Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 04:20 AM EDT

PDB ID	:	7RIE
Title	:	Plasmodium falciparum M17 in complex with inhibitor MIPS2571
Authors	:	Webb, C.T.; McGowan, S.
Deposited on	:	2021-07-19
Resolution	:	2.49 Å(reported)

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

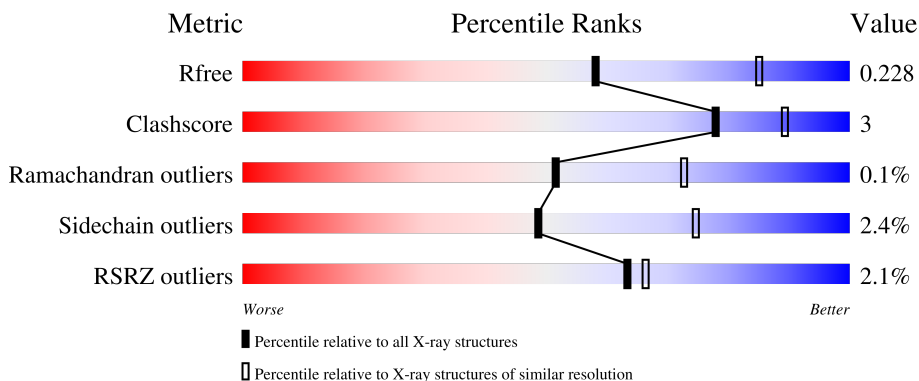|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.49 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.
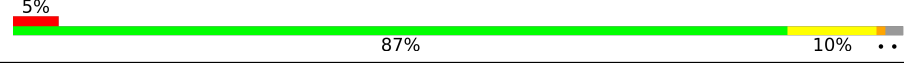
Metric	Percentile Ranks	Value
Rfree		0.228
Clashscore		3
Ramachandran outliers		0.1%
Sidechain outliers		2.4%
RSRZ outliers		2.1%

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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	527	91% 7% ··
1	B	527	6% 87% 10% ··
1	C	527	2% 89% 9% ··
1	D	527	.% 91% 6% ·
1	E	527	.% 88% 9% ·

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Mol	Chain	Length	Quality of chain
1	F	527	2% / 87% / 9%
1	G	527	% / 93% / 6%
1	H	527	5% / 87% / 10%
1	I	527	2% / 91% / 7%
1	J	527	% / 90% / 7%
1	K	527	% / 90% / 6%
1	L	527	4% / 86% / 10%

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 49071 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called M17 leucyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total 3993	C 2565	N 643	O 765	S 20	0	1	0
1	B	518	Total 3892	C 2505	N 629	O 738	S 20	0	0	0
1	C	518	Total 3942	C 2532	N 635	O 755	S 20	0	0	0
1	D	513	Total 3916	C 2522	N 633	O 741	S 20	0	0	0
1	E	511	Total 3885	C 2499	N 624	O 743	S 19	0	0	0
1	F	510	Total 3839	C 2472	N 617	O 731	S 19	0	0	0
1	G	519	Total 3987	C 2559	N 640	O 768	S 20	0	1	0
1	H	518	Total 3900	C 2512	N 630	O 738	S 20	0	0	0
1	I	518	Total 3951	C 2542	N 637	O 752	S 20	0	0	0
1	J	516	Total 3944	C 2540	N 638	O 746	S 20	0	0	0
1	K	512	Total 3908	C 2513	N 626	O 750	S 19	0	0	0
1	L	510	Total 3859	C 2484	N 620	O 736	S 19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

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

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

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

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

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO_3).
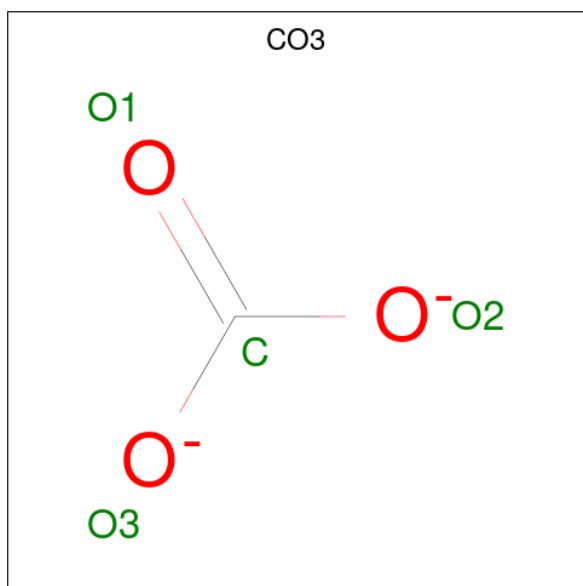
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 4	C 1	O 3	0	0
2	B	1	Total 4	C 1	O 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 4	C 1	O 3	0	0
2	D	1	Total 4	C 1	O 3	0	0
2	E	1	Total 4	C 1	O 3	0	0
2	F	1	Total 4	C 1	O 3	0	0
2	G	1	Total 4	C 1	O 3	0	0
2	H	1	Total 4	C 1	O 3	0	0
2	I	1	Total 4	C 1	O 3	0	0
2	J	1	Total 4	C 1	O 3	0	0
2	K	1	Total 4	C 1	O 3	0	0
2	L	1	Total 4	C 1	O 3	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 4 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).
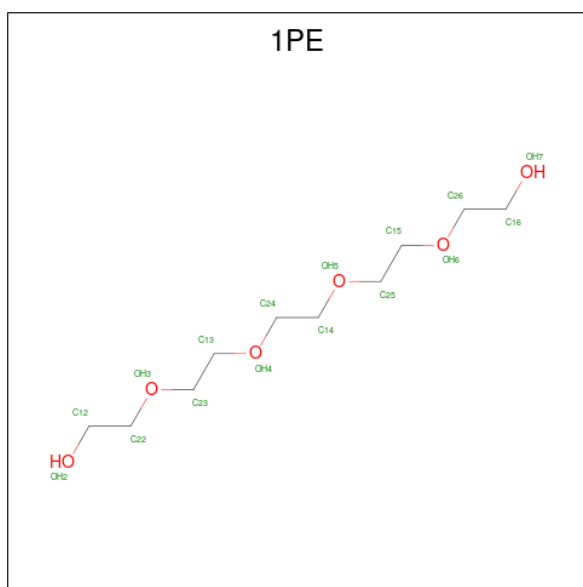
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 10	C 6	O 4	0	0
4	B	1	Total 10	C 6	O 4	0	0
4	C	1	Total 8	C 5	O 3	0	0
4	C	1	Total 8	C 5	O 3	0	0
4	E	1	Total 10	C 6	O 4	0	0
4	I	1	Total 10	C 6	O 4	0	0
4	J	1	Total 10	C 6	O 4	0	0
4	K	1	Total 13	C 8	O 5	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total 10	C 6	O 4	0	0

- Molecule 5 is N-{(1R)-2-(hydroxyamino)-1-[4'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]-2-oxoethyl}-2,2-dimethylpropanamide (three-letter code: 5IF) (formula: $C_{20}H_{24}N_2O_4$) (labeled as "Ligand of Interest" by depositor).
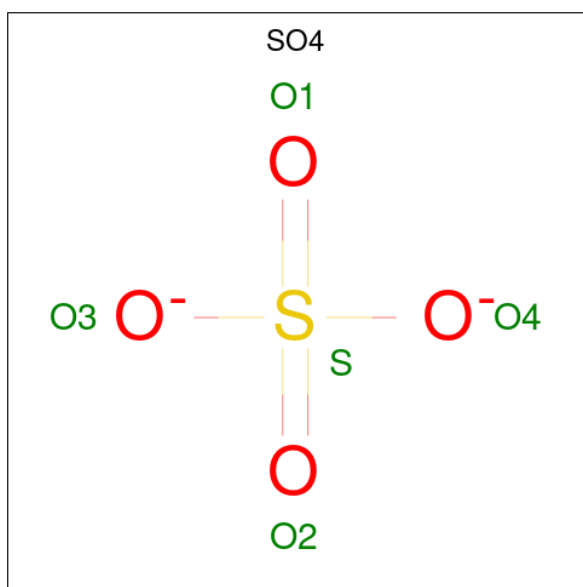

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total 26	C 20	N 2	O 4	0	0
5	B	1	Total 26	C 20	N 2	O 4	0	0
5	C	1	Total 26	C 20	N 2	O 4	0	0
5	D	1	Total 26	C 20	N 2	O 4	0	0
5	E	1	Total 26	C 20	N 2	O 4	0	0
5	F	1	Total 26	C 20	N 2	O 4	0	0
5	G	1	Total 26	C 20	N 2	O 4	0	0
5	H	1	Total 26	C 20	N 2	O 4	0	0
5	I	1	Total 26	C 20	N 2	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			26	20	2	4		
5	K	1	Total	C	N	O	0	0
			26	20	2	4		
5	L	1	Total	C	N	O	0	0
			26	20	2	4		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total 5	O 4	S 1	0	0
6	K	1	Total 5	O 4	S 1	0	0
6	L	1	Total 5	O 4	S 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	127	Total 127	O 127	0	0
7	B	84	Total 84	O 84	0	0
7	C	118	Total 118	O 118	0	0
7	D	164	Total 164	O 164	0	0
7	E	139	Total 139	O 139	0	0
7	F	97	Total 97	O 97	0	0
7	G	128	Total 128	O 128	0	0
7	H	112	Total 112	O 112	0	0
7	I	144	Total 144	O 144	0	0
7	J	144	Total 144	O 144	0	0
7	K	153	Total 153	O 153	0	0
7	L	117	Total 117	O 117	0	0

3 Residue-property plots ⓘ

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

• Molecule 1: M17 leucyl aminopeptidase
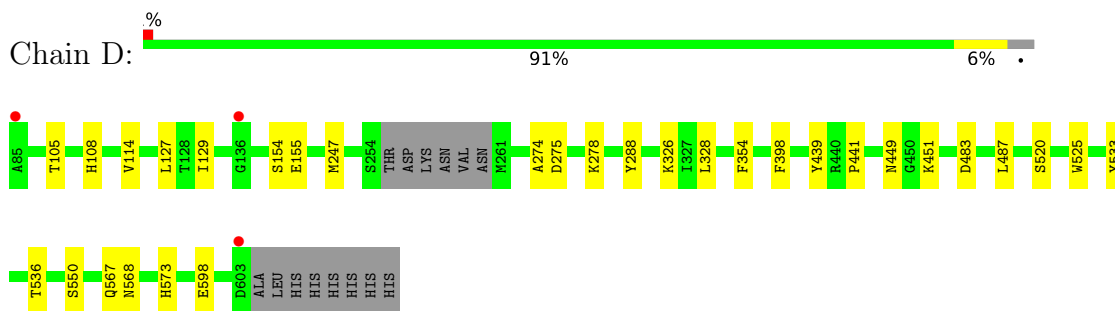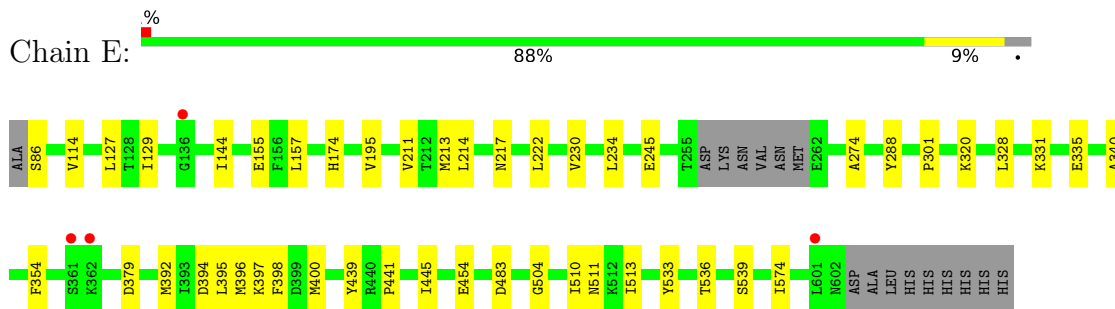
Chain A:
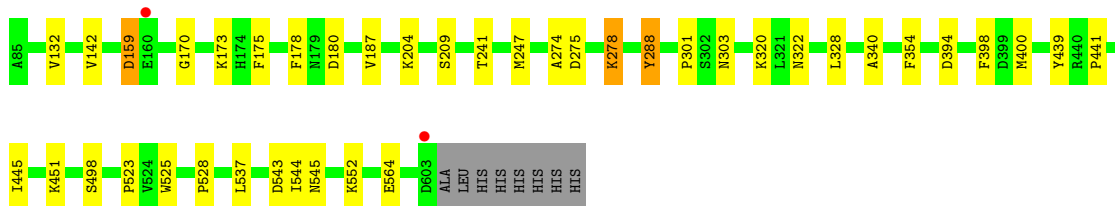
• Molecule 1: M17 leucyl aminopeptidase

