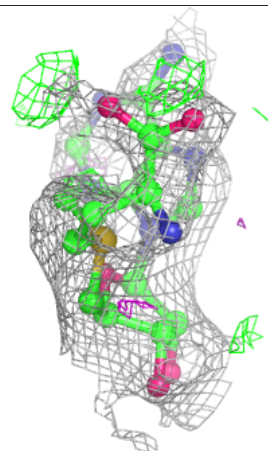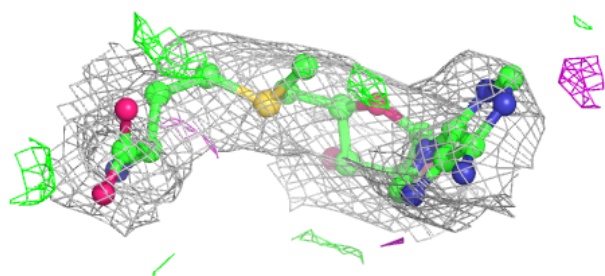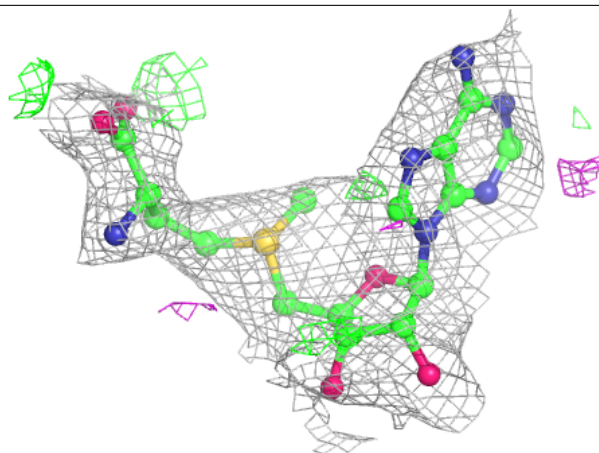
Electron density around SAM B 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
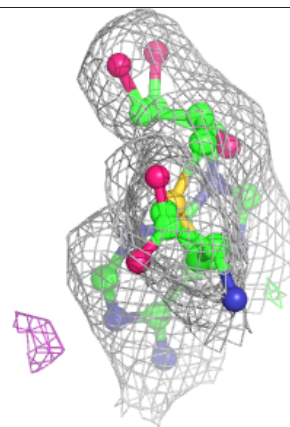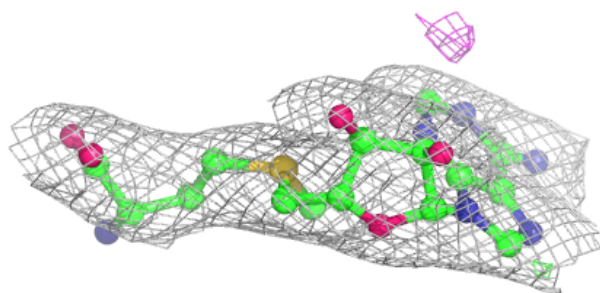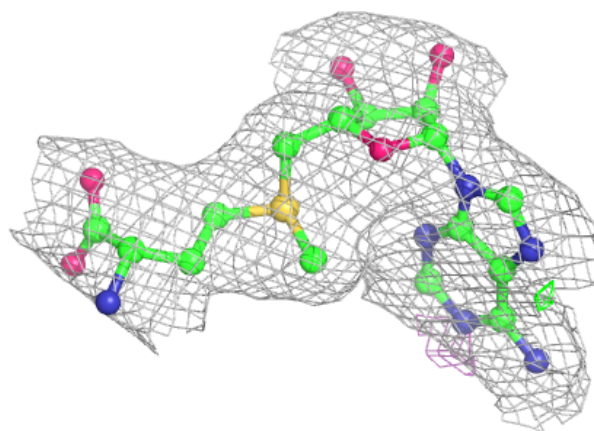
Electron density around SAM C 406:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