Chain B:
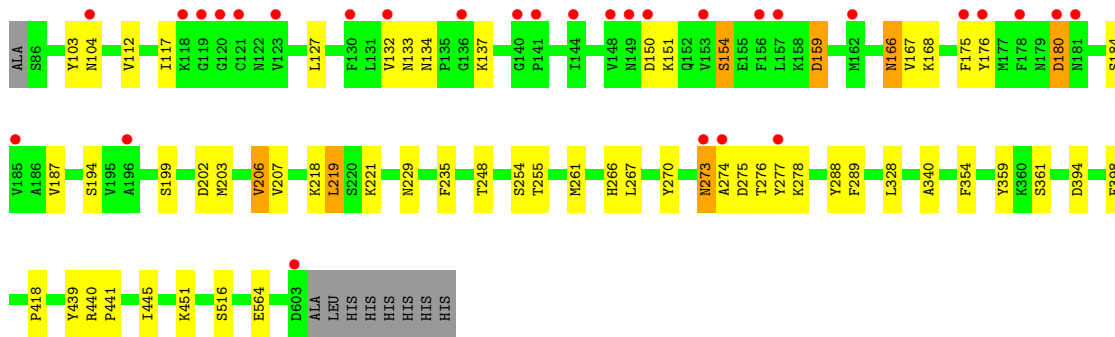
• Molecule 1: M17 leucyl aminopeptidase

Chain C:
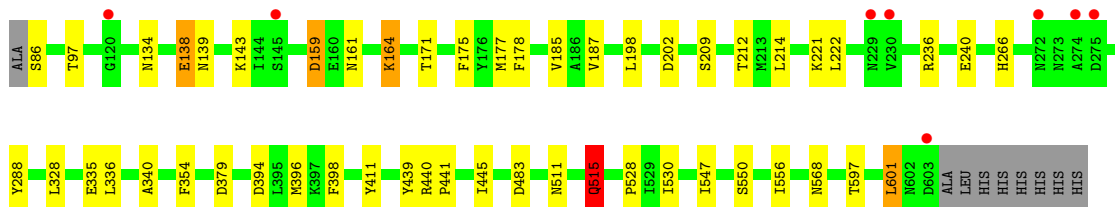
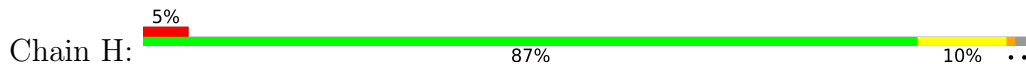• Molecule 1: M17 leucyl aminopeptidase

Chain D:

• Molecule 1: M17 leucyl aminopeptidase

Chain E:

• Molecule 1: M17 leucyl aminopeptidase
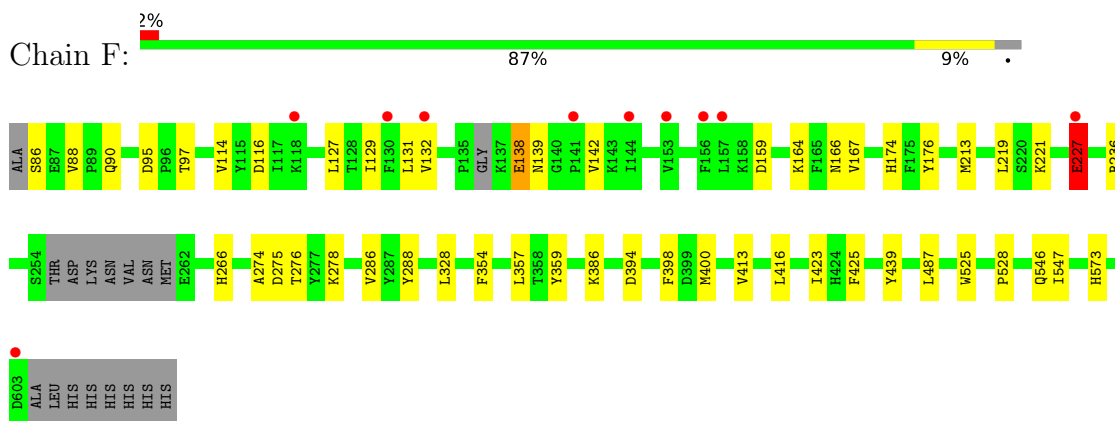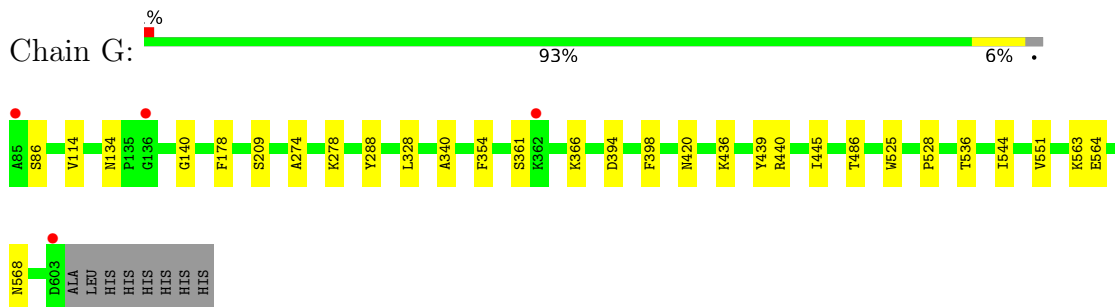
Chain F:

• Molecule 1: M17 leucyl aminopeptidase

Chain G:

• Molecule 1: M17 leucyl aminopeptidase

Chain H:

• Molecule 1: M17 leucyl aminopeptidase
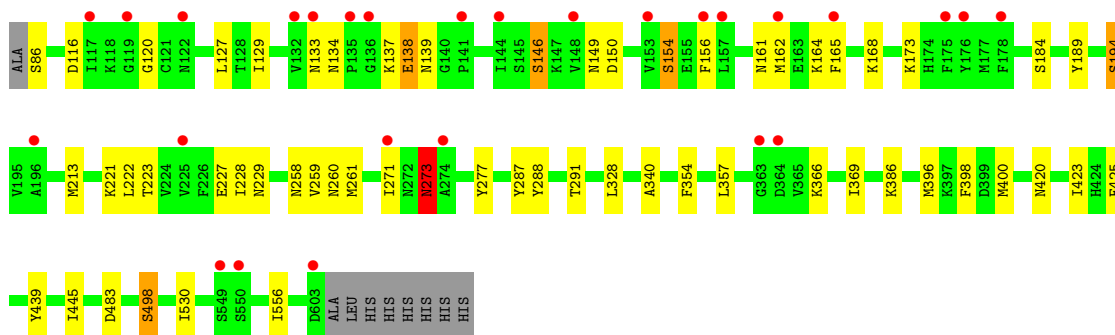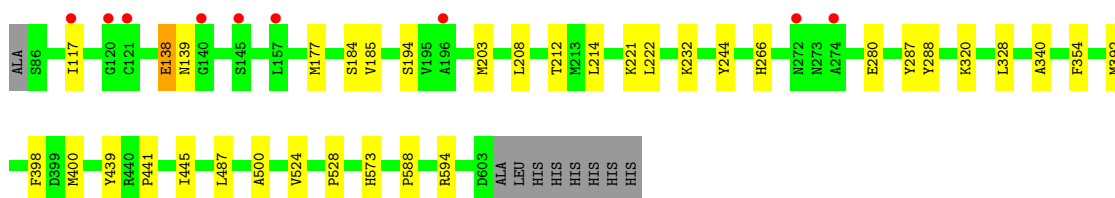
Chain I:

• Molecule 1: M17 leucyl aminopeptidase

Chain J:

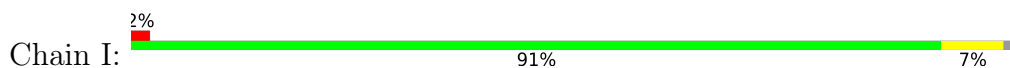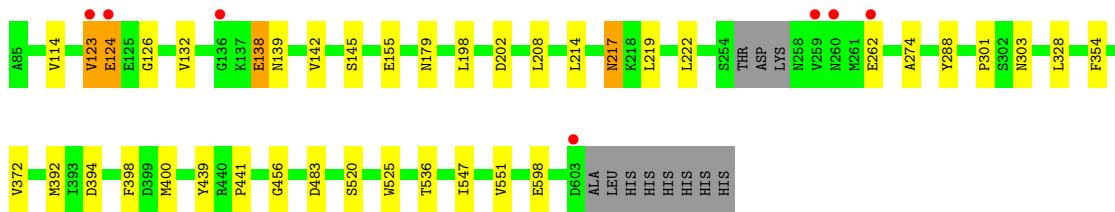• Molecule 1: M17 leucyl aminopeptidase

Chain K:

• Molecule 1: M17 leucyl aminopeptidase
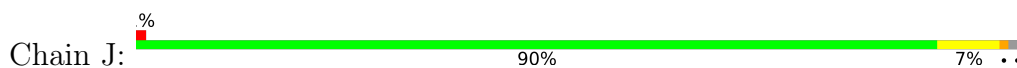
Chain L:
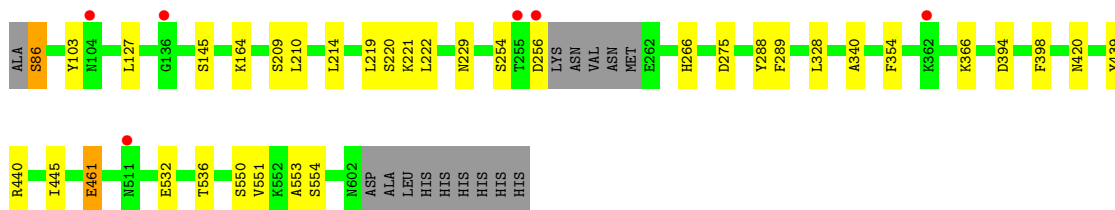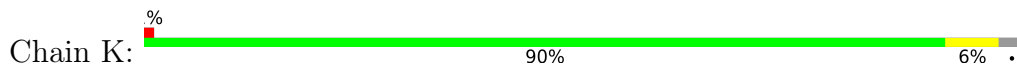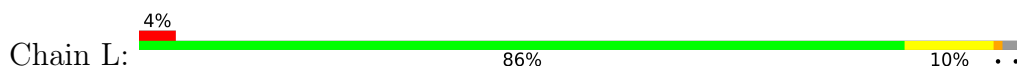
M213 D216 L219 V230 D231 K232 N233 L234 F235 S254 THR ASP LYS ASN VAL ASN MET E262 V269 Y270 I271 N272 N273 A274 D275 T276 E279 Y288 L328 A340 K353 F354 S361 K366 K367 F398 D399 M400 V413 E419 N420 I423 Y439

R440 P441 I445 S520 W525 P528 Y533 T536 S550 N568 L595 E598 D603 ALA LEU HIS HIS HIS HIS HIS HIS
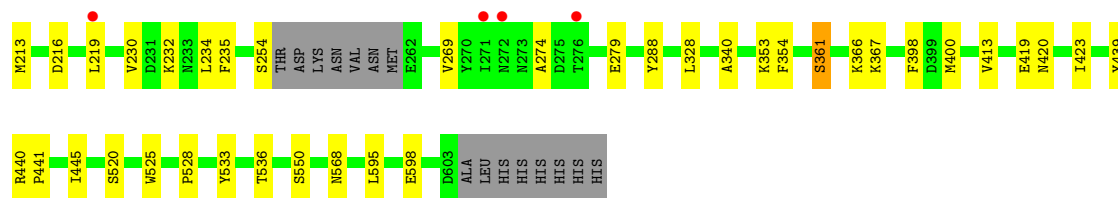
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	175.29Å 175.86Å 234.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 2.49 48.80 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.75-2.49) 92.8 (48.80-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.32 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.195 , 0.229 0.194 , 0.228	Depositor DCC
R_{free} test set	12437 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	36.3	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	49071	wwPDB-VP
Average B, all atoms (Å^2)	43.0	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 45.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2381e-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: SO4, ZN, 5IF, 1PE, CO3

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	0.27	0/4071	0.47	2/5521 (0.0%)
1	B	0.27	0/3970	0.47	1/5398 (0.0%)
1	C	0.32	1/4020 (0.0%)	0.50	3/5459 (0.1%)
1	D	0.24	0/3993	0.43	0/5416
1	E	0.25	0/3962	0.43	0/5382
1	F	0.30	1/3915 (0.0%)	0.47	1/5325 (0.0%)
1	G	0.25	0/4068	0.44	0/5518
1	H	0.29	1/3978 (0.0%)	0.46	0/5407
1	I	0.27	0/4029	0.44	0/5467
1	J	0.36	4/4021 (0.1%)	0.54	6/5451 (0.1%)
1	K	0.27	0/3985	0.45	0/5411
1	L	0.24	0/3935	0.44	0/5348
All	All	0.28	7/47947 (0.0%)	0.46	13/65103 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	C	0	1
1	H	0	1
All	All	0	4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	124	GLU	CD-OE2	8.62	1.35	1.25
1	J	262	GLU	CD-OE2	7.39	1.33	1.25
1	J	262	GLU	CG-CD	7.38	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	227	GLU	CG-CD	7.25	1.62	1.51
1	J	262	GLU	CD-OE1	6.68	1.32	1.25
1	C	515	GLN	CD-NE2	6.29	1.48	1.32
1	H	273	ASN	CG-OD1	6.12	1.37	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	123	VAL	C-N-CA	-13.44	88.10	121.70
1	J	124	GLU	OE1-CD-OE2	8.93	134.01	123.30
1	J	124	GLU	CG-CD-OE1	-8.32	101.66	118.30
1	F	227	GLU	CA-CB-CG	7.70	130.34	113.40
1	J	262	GLU	OE1-CD-OE2	6.31	130.87	123.30
1	J	262	GLU	CB-CA-C	5.89	122.18	110.40
1	C	515	GLN	CB-CA-C	5.70	121.81	110.40
1	C	335	GLU	OE1-CD-OE2	5.70	130.13	123.30
1	C	515	GLN	N-CA-CB	-5.61	100.50	110.60
1	J	262	GLU	CA-CB-CG	5.34	125.14	113.40
1	A	552	LYS	CB-CG-CD	5.32	125.44	111.60
1	B	104	ASN	C-N-CA	-5.25	108.59	121.70
1	A	552	LYS	N-CA-CB	5.16	119.89	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	180	ASP	Peptide
1	B	273	ASN	Peptide
1	C	515	GLN	Sidechain
1	H	273	ASN	Sidechain

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	3993	0	3929	22	1
1	B	3892	0	3764	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3942	0	3842	32	0
1	D	3916	0	3855	14	0
1	E	3885	0	3783	26	0
1	F	3839	0	3707	28	0
1	G	3987	0	3913	15	1
1	H	3900	0	3786	27	0
1	I	3951	0	3878	16	0
1	J	3944	0	3889	24	0
1	K	3908	0	3815	15	0
1	L	3859	0	3745	31	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	1	0
2	D	4	0	0	0	0
2	E	4	0	0	1	0
2	F	4	0	0	1	0
2	G	4	0	0	0	0
2	H	4	0	0	1	0
2	I	4	0	0	1	0
2	J	4	0	0	0	0
2	K	4	0	0	1	0
2	L	4	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
4	A	10	0	12	1	0
4	B	10	0	13	0	0
4	C	16	0	16	1	0
4	E	10	0	12	1	0
4	I	10	0	12	1	0
4	J	10	0	12	0	0
4	K	13	0	17	0	0
4	L	10	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	26	0	0	0	0
5	B	26	0	0	0	0
5	C	26	0	0	1	0
5	D	26	0	0	0	0
5	E	26	0	0	1	0
5	F	26	0	0	2	0
5	G	26	0	0	0	0
5	H	26	0	0	1	0
5	I	26	0	0	1	0
5	J	26	0	0	0	0
5	K	26	0	0	1	0
5	L	26	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	E	10	0	0	0	0
6	F	5	0	0	0	0
6	G	15	0	0	0	0
6	H	5	0	0	1	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
7	A	127	0	0	1	0
7	B	84	0	0	1	0
7	C	118	0	0	5	0
7	D	164	0	0	0	0
7	E	139	0	0	2	0
7	F	97	0	0	1	0
7	G	128	0	0	3	0
7	H	112	0	0	0	0
7	I	144	0	0	1	0
7	J	144	0	0	0	0
7	K	153	0	0	3	0
7	L	117	0	0	2	0
All	All	49071	0	46010	268	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 3.