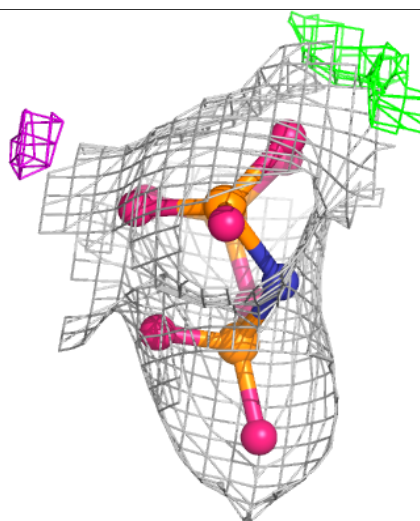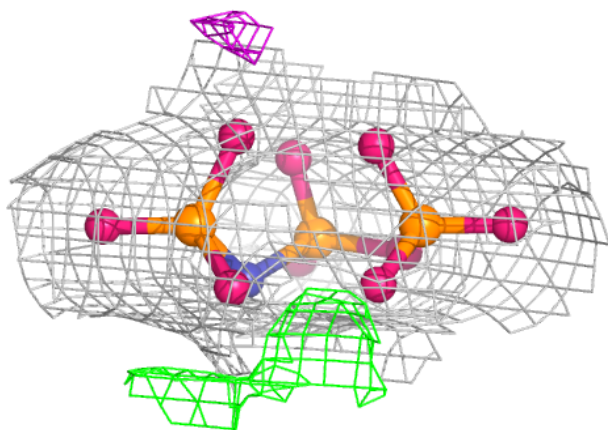and green (positive)
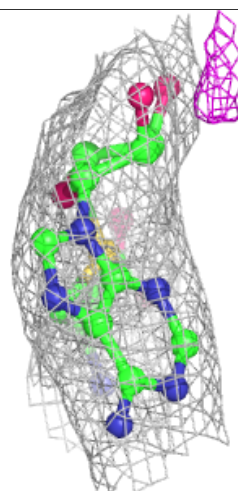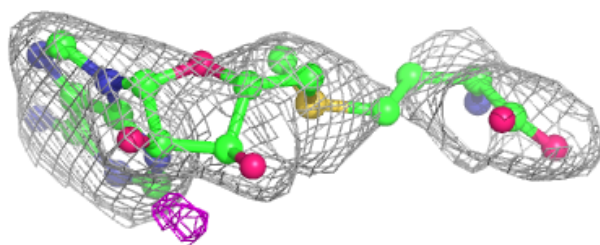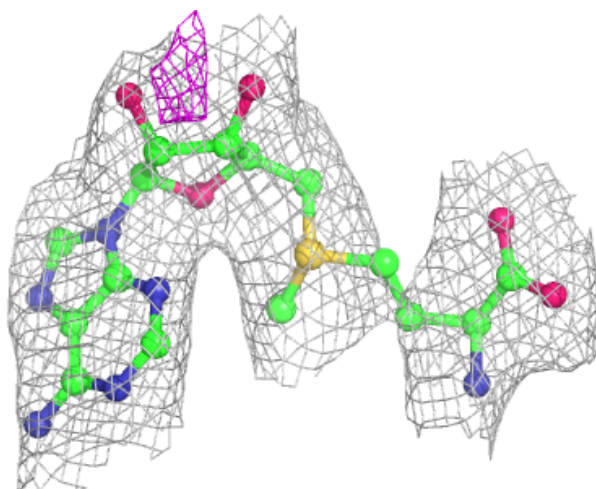
Electron density around SAM D 402:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