All (268) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:GLN:HE21	1:C:515:GLN:HA	0.97	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:GLN:HA	1:C:515:GLN:NE2	1.74	1.03
1:J:124:GLU:OE1	1:J:179:ASN:ND2	2.08	0.84
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.59	0.83
1:C:511:ASN:O	1:C:515:GLN:HB2	1.81	0.80
1:C:97:THR:O	7:C:801:HOH:O	1.99	0.80
1:B:273:ASN:ND2	1:B:276:THR:OG1	2.14	0.78
1:I:221:LYS:HG3	1:I:266:HIS:HB2	1.66	0.78
1:H:173:LYS:NZ	1:L:216:ASP:O	2.19	0.75
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.70	0.74
1:C:515:GLN:HE21	1:C:515:GLN:CA	1.89	0.74
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.69	0.74
1:E:230:VAL:HG13	1:E:234:LEU:HB3	1.70	0.72
1:K:461:GLU:OE2	7:K:801:HOH:O	2.10	0.70
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.58	0.68
1:K:86:SER:N	7:K:802:HOH:O	2.27	0.68
1:H:150:ASP:O	1:H:154:SER:OG	2.11	0.67
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.61	0.66
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.78	0.65
1:B:274:ALA:O	1:B:278:LYS:HG3	1.96	0.65
1:C:221:LYS:HG3	1:C:266:HIS:HB2	1.79	0.65
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.63	0.64
2:E:701:CO3:O3	5:E:707:5IF:O11	2.15	0.64
1:B:440:ARG:NH2	7:B:802:HOH:O	2.31	0.64
1:J:217:ASN:HD21	1:J:219:LEU:HD12	1.63	0.64
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.79	0.63
1:C:214:LEU:HD21	1:C:222:LEU:HD22	1.79	0.63
2:C:701:CO3:O2	5:C:707:5IF:O11	2.16	0.63
2:F:701:CO3:O3	5:F:705:5IF:O11	2.16	0.63
1:J:132:VAL:HG21	1:J:142:VAL:HG13	1.81	0.63
1:B:117:ILE:HD12	1:B:270:TYR:HB3	1.80	0.63
1:G:366:LYS:HG3	1:G:420:ASN:HB3	1.79	0.63
2:I:701:CO3:O3	5:I:705:5IF:O11	2.17	0.62
1:F:275:ASP:HA	1:F:278:LYS:HD2	1.80	0.62
1:H:129:ILE:HD11	1:H:213:MET:HE1	1.80	0.62
1:J:114:VAL:HG12	1:J:274:ALA:HB1	1.82	0.62
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.82	0.61
2:H:701:CO3:O1	5:H:705:5IF:O11	2.19	0.61
1:F:132:VAL:HG12	1:F:227:GLU:HG2	1.84	0.60
1:A:173:LYS:NZ	7:A:805:HOH:O	2.33	0.60
1:F:286:VAL:HG11	1:F:416:LEU:HD13	1.84	0.60
1:B:133:ASN:OD1	1:B:134:ASN:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:ASN:O	1:H:164:LYS:HE3	2.02	0.59
2:K:701:CO3:O3	5:K:706:5IF:O11	2.20	0.59
1:F:174:HIS:HB3	1:F:213:MET:HE1	1.83	0.59
1:D:275:ASP:HA	1:D:278:LYS:HD2	1.84	0.59
1:H:133:ASN:HB2	1:H:228:ILE:HG22	1.83	0.59
1:L:135:PRO:O	1:L:137:LYS:N	2.35	0.59
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.85	0.58
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.86	0.57
1:F:221:LYS:HG3	1:F:266:HIS:HB2	1.85	0.57
1:G:134:ASN:HD22	1:G:140:GLY:HA3	1.69	0.57
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.86	0.57
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.87	0.57
1:F:131:LEU:O	1:F:227:GLU:HB3	2.04	0.56
1:E:511:ASN:ND2	7:E:803:HOH:O	2.37	0.56
1:K:366:LYS:HG3	1:K:420:ASN:HB3	1.87	0.56
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.88	0.56
1:E:513:ILE:HD12	1:E:574:ILE:HD11	1.87	0.56
1:B:199:SER:HB3	1:B:202:ASP:H	1.70	0.56
1:I:214:LEU:HD21	1:I:222:LEU:HD22	1.88	0.55
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.89	0.55
1:E:504:GLY:HA3	1:E:510:ILE:HD11	1.89	0.54
1:A:274:ALA:O	1:A:278:LYS:HB2	2.08	0.54
1:B:273:ASN:O	1:B:277:TYR:CD2	2.61	0.54
1:H:221:LYS:HG2	1:H:222:LEU:N	2.22	0.54
1:L:533:TYR:O	1:L:536:THR:HG22	2.08	0.54
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.90	0.53
1:B:150:ASP:O	1:B:154:SER:OG	2.23	0.53
1:H:287:TYR:O	1:H:291:THR:HG23	2.09	0.53
1:K:440:ARG:NH1	7:K:809:HOH:O	2.39	0.53
1:C:440:ARG:NH2	7:C:803:HOH:O	2.42	0.53
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.91	0.52
1:H:221:LYS:HD3	1:H:223:THR:OG1	2.09	0.52
1:H:139:ASN:ND2	1:H:168:LYS:HG3	2.24	0.52
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.92	0.52
1:F:127:LEU:HD21	1:F:213:MET:HE2	1.91	0.51
1:J:217:ASN:HD21	1:J:219:LEU:HB2	1.75	0.51
1:C:411:TYR:HE1	4:C:705:1PE:H151	1.75	0.51
1:D:105:THR:H	1:D:108:HIS:HD2	1.58	0.51
1:I:320:LYS:HB3	4:I:704:1PE:H152	1.92	0.51
1:B:175:PHE:HD1	1:F:176:TYR:HB2	1.75	0.51
1:E:331:LYS:O	1:E:335:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:126:GLY:HA2	1:J:219:LEU:HD22	1.91	0.51
1:K:127:LEU:HB3	1:K:219:LEU:HD13	1.92	0.51
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.92	0.51
1:B:221:LYS:HG3	1:B:266:HIS:HB2	1.93	0.51
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.92	0.50
1:I:287:TYR:CD2	1:I:594:ARG:HG2	2.47	0.50
1:C:530:ILE:HD12	1:C:556:ILE:HD13	1.94	0.50
1:B:202:ASP:O	1:B:206:VAL:HG12	2.12	0.50
1:E:392:MET:HE2	1:E:395:LEU:HB2	1.93	0.50
1:J:214:LEU:HD21	1:J:222:LEU:HD22	1.92	0.50
1:C:547:ILE:HD11	7:C:914:HOH:O	2.12	0.50
1:L:361:SER:OG	1:L:419:GLU:HA	2.12	0.50
1:C:86:SER:N	7:C:805:HOH:O	2.45	0.49
1:C:597:THR:HG22	1:C:601:LEU:HD22	1.93	0.49
1:L:366:LYS:O	1:L:367:LYS:HD2	2.12	0.49
1:L:440:ARG:NH1	7:L:805:HOH:O	2.44	0.49
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.93	0.49
1:A:247:MET:HG3	1:A:288:TYR:OH	2.12	0.49
1:L:127:LEU:HB2	1:L:219:LEU:HD22	1.94	0.49
1:J:198:LEU:HD22	1:J:202:ASP:HB3	1.94	0.49
1:J:536:THR:HG21	1:J:551:VAL:HG23	1.94	0.49
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.94	0.49
1:B:203:MET:HE2	1:B:207:VAL:HG23	1.95	0.49
1:H:258:ASN:O	1:H:260:ASN:N	2.46	0.49
1:H:273:ASN:O	1:H:277:TYR:HD1	1.95	0.49
1:J:126:GLY:C	1:J:219:LEU:HD13	2.34	0.48
1:L:232:LYS:NZ	1:L:279:GLU:OE2	2.41	0.48
1:E:213:MET:O	1:E:217:ASN:ND2	2.27	0.48
1:I:232:LYS:NZ	1:I:280:GLU:OE2	2.36	0.48
1:J:456:GLY:HA3	1:J:547:ILE:HD11	1.96	0.48
1:E:144:ILE:HG13	1:E:157:LEU:HD22	1.96	0.48
1:L:366:LYS:HG3	1:L:420:ASN:HB3	1.96	0.47
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.95	0.47
1:G:440:ARG:NH1	7:G:807:HOH:O	2.46	0.47
1:C:161:ASN:O	1:C:164:LYS:HE3	2.15	0.47
1:K:214:LEU:HD21	1:K:222:LEU:HD22	1.97	0.47
1:B:451:LYS:NZ	1:B:564:GLU:O	2.46	0.47
1:J:124:GLU:CD	1:J:179:ASN:HD22	2.07	0.47
1:L:413:VAL:HG11	1:L:423:ILE:HD13	1.96	0.47
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.97	0.47
1:E:454:GLU:OE1	1:E:539:SER:OG	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.97	0.46
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.97	0.46
1:A:170:GLY:O	1:A:209:SER:OG	2.25	0.46
1:K:103:TYR:HA	1:K:289:PHE:CZ	2.50	0.46
1:L:210:LEU:HA	1:L:213:MET:HE2	1.97	0.46
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.96	0.46
1:E:127:LEU:HD11	1:E:129:ILE:HD11	1.96	0.46
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.98	0.46
1:B:175:PHE:N	1:B:187:VAL:O	2.44	0.46
1:C:97:THR:HB	7:C:801:HOH:O	2.15	0.46
1:B:273:ASN:O	1:B:277:TYR:HD2	1.99	0.46
1:C:138:GLU:O	1:C:139:ASN:HB2	2.16	0.46
1:H:146:SER:OG	1:H:227:GLU:OE2	2.31	0.46
1:A:320:LYS:HB3	4:A:704:1PE:H231	1.98	0.46
1:L:138:GLU:O	1:L:139:ASN:HB2	2.16	0.46
1:L:230:VAL:HG13	1:L:234:LEU:HB3	1.98	0.46
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.98	0.46
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.98	0.46
1:F:413:VAL:HG11	1:F:423:ILE:HD13	1.98	0.46
1:K:221:LYS:HG3	1:K:266:HIS:HB2	1.97	0.46
1:D:326:LYS:HB3	1:D:326:LYS:HE2	1.68	0.45
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.98	0.45
1:F:88:VAL:HG21	1:F:97:THR:HA	1.98	0.45
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.98	0.45
1:B:132:VAL:HG23	1:B:167:VAL:HG23	1.98	0.45
1:B:166:ASN:OD1	1:B:168:LYS:HB2	2.17	0.45
1:F:132:VAL:HG23	1:F:167:VAL:HG12	1.98	0.45
1:F:386:LYS:NZ	5:F:705:5IF:O12	2.48	0.45
1:H:498:SER:OG	1:K:532:GLU:OE1	2.33	0.45
1:K:536:THR:HG21	1:K:551:VAL:HG23	1.98	0.45
1:A:537:LEU:HA	1:A:545:ASN:HB2	1.99	0.45
1:B:359:TYR:OH	1:B:418:PRO:O	2.21	0.45
1:L:107:ILE:HA	1:L:110:ILE:HD12	1.97	0.45
1:B:151:LYS:N	1:B:180:ASP:OD2	2.47	0.45
1:D:533:TYR:O	1:D:536:THR:HG22	2.16	0.45
1:J:123:VAL:HG12	1:J:123:VAL:O	2.17	0.45
1:J:217:ASN:ND2	1:J:219:LEU:HD12	2.29	0.45
1:E:301:PRO:HA	1:E:397:LYS:HD3	1.99	0.45
1:C:177:MET:HG2	1:C:185:VAL:HG23	1.99	0.45
1:E:533:TYR:O	1:E:536:THR:HG22	2.16	0.44
1:B:112:VAL:HG22	1:B:267:LEU:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LYS:HG3	1:F:164:LYS:HA	1.99	0.44
1:B:441:PRO:HB2	1:C:394:ASP:HA	1.98	0.44
1:E:129:ILE:HD11	1:E:213:MET:HE1	2.00	0.44
1:L:232:LYS:HE2	1:L:232:LYS:HB3	1.50	0.44
1:A:498:SER:O	1:A:523:PRO:HG2	2.17	0.44
1:B:103:TYR:HA	1:B:289:PHE:CZ	2.53	0.44
1:F:114:VAL:HG12	1:F:274:ALA:HB1	1.99	0.44
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.98	0.44
1:B:235:PHE:CE2	1:B:277:TYR:HB3	2.52	0.44
1:C:336:LEU:HA	1:C:336:LEU:HD23	1.78	0.44
1:G:486:THR:HB	7:G:903:HOH:O	2.16	0.44
1:E:195:VAL:HG22	7:E:816:HOH:O	2.18	0.43
1:H:165:PHE:HB3	1:H:189:TYR:OH	2.18	0.43
1:I:528:PRO:HB3	1:J:525:TRP:CZ3	2.53	0.43
1:B:159:ASP:OD1	1:B:159:ASP:N	2.50	0.43
1:C:175:PHE:N	1:C:187:VAL:O	2.45	0.43
1:A:175:PHE:N	1:A:187:VAL:O	2.44	0.43
1:A:451:LYS:HE3	1:A:564:GLU:O	2.18	0.43
1:C:198:LEU:HD22	1:C:202:ASP:HB3	2.01	0.43
1:C:209:SER:O	1:C:212:THR:OG1	2.33	0.43
1:I:208:LEU:O	1:I:212:THR:HG23	2.18	0.43
1:L:254:SER:O	1:L:254:SER:OG	2.30	0.43
1:D:114:VAL:HG12	1:D:274:ALA:HB1	2.00	0.43
1:A:159:ASP:N	1:A:159:ASP:OD1	2.50	0.43
1:D:449:ASN:HD21	1:D:451:LYS:HD2	1.83	0.43
1:E:211:VAL:HG21	1:E:245:GLU:HB2	2.01	0.43
1:F:90:GLN:HB3	1:F:95:ASP:HB2	2.00	0.43
1:E:379:ASP:O	1:E:396:MET:HG3	2.18	0.43
1:J:394:ASP:HA	1:L:441:PRO:HB2	2.01	0.43
1:A:528:PRO:HB3	1:F:525:TRP:CZ3	2.53	0.43
1:I:138:GLU:O	1:I:139:ASN:HB2	2.18	0.43
1:B:248:THR:HB	1:B:261:MET:HE1	2.01	0.43
1:E:174:HIS:HB3	1:E:213:MET:HE3	2.01	0.43
1:H:138:GLU:HA	1:H:194:SER:HB3	2.00	0.43
1:I:487:LEU:HD22	1:I:573:HIS:CE1	2.54	0.43
1:A:340:ALA:HA	1:A:445:ILE:HD12	2.00	0.42
1:I:500:ALA:HB3	1:I:524:VAL:HG22	2.01	0.42
1:C:379:ASP:O	1:C:396:MET:HG3	2.19	0.42
1:L:127:LEU:HD11	1:L:129:ILE:HD11	2.01	0.42
1:F:357:LEU:HB2	1:F:425:PHE:HB2	2.01	0.42
1:F:359:TYR:HD2	1:F:423:ILE:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LYS:HB2	1:C:143:LYS:HE3	1.74	0.42
1:E:320:LYS:HB3	4:E:706:1PE:H132	2.00	0.42
1:F:546:GLN:HG2	1:F:547:ILE:HG23	2.02	0.42
1:G:436:LYS:HG2	6:H:704:SO4:O2	2.20	0.42
1:L:88:VAL:HG21	1:L:97:THR:HA	2.01	0.42
1:B:176:TYR:CE1	1:B:184:SER:HB2	2.55	0.42
1:D:105:THR:H	1:D:108:HIS:CD2	2.37	0.42
1:F:138:GLU:O	1:F:139:ASN:HB2	2.19	0.42
1:F:487:LEU:HD22	1:F:573:HIS:CE1	2.54	0.42
1:A:441:PRO:HB2	1:B:394:ASP:HA	2.01	0.42
1:A:544:ILE:HD12	1:A:564:GLU:HG3	2.02	0.42
1:H:366:LYS:HG3	1:H:420:ASN:HB3	2.01	0.42
1:C:134:ASN:HD22	1:C:134:ASN:HA	1.71	0.42
1:F:174:HIS:HB3	1:F:213:MET:CE	2.49	0.42
1:G:528:PRO:HB3	1:L:525:TRP:CZ3	2.54	0.42
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.20	0.42
1:A:394:ASP:HA	1:C:441:PRO:HB2	2.01	0.42
1:H:369:ILE:HB	1:H:423:ILE:HD13	2.01	0.42
1:J:138:GLU:O	1:J:139:ASN:HB2	2.20	0.42
1:K:210:LEU:HD12	1:K:210:LEU:HA	1.92	0.42
1:E:129:ILE:CD1	1:E:213:MET:HE1	2.50	0.42
1:L:90:GLN:HB3	1:L:95:ASP:HB2	2.01	0.42
1:L:235:PHE:CE1	1:L:269:VAL:HG11	2.55	0.42
1:A:525:TRP:CZ3	1:F:528:PRO:HB3	2.55	0.41
1:C:528:PRO:HB3	1:D:525:TRP:CZ3	2.54	0.41
1:D:127:LEU:HD11	1:D:129:ILE:HD11	2.02	0.41
1:E:340:ALA:HA	1:E:445:ILE:HD12	2.01	0.41
1:G:114:VAL:HG22	1:G:274:ALA:HB1	2.02	0.41
1:H:120:GLY:HA3	1:H:149:ASN:OD1	2.20	0.41
1:C:340:ALA:HA	1:C:445:ILE:HD12	2.02	0.41
1:B:127:LEU:HB2	1:B:219:LEU:HD22	2.02	0.41
1:B:254:SER:OG	1:B:255:THR:N	2.54	0.41
1:F:129:ILE:HD11	1:F:213:MET:HE2	2.02	0.41
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.56	0.41
1:I:177:MET:HG2	1:I:185:VAL:HG23	2.03	0.41
1:I:320:LYS:NZ	7:I:809:HOH:O	2.48	0.41
1:K:551:VAL:HG12	1:K:553:ALA:H	1.85	0.41
1:E:114:VAL:HG12	1:E:274:ALA:HB1	2.02	0.41
1:I:244:TYR:OH	1:I:588:PRO:O	2.38	0.41
1:H:386:LYS:HE3	1:H:396:MET:HG3	2.03	0.41
1:L:142:VAL:HG23	1:L:165:PHE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:116:ASP:HA	1:H:271:ILE:O	2.19	0.41
1:H:127:LEU:CD2	1:H:129:ILE:HG12	2.50	0.41
1:J:219:LEU:HD23	1:J:219:LEU:HA	1.93	0.41
1:A:204:LYS:HG2	1:A:241:THR:HG21	2.02	0.41
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.29	0.41
1:F:236:ARG:NH2	7:F:802:HOH:O	2.34	0.41
1:G:361:SER:HB3	7:G:802:HOH:O	2.21	0.41
1:H:530:ILE:HD12	1:H:556:ILE:HD13	2.02	0.41
1:J:301:PRO:HB2	1:J:303:ASN:OD1	2.21	0.41
1:A:543:ASP:OD2	1:B:254:SER:OG	2.30	0.41
1:C:159:ASP:OD1	1:C:159:ASP:N	2.54	0.41
1:B:275:ASP:HA	1:B:278:LYS:HD2	2.03	0.40
1:H:258:ASN:HB2	1:H:261:MET:HB3	2.03	0.40
1:D:487:LEU:HD22	1:D:573:HIS:CE1	2.56	0.40
1:J:372:VAL:O	1:J:483:ASP:HA	2.20	0.40
1:F:132:VAL:HG21	1:F:142:VAL:HG13	2.04	0.40
1:G:544:ILE:HD12	1:G:564:GLU:HG3	2.03	0.40
1:L:235:PHE:HE1	1:L:269:VAL:HG11	1.86	0.40
1:G:536:THR:HG21	1:G:551:VAL:CG2	2.52	0.40
1:H:138:GLU:HA	1:H:194:SER:CB	2.52	0.40
1:L:353:LYS:NZ	7:L:819:HOH:O	2.54	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:A:180:ASP:O	1:G:278:LYS:NZ[2_665]	2.11	0.09

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/527 (98%)	501 (97%)	17 (3%)	0	100	100
1	B	516/527 (98%)	498 (96%)	17 (3%)	1 (0%)	47	68
1	C	516/527 (98%)	501 (97%)	14 (3%)	1 (0%)	47	68
1	D	509/527 (97%)	499 (98%)	10 (2%)	0	100	100
1	E	507/527 (96%)	494 (97%)	13 (3%)	0	100	100
1	F	504/527 (96%)	491 (97%)	12 (2%)	1 (0%)	47	68
1	G	518/527 (98%)	502 (97%)	16 (3%)	0	100	100
1	H	516/527 (98%)	493 (96%)	20 (4%)	3 (1%)	25	43
1	I	516/527 (98%)	503 (98%)	12 (2%)	1 (0%)	47	68
1	J	512/527 (97%)	496 (97%)	15 (3%)	1 (0%)	47	68
1	K	508/527 (96%)	495 (97%)	13 (3%)	0	100	100
1	L	504/527 (96%)	491 (97%)	12 (2%)	1 (0%)	47	68
All	All	6144/6324 (97%)	5964 (97%)	171 (3%)	9 (0%)	51	73

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	138	GLU
1	H	137	LYS
1	I	138	GLU
1	J	138	GLU
1	L	138	GLU
1	B	137	LYS
1	C	138	GLU
1	F	138	GLU
1	H	259	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/454 (94%)	419 (98%)	8 (2%)	57	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
1	B	403/454 (89%)	391 (97%)	12 (3%)	41	68	
1	C	417/454 (92%)	406 (97%)	11 (3%)	46	72	
1	D	415/454 (91%)	406 (98%)	9 (2%)	52	77	
1	E	410/454 (90%)	404 (98%)	6 (2%)	65	85	
1	F	400/454 (88%)	389 (97%)	11 (3%)	43	70	
1	G	427/454 (94%)	420 (98%)	7 (2%)	62	84	
1	H	405/454 (89%)	390 (96%)	15 (4%)	34	60	
1	I	419/454 (92%)	410 (98%)	9 (2%)	53	78	
1	J	418/454 (92%)	410 (98%)	8 (2%)	57	80	
1	K	415/454 (91%)	400 (96%)	15 (4%)	35	61	
1	L	406/454 (89%)	396 (98%)	10 (2%)	47	73	
All	All	4962/5448 (91%)	4841 (98%)	121 (2%)	49	74	

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	ASP
1	A	275	ASP
1	A	278	LYS
1	A	288	TYR
1	A	322	ASN
1	A	398	PHE
1	A	400	MET
1	A	439	TYR
1	B	154	SER
1	B	159	ASP
1	B	166	ASN
1	B	194	SER
1	B	206	VAL
1	B	219	LEU
1	B	229	ASN
1	B	288	TYR
1	B	361	SER
1	B	398	PHE
1	B	439	TYR
1	B	516	SER
1	C	159	ASP
1	C	164	LYS

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Mol	Chain	Res	Type
1	C	171	THR
1	C	288	TYR
1	C	398	PHE
1	C	439	TYR
1	C	483	ASP
1	C	515	GLN
1	C	550	SER
1	C	568	ASN
1	C	601	LEU
1	D	154	SER
1	D	247	MET
1	D	288	TYR
1	D	398	PHE
1	D	439	TYR
1	D	483	ASP
1	D	550	SER
1	D	567	GLN
1	D	568	ASN
1	E	86	SER
1	E	288	TYR
1	E	398	PHE
1	E	400	MET
1	E	439	TYR
1	E	483	ASP
1	F	86	SER
1	F	116	ASP
1	F	159	ASP
1	F	166	ASN
1	F	219	LEU
1	F	227	GLU
1	F	276	THR
1	F	288	TYR
1	F	398	PHE
1	F	400	MET
1	F	439	TYR
1	G	86	SER
1	G	209	SER
1	G	288	TYR
1	G	398	PHE
1	G	439	TYR
1	G	563	LYS
1	G	568	ASN

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Mol	Chain	Res	Type
1	H	86	SER
1	H	134	ASN
1	H	146	SER
1	H	154	SER
1	H	156	PHE
1	H	162	MET
1	H	184	SER
1	H	194	SER
1	H	229	ASN
1	H	288	TYR
1	H	398	PHE
1	H	400	MET
1	H	439	TYR
1	H	483	ASP
1	H	498	SER
1	I	117	ILE
1	I	184	SER
1	I	194	SER
1	I	203	MET
1	I	288	TYR
1	I	392	MET
1	I	398	PHE
1	I	400	MET
1	I	439	TYR
1	J	145	SER
1	J	208	LEU
1	J	217	ASN
1	J	288	TYR
1	J	392	MET
1	J	398	PHE
1	J	400	MET
1	J	439	TYR
1	K	86	SER
1	K	145	SER
1	K	164	LYS
1	K	209	SER
1	K	220	SER
1	K	229	ASN
1	K	254	SER
1	K	256	ASP
1	K	275	ASP
1	K	288	TYR