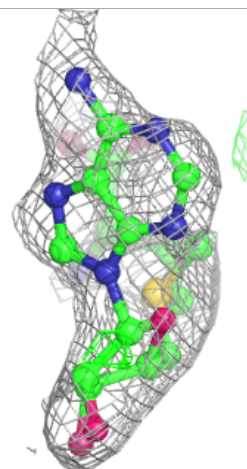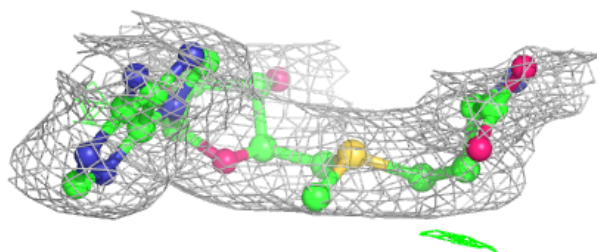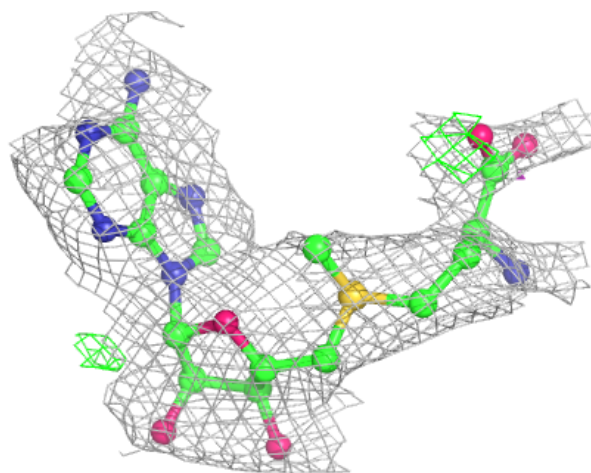
Electron density around SAM D 403:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
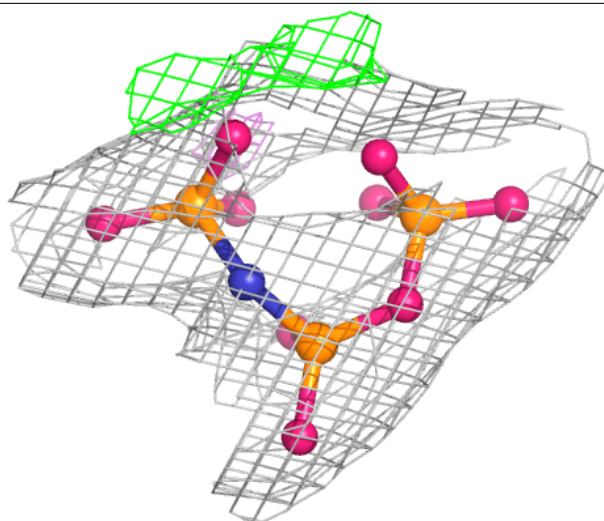$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
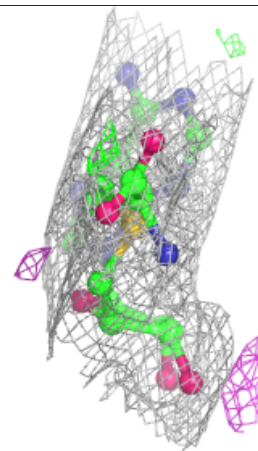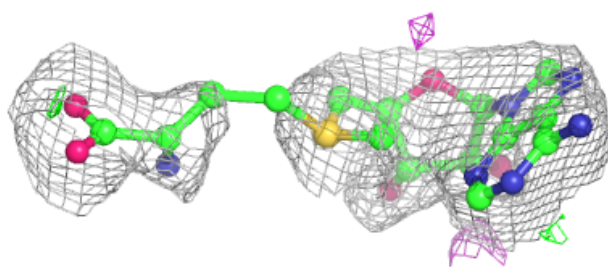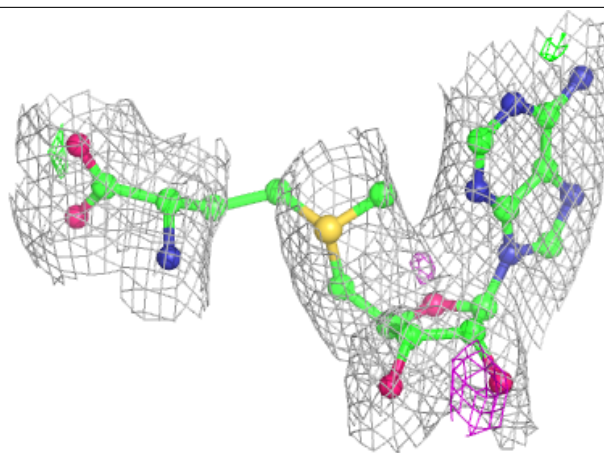