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Mol	Chain	Res	Type
1	K	398	PHE
1	K	439	TYR
1	K	461	GLU
1	K	550	SER
1	K	554	SER
1	L	88	VAL
1	L	177	MET
1	L	288	TYR
1	L	361	SER
1	L	398	PHE
1	L	400	MET
1	L	439	TYR
1	L	550	SER
1	L	568	ASN
1	L	595	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	602	ASN
1	B	139	ASN
1	B	273	ASN
1	C	273	ASN
1	C	515	GLN
1	D	108	HIS
1	D	515	GLN
1	F	272	ASN
1	G	134	ASN
1	H	113	GLN
1	H	134	ASN
1	H	515	GLN
1	I	319	GLN
1	I	515	GLN
1	L	139	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 68 ligands modelled in this entry, 24 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
5	5IF	B	706	3	27,27,27	2.14	4 (14%)	37,38,38	1.04	1 (2%)
2	CO3	A	701	-	2,3,3	0.40	0	2,3,3	0.16	0
2	CO3	H	701	-	2,3,3	0.40	0	2,3,3	0.14	0
2	CO3	I	701	-	2,3,3	0.41	0	2,3,3	0.24	0
5	5IF	E	707	3	27,27,27	2.15	4 (14%)	37,38,38	1.11	2 (5%)
6	SO4	L	704	-	4,4,4	0.15	0	6,6,6	0.06	0
5	5IF	D	704	3	27,27,27	2.13	4 (14%)	37,38,38	1.01	1 (2%)
2	CO3	E	701	-	2,3,3	0.41	0	2,3,3	0.20	0
5	5IF	F	705	3	27,27,27	2.14	4 (14%)	37,38,38	1.10	1 (2%)
6	SO4	E	704	-	4,4,4	0.15	0	6,6,6	0.05	0
2	CO3	K	701	-	2,3,3	0.41	0	2,3,3	0.21	0
2	CO3	J	701	-	2,3,3	0.39	0	2,3,3	0.15	0
2	CO3	C	701	-	2,3,3	0.41	0	2,3,3	0.24	0
4	1PE	C	705	-	7,7,15	0.16	0	6,6,14	0.15	0
5	5IF	A	705	3	27,27,27	2.13	4 (14%)	37,38,38	1.08	1 (2%)
5	5IF	H	705	3	27,27,27	2.14	4 (14%)	37,38,38	1.13	2 (5%)
6	SO4	E	705	-	4,4,4	0.14	0	6,6,6	0.04	0
4	1PE	B	705	-	9,9,15	0.11	0	8,8,14	0.13	0
2	CO3	G	701	-	2,3,3	0.40	0	2,3,3	0.21	0
4	1PE	E	706	-	9,9,15	0.10	0	8,8,14	0.17	0
6	SO4	H	704	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	SO4	G	704	-	4,4,4	0.14	0	6,6,6	0.06	0
6	SO4	G	705	-	4,4,4	0.15	0	6,6,6	0.05	0
2	CO3	F	701	-	2,3,3	0.40	0	2,3,3	0.18	0
5	5IF	K	706	3	27,27,27	2.13	4 (14%)	37,38,38	1.07	1 (2%)
6	SO4	C	704	-	4,4,4	0.14	0	6,6,6	0.05	0
4	1PE	C	706	-	7,7,15	0.15	0	6,6,14	0.13	0
4	1PE	J	704	-	9,9,15	0.10	0	8,8,14	0.17	0
2	CO3	D	701	-	2,3,3	0.40	0	2,3,3	0.18	0
5	5IF	J	705	3	27,27,27	2.12	4 (14%)	37,38,38	1.05	1 (2%)
5	5IF	C	707	3	27,27,27	2.13	4 (14%)	37,38,38	1.08	1 (2%)
4	1PE	L	705	-	9,9,15	0.11	0	8,8,14	0.17	0
6	SO4	G	706	-	4,4,4	0.13	0	6,6,6	0.08	0
4	1PE	K	705	-	12,12,15	0.10	0	11,11,14	0.13	0
4	1PE	A	704	-	9,9,15	0.10	0	8,8,14	0.16	0
6	SO4	K	704	-	4,4,4	0.14	0	6,6,6	0.05	0
5	5IF	G	707	3	27,27,27	2.13	4 (14%)	37,38,38	1.02	1 (2%)
6	SO4	F	704	-	4,4,4	0.14	0	6,6,6	0.06	0
2	CO3	L	701	-	2,3,3	0.40	0	2,3,3	0.19	0
5	5IF	I	705	3	27,27,27	2.13	4 (14%)	37,38,38	1.13	2 (5%)
2	CO3	B	701	-	2,3,3	0.41	0	2,3,3	0.19	0
6	SO4	B	704	-	4,4,4	0.13	0	6,6,6	0.07	0
5	5IF	L	706	3	27,27,27	2.14	4 (14%)	37,38,38	1.07	1 (2%)
4	1PE	I	704	-	9,9,15	0.11	0	8,8,14	0.17	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5IF	B	706	3	-	2/26/26/26	0/2/2/2
5	5IF	E	707	3	-	4/26/26/26	0/2/2/2
5	5IF	D	704	3	-	3/26/26/26	0/2/2/2
5	5IF	F	705	3	-	4/26/26/26	0/2/2/2
4	1PE	C	705	-	-	3/5/5/13	-
5	5IF	A	705	3	-	2/26/26/26	0/2/2/2
5	5IF	H	705	3	-	3/26/26/26	0/2/2/2
4	1PE	B	705	-	-	1/7/7/13	-
4	1PE	E	706	-	-	3/7/7/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5IF	K	706	3	-	4/26/26/26	0/2/2/2
4	1PE	C	706	-	-	3/5/5/13	-
4	1PE	J	704	-	-	1/7/7/13	-
5	5IF	J	705	3	-	2/26/26/26	0/2/2/2
5	5IF	C	707	3	-	3/26/26/26	0/2/2/2
4	1PE	L	705	-	-	5/7/7/13	-
4	1PE	K	705	-	-	3/10/10/13	-
4	1PE	A	704	-	-	1/7/7/13	-
5	5IF	G	707	3	-	2/26/26/26	0/2/2/2
5	5IF	I	705	3	-	2/26/26/26	0/2/2/2
5	5IF	L	706	3	-	2/26/26/26	0/2/2/2
4	1PE	I	704	-	-	2/7/7/13	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	707	5IF	C09-N10	8.87	1.45	1.33
5	L	706	5IF	C09-N10	8.79	1.45	1.33
5	B	706	5IF	C09-N10	8.78	1.45	1.33
5	F	705	5IF	C09-N10	8.78	1.45	1.33
5	I	705	5IF	C09-N10	8.75	1.45	1.33
5	G	707	5IF	C09-N10	8.74	1.45	1.33
5	C	707	5IF	C09-N10	8.73	1.45	1.33
5	A	705	5IF	C09-N10	8.73	1.45	1.33
5	H	705	5IF	C09-N10	8.73	1.45	1.33
5	K	706	5IF	C09-N10	8.70	1.45	1.33
5	D	704	5IF	C09-N10	8.69	1.45	1.33
5	J	705	5IF	C09-N10	8.69	1.45	1.33
5	H	705	5IF	C02-N07	5.76	1.45	1.34
5	F	705	5IF	C02-N07	5.75	1.45	1.34
5	K	706	5IF	C02-N07	5.71	1.45	1.34
5	D	704	5IF	C02-N07	5.70	1.45	1.34
5	G	707	5IF	C02-N07	5.70	1.45	1.34
5	A	705	5IF	C02-N07	5.68	1.45	1.34
5	C	707	5IF	C02-N07	5.67	1.45	1.34
5	L	706	5IF	C02-N07	5.66	1.45	1.34
5	B	706	5IF	C02-N07	5.65	1.45	1.34
5	E	707	5IF	C02-N07	5.65	1.45	1.34
5	I	705	5IF	C02-N07	5.65	1.45	1.34
5	J	705	5IF	C02-N07	5.60	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	I	705	5IF	O12-C09	-2.42	1.18	1.23
5	E	707	5IF	O01-C02	-2.40	1.18	1.22
5	C	707	5IF	O12-C09	-2.39	1.18	1.23
5	K	706	5IF	O12-C09	-2.37	1.18	1.23
5	H	705	5IF	O01-C02	-2.36	1.18	1.22
5	E	707	5IF	O12-C09	-2.36	1.18	1.23
5	F	705	5IF	O12-C09	-2.36	1.18	1.23
5	B	706	5IF	O01-C02	-2.35	1.18	1.22
5	J	705	5IF	O12-C09	-2.35	1.18	1.23
5	H	705	5IF	O12-C09	-2.34	1.18	1.23
5	L	706	5IF	O01-C02	-2.34	1.18	1.22
5	B	706	5IF	O12-C09	-2.34	1.18	1.23
5	K	706	5IF	O01-C02	-2.33	1.18	1.22
5	L	706	5IF	O12-C09	-2.33	1.18	1.23
5	D	704	5IF	O01-C02	-2.33	1.18	1.22
5	D	704	5IF	O12-C09	-2.32	1.18	1.23
5	F	705	5IF	O01-C02	-2.32	1.18	1.22
5	A	705	5IF	O12-C09	-2.31	1.18	1.23
5	A	705	5IF	O01-C02	-2.31	1.18	1.22
5	J	705	5IF	O01-C02	-2.31	1.18	1.22
5	G	707	5IF	O01-C02	-2.31	1.18	1.22
5	I	705	5IF	O01-C02	-2.27	1.18	1.22
5	G	707	5IF	O12-C09	-2.26	1.18	1.23
5	C	707	5IF	O01-C02	-2.21	1.19	1.22

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	705	5IF	O12-C09-N10	-3.27	119.03	123.27
5	E	707	5IF	O12-C09-N10	-3.19	119.14	123.27
5	C	707	5IF	O12-C09-N10	-2.94	119.47	123.27
5	F	705	5IF	O12-C09-N10	-2.93	119.48	123.27
5	K	706	5IF	O12-C09-N10	-2.87	119.55	123.27
5	H	705	5IF	O12-C09-N10	-2.86	119.56	123.27
5	B	706	5IF	O12-C09-N10	-2.76	119.70	123.27
5	D	704	5IF	O12-C09-N10	-2.61	119.90	123.27
5	G	707	5IF	O12-C09-N10	-2.59	119.92	123.27
5	A	705	5IF	O12-C09-N10	-2.47	120.08	123.27
5	J	705	5IF	O12-C09-N10	-2.38	120.19	123.27
5	L	706	5IF	O12-C09-N10	-2.36	120.22	123.27
5	I	705	5IF	C08-C09-N10	2.24	122.63	116.82
5	E	707	5IF	C08-C09-N10	2.20	122.51	116.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	705	5IF	C08-N07-C02	2.12	124.23	120.45

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	707	5IF	C08-C09-N10-O11
5	C	707	5IF	O12-C09-N10-O11
5	E	707	5IF	C08-C09-N10-O11
5	E	707	5IF	O12-C09-N10-O11
5	F	705	5IF	C08-C09-N10-O11
5	F	705	5IF	O12-C09-N10-O11
5	H	705	5IF	C08-C09-N10-O11
5	H	705	5IF	O12-C09-N10-O11
5	I	705	5IF	C08-C09-N10-O11
5	I	705	5IF	O12-C09-N10-O11
5	K	706	5IF	C08-C09-N10-O11
5	K	706	5IF	O12-C09-N10-O11
4	L	705	1PE	OH5-C14-C24-OH4
4	B	705	1PE	OH6-C15-C25-OH5
4	C	705	1PE	OH6-C15-C25-OH5
4	K	705	1PE	OH6-C15-C25-OH5
4	E	706	1PE	OH6-C15-C25-OH5
4	K	705	1PE	OH7-C16-C26-OH6
4	L	705	1PE	OH4-C13-C23-OH3
4	C	706	1PE	OH6-C15-C25-OH5
4	E	706	1PE	C23-C13-OH4-C24
4	I	704	1PE	C15-C25-OH5-C14
4	I	704	1PE	C23-C13-OH4-C24
4	C	705	1PE	C15-C25-OH5-C14
4	C	705	1PE	C24-C14-OH5-C25
4	L	705	1PE	C14-C24-OH4-C13
4	C	706	1PE	OH5-C14-C24-OH4
4	E	706	1PE	OH4-C13-C23-OH3
4	L	705	1PE	OH6-C15-C25-OH5
5	D	704	5IF	N07-C08-C09-O12
4	L	705	1PE	C24-C14-OH5-C25
5	A	705	5IF	N07-C08-C09-O12
5	B	706	5IF	N07-C08-C09-N10
5	B	706	5IF	N07-C08-C09-O12
5	D	704	5IF	N07-C08-C09-N10
5	E	707	5IF	N07-C08-C09-N10

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Mol	Chain	Res	Type	Atoms
5	F	705	5IF	N07-C08-C09-N10
5	H	705	5IF	N07-C08-C09-N10
5	J	705	5IF	N07-C08-C09-O12
4	K	705	1PE	C25-C15-OH6-C26
5	A	705	5IF	N07-C08-C09-N10
5	C	707	5IF	N07-C08-C09-N10
5	E	707	5IF	N07-C08-C09-O12
5	F	705	5IF	N07-C08-C09-O12
5	G	707	5IF	N07-C08-C09-N10
5	G	707	5IF	N07-C08-C09-O12
5	K	706	5IF	N07-C08-C09-N10
5	K	706	5IF	N07-C08-C09-O12
5	L	706	5IF	N07-C08-C09-O12
4	A	704	1PE	C24-C14-OH5-C25
4	J	704	1PE	OH6-C15-C25-OH5
5	D	704	5IF	C13-C08-C09-O12
5	J	705	5IF	N07-C08-C09-N10
5	L	706	5IF	N07-C08-C09-N10
4	C	706	1PE	C25-C15-OH6-C26

There are no ring outliers.

17 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	701	CO3	1	0
2	I	701	CO3	1	0
5	E	707	5IF	1	0
2	E	701	CO3	1	0
5	F	705	5IF	2	0
2	K	701	CO3	1	0
2	C	701	CO3	1	0
4	C	705	1PE	1	0
5	H	705	5IF	1	0
4	E	706	1PE	1	0
6	H	704	SO4	1	0
2	F	701	CO3	1	0
5	K	706	5IF	1	0
5	C	707	5IF	1	0
4	A	704	1PE	1	0
5	I	705	5IF	1	0
4	I	704	1PE	1	0

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

Ligand 5IF B 706

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF E 707

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF D 704

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF F 705

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF A 705

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF H 705

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF K 706

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF J 705

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF C 707

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF G 707

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF I 705

Bond lengths

Bond angles

Torsions

Rings

Ligand 5IF L 706

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	519/527 (98%)	-0.32	2 (0%)	92	93	29, 39, 57, 71	0
1	B	518/527 (98%)	0.14	30 (5%)	23	24	27, 46, 90, 99	0
1	C	518/527 (98%)	-0.23	8 (1%)	73	75	27, 40, 64, 86	0
1	D	513/527 (97%)	-0.43	3 (0%)	89	90	29, 39, 55, 74	0
1	E	511/527 (96%)	-0.35	4 (0%)	86	87	32, 40, 55, 81	0
1	F	510/527 (96%)	-0.09	10 (1%)	65	68	32, 45, 78, 96	0
1	G	519/527 (98%)	-0.33	4 (0%)	86	87	25, 38, 59, 74	0
1	H	518/527 (98%)	-0.04	27 (5%)	27	29	26, 39, 82, 94	0
1	I	518/527 (98%)	-0.20	9 (1%)	70	72	24, 37, 67, 83	0
1	J	516/527 (97%)	-0.42	7 (1%)	75	77	28, 36, 52, 98	0
1	K	512/527 (97%)	-0.39	6 (1%)	79	80	27, 38, 53, 69	0
1	L	510/527 (96%)	-0.08	19 (3%)	41	45	29, 43, 73, 86	0
All	All	6182/6324 (97%)	-0.23	129 (2%)	63	66	24, 40, 71, 99	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	603	ASP	6.5
1	H	157	LEU	6.3
1	J	260	ASN	6.2
1	B	141	PRO	6.1
1	B	144	ILE	5.1
1	L	153	VAL	4.8
1	J	259	VAL	4.7
1	B	119	GLY	4.4
1	L	121	CYS	4.0
1	H	176	TYR	4.0
1	H	153	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	603	ASP	3.9
1	B	196	ALA	3.7
1	B	175	PHE	3.6
1	H	549	SER	3.6
1	B	176	TYR	3.6
1	F	144	ILE	3.5
1	B	130	PHE	3.5
1	B	104	ASN	3.5
1	L	148	VAL	3.5
1	A	603	ASP	3.4
1	F	153	VAL	3.4
1	B	273	ASN	3.4
1	B	274	ALA	3.4
1	B	180	ASP	3.3
1	B	181	ASN	3.3
1	F	118	LYS	3.3
1	B	121	CYS	3.3
1	H	117	ILE	3.2
1	I	274	ALA	3.2
1	E	362	LYS	3.2
1	B	148	VAL	3.2
1	F	132	VAL	3.2
1	C	603	ASP	3.2
1	K	256	ASP	3.2
1	L	144	ILE	3.1
1	D	136	GLY	3.1
1	J	136	GLY	3.1
1	L	157	LEU	3.0
1	H	156	PHE	3.0
1	B	185	VAL	2.9
1	J	124	GLU	2.9
1	F	157	LEU	2.9
1	H	603	ASP	2.9
1	L	178	PHE	2.9
1	C	229	ASN	2.9
1	B	118	LYS	2.9
1	I	196	ALA	2.9
1	B	153	VAL	2.8
1	L	219	LEU	2.8
1	H	122	ASN	2.8
1	L	161	ASN	2.8
1	J	123	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	140	GLY	2.8
1	G	136	GLY	2.8
1	L	272	ASN	2.8
1	H	165	PHE	2.7
1	E	136	GLY	2.7
1	L	156	PHE	2.7
1	H	162	MET	2.7
1	K	362	LYS	2.7
1	B	178	PHE	2.7
1	I	140	GLY	2.7
1	K	136	GLY	2.7
1	L	126	GLY	2.6
1	I	157	LEU	2.6
1	H	363	GLY	2.6
1	F	603	ASP	2.6
1	B	123	VAL	2.6
1	I	117	ILE	2.6
1	H	175	PHE	2.5
1	L	117	ILE	2.5
1	I	120	GLY	2.5
1	C	274	ALA	2.5
1	C	230	VAL	2.5
1	B	162	MET	2.5
1	G	85	ALA	2.5
1	C	272	ASN	2.5
1	L	185	VAL	2.5
1	B	120	GLY	2.5
1	H	225	VAL	2.5
1	B	156	PHE	2.5
1	I	272	ASN	2.5
1	H	119	GLY	2.4
1	H	141	PRO	2.4
1	E	601	LEU	2.4
1	F	156	PHE	2.4
1	D	85	ALA	2.4
1	I	145	SER	2.4
1	H	136	GLY	2.4
1	L	271	ILE	2.4
1	L	150	ASP	2.4
1	K	511	ASN	2.4
1	J	603	ASP	2.3
1	F	141	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	145	SER	2.3
1	H	196	ALA	2.3
1	B	132	VAL	2.3
1	L	149	ASN	2.3
1	H	274	ALA	2.2
1	L	276	THR	2.2
1	H	148	VAL	2.2
1	H	178	PHE	2.2
1	K	255	THR	2.2
1	J	262	GLU	2.2
1	B	157	LEU	2.2
1	A	160	GLU	2.2
1	H	550	SER	2.2
1	K	104	ASN	2.2
1	C	145	SER	2.1
1	H	132	VAL	2.1
1	B	150	ASP	2.1
1	B	136	GLY	2.1
1	F	130	PHE	2.1
1	C	275	ASP	2.1
1	F	227	GLU	2.1
1	H	133	ASN	2.1
1	H	144	ILE	2.1
1	H	135	PRO	2.1
1	B	277	TYR	2.1
1	B	149	ASN	2.1
1	I	121	CYS	2.1
1	B	603	ASP	2.0
1	C	120	GLY	2.0
1	E	361	SER	2.0
1	H	364	ASP	2.0
1	G	362	LYS	2.0
1	L	146	SER	2.0
1	H	271	ILE	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	1PE	C	705	8/16	0.81	0.24	46,54,58,65	0
4	1PE	L	705	10/16	0.82	0.26	55,62,69,72	0
4	1PE	B	705	10/16	0.84	0.18	54,62,67,68	0
4	1PE	C	706	8/16	0.87	0.23	46,53,64,66	0
4	1PE	A	704	10/16	0.89	0.17	39,48,54,55	0
6	SO4	C	704	5/5	0.89	0.14	87,87,97,100	0
6	SO4	E	705	5/5	0.89	0.14	77,81,89,92	0
4	1PE	K	705	13/16	0.90	0.17	41,50,58,59	0
4	1PE	I	704	10/16	0.90	0.19	39,46,55,56	0
6	SO4	G	705	5/5	0.91	0.19	59,60,75,83	0
4	1PE	J	704	10/16	0.92	0.15	43,47,55,62	0
4	1PE	E	706	10/16	0.92	0.15	42,52,57,64	0
6	SO4	K	704	5/5	0.92	0.25	51,58,70,72	0
5	5IF	H	705	26/26	0.93	0.15	28,34,46,49	0
6	SO4	G	706	5/5	0.93	0.34	51,56,74,76	0
5	5IF	K	706	26/26	0.93	0.16	31,36,44,54	0
2	CO3	E	701	4/4	0.94	0.19	34,36,39,43	0
5	5IF	E	707	26/26	0.94	0.16	27,39,48,59	0
6	SO4	F	704	5/5	0.94	0.32	59,63,72,73	0
5	5IF	C	707	26/26	0.95	0.17	28,35,41,46	0
5	5IF	I	705	26/26	0.95	0.16	26,32,44,46	0
6	SO4	G	704	5/5	0.95	0.19	39,42,44,51	5
5	5IF	F	705	26/26	0.96	0.15	32,37,51,53	0
5	5IF	B	706	26/26	0.96	0.14	28,37,42,51	0
2	CO3	L	701	4/4	0.96	0.12	31,31,33,36	0
5	5IF	D	704	26/26	0.96	0.15	28,33,42,53	0
5	5IF	L	706	26/26	0.96	0.14	25,35,43,48	0
2	CO3	C	701	4/4	0.96	0.14	32,34,37,37	0
2	CO3	K	701	4/4	0.97	0.14	32,34,36,38	0
2	CO3	I	701	4/4	0.97	0.12	30,31,31,32	0
3	ZN	G	702	1/1	0.97	0.10	39,39,39,39	0
5	5IF	G	707	26/26	0.97	0.14	26,33,40,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	5IF	A	705	26/26	0.97	0.14	29,36,44,53	0
3	ZN	K	703	1/1	0.97	0.10	38,38,38,38	0
5	5IF	J	705	26/26	0.97	0.14	27,31,39,50	0
2	CO3	J	701	4/4	0.97	0.11	31,33,34,36	0
2	CO3	A	701	4/4	0.98	0.12	33,36,40,45	0
3	ZN	B	703	1/1	0.98	0.07	38,38,38,38	0
3	ZN	E	703	1/1	0.98	0.10	39,39,39,39	0
2	CO3	F	701	4/4	0.98	0.10	33,36,36,38	0
3	ZN	H	703	1/1	0.98	0.09	35,35,35,35	0
3	ZN	J	703	1/1	0.98	0.07	32,32,32,32	0
2	CO3	H	701	4/4	0.98	0.10	29,33,34,35	0
3	ZN	J	702	1/1	0.99	0.08	34,34,34,34	0
3	ZN	A	703	1/1	0.99	0.09	36,36,36,36	0
3	ZN	K	702	1/1	0.99	0.10	38,38,38,38	0
3	ZN	B	702	1/1	0.99	0.08	39,39,39,39	0
3	ZN	L	702	1/1	0.99	0.11	37,37,37,37	0
3	ZN	L	703	1/1	0.99	0.09	34,34,34,34	0
2	CO3	G	701	4/4	0.99	0.11	31,32,34,36	0
3	ZN	C	702	1/1	0.99	0.12	37,37,37,37	0
3	ZN	C	703	1/1	0.99	0.10	34,34,34,34	0
3	ZN	E	702	1/1	0.99	0.12	41,41,41,41	0
6	SO4	B	704	5/5	0.99	0.11	28,31,37,37	0
2	CO3	B	701	4/4	0.99	0.16	34,35,35,39	0
6	SO4	E	704	5/5	0.99	0.13	35,39,41,49	0
3	ZN	F	702	1/1	0.99	0.10	38,38,38,38	0
2	CO3	D	701	4/4	0.99	0.10	33,35,36,37	0
3	ZN	G	703	1/1	0.99	0.09	31,31,31,31	0
3	ZN	H	702	1/1	0.99	0.09	36,36,36,36	0
3	ZN	A	702	1/1	0.99	0.09	39,39,39,39	0
6	SO4	H	704	5/5	0.99	0.11	30,30,32,35	0
3	ZN	I	703	1/1	0.99	0.09	31,31,31,31	0
6	SO4	L	704	5/5	0.99	0.12	29,35,42,42	0
3	ZN	I	702	1/1	1.00	0.12	35,35,35,35	0
3	ZN	D	702	1/1	1.00	0.10	38,38,38,38	0
3	ZN	F	703	1/1	1.00	0.11	35,35,35,35	0
3	ZN	D	703	1/1	1.00	0.08	38,38,38,38	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.
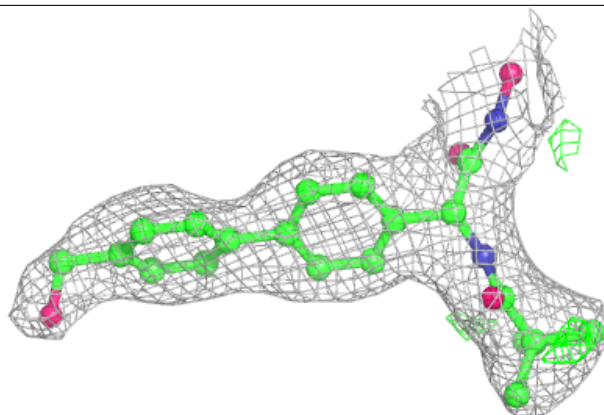
Electron density around 5IF H 705:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
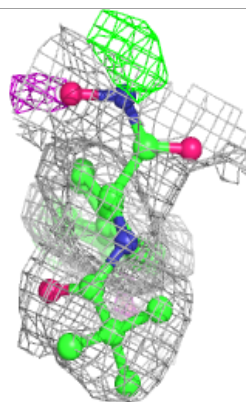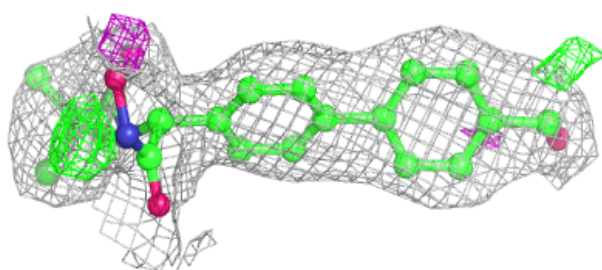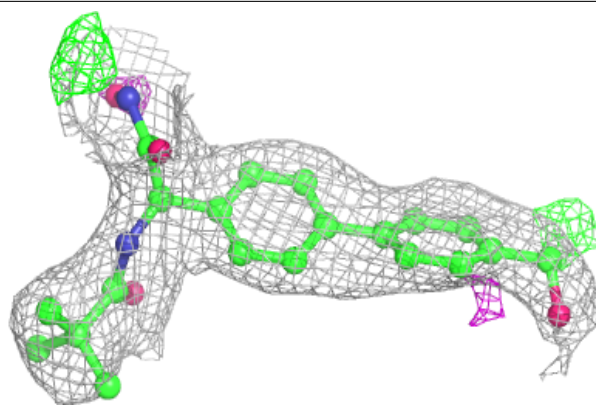
Electron density around 5IF K 706:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
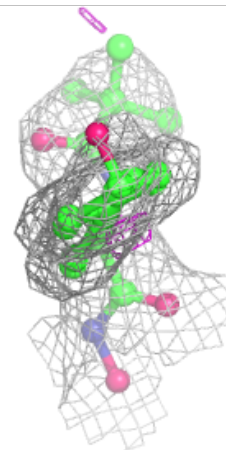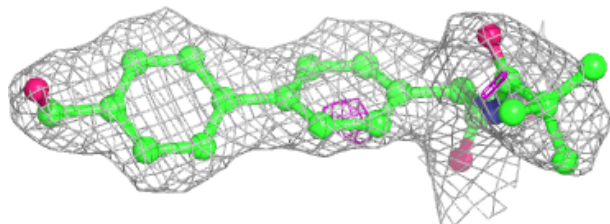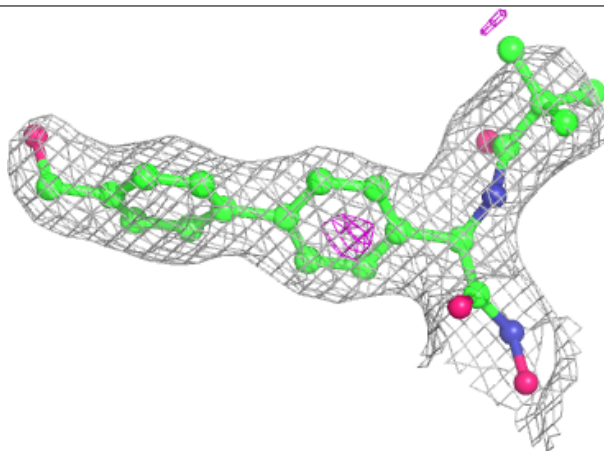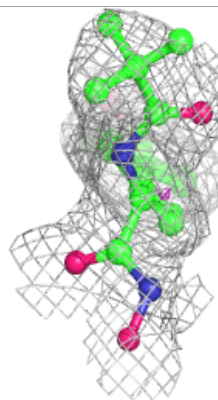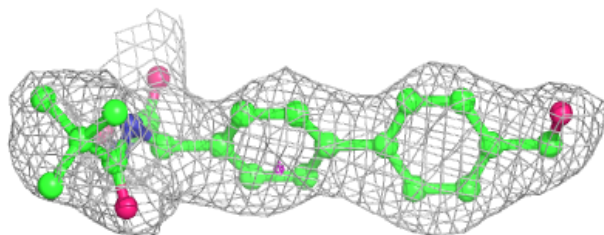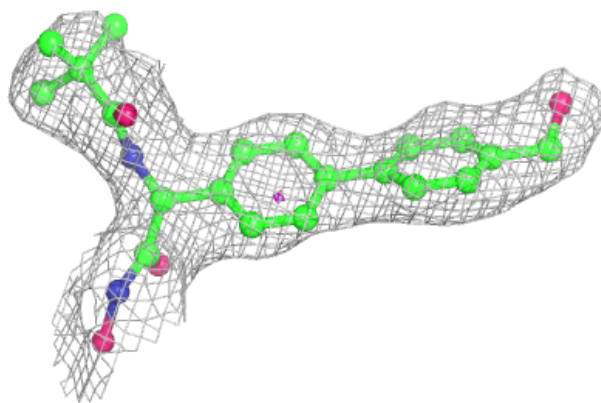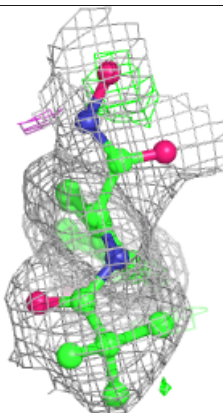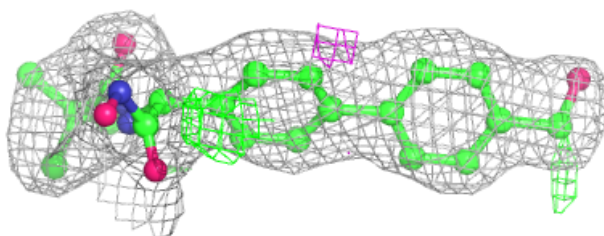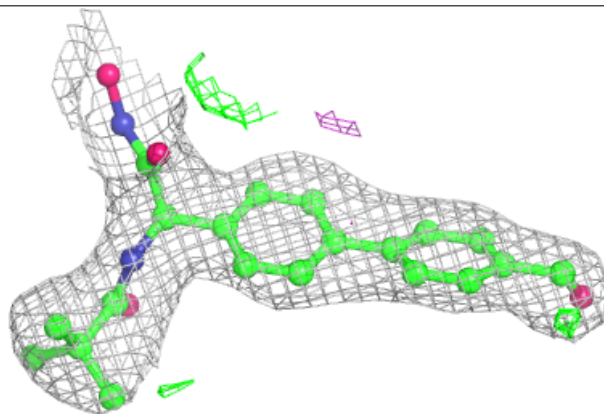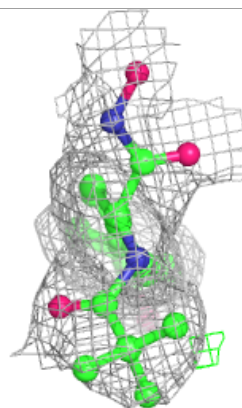$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
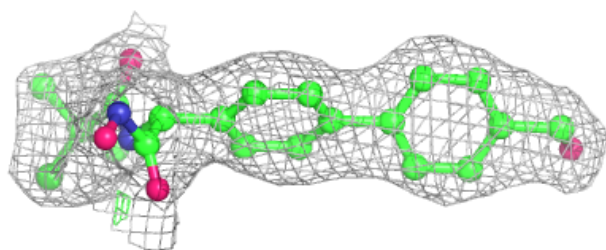and green (positive)
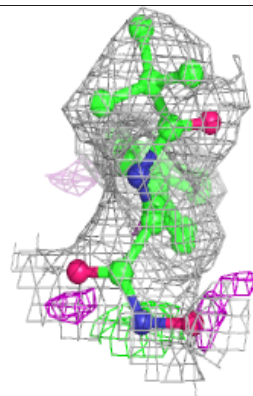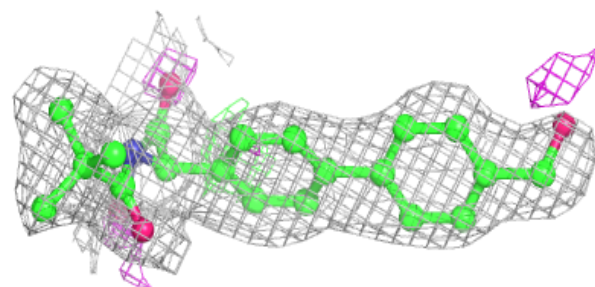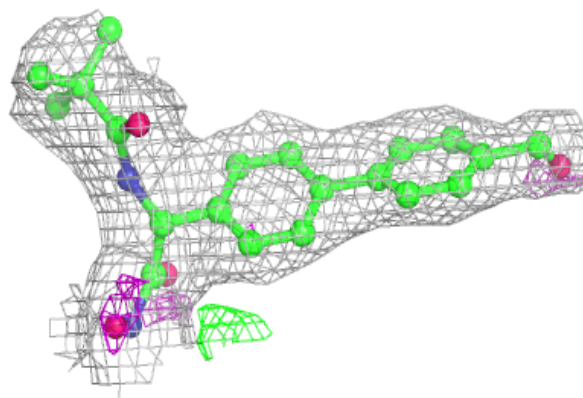
Electron density around 5IF E 707:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
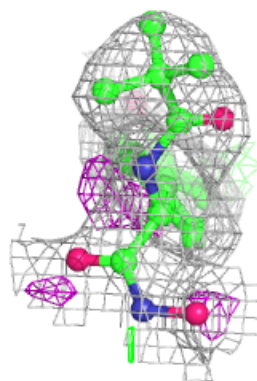