Electron density around PPK E 409:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
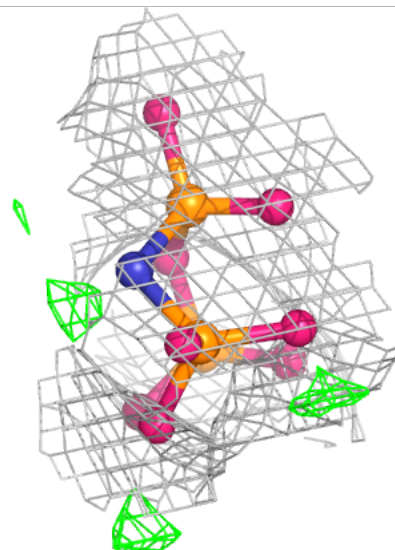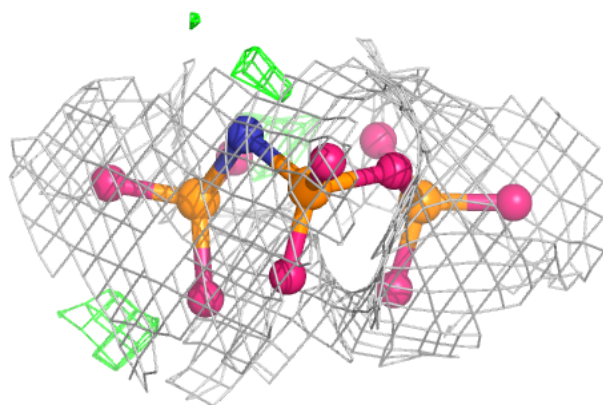
Electron density around SAM B 402:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
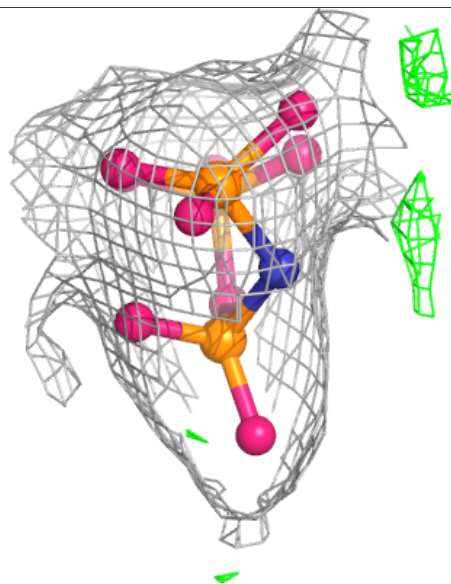
Electron density around PPK E 405:

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

Electron density around PPK G 409:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
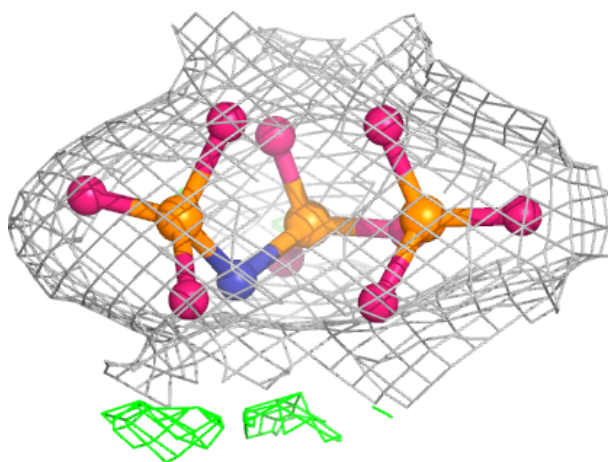and green (positive)

Electron density around PPK A 405:

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

Electron density around PPK C 405:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
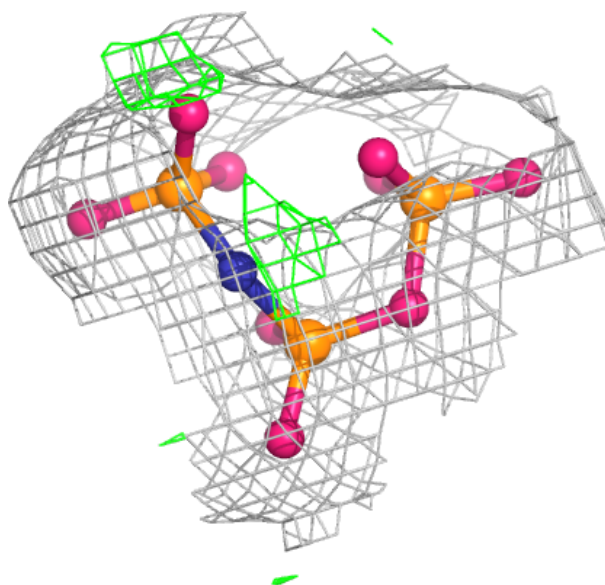mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
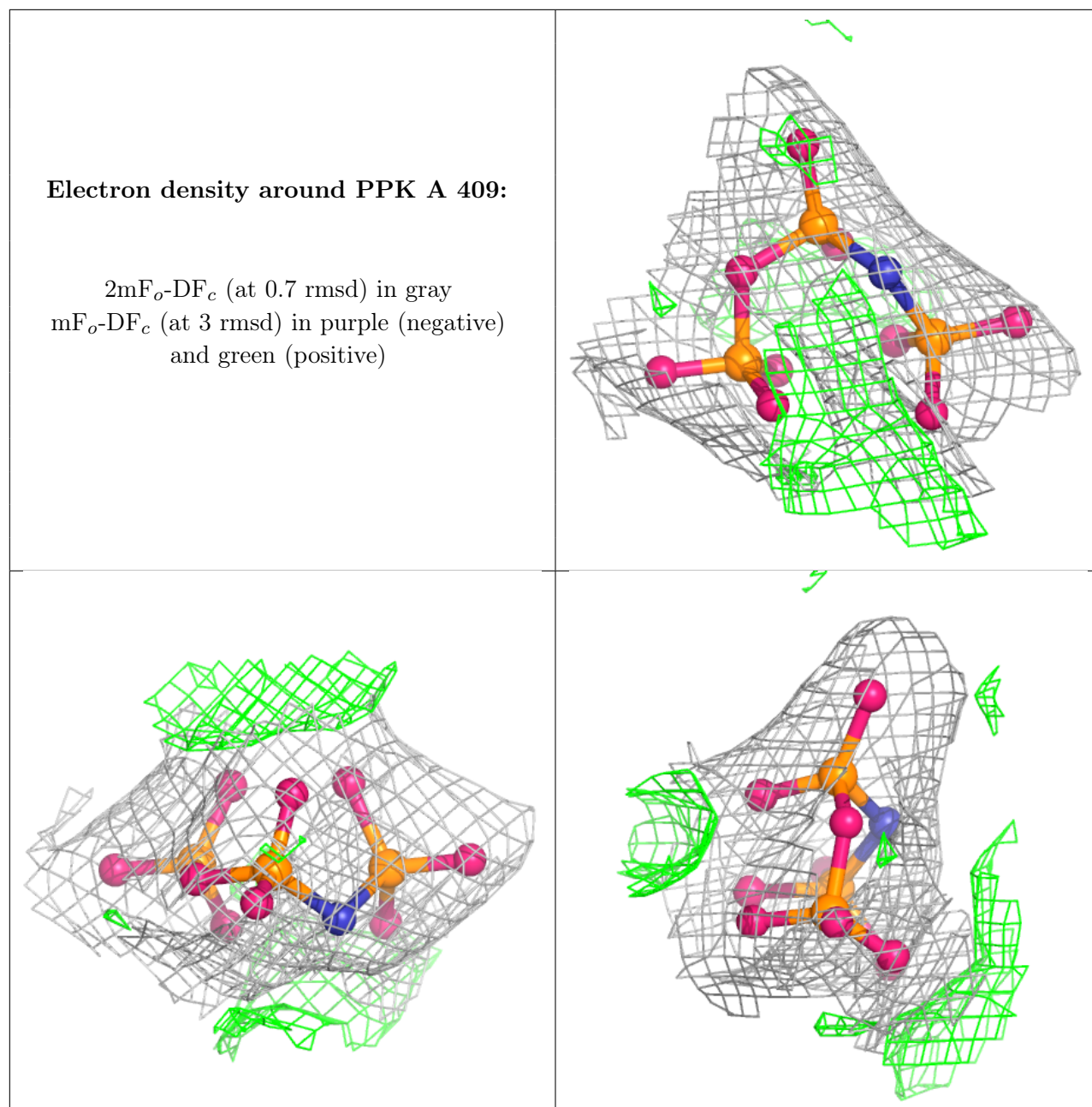
Electron density around PPK C 408:

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

Electron density around PPK G 404:

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

Electron density around PPK A 409:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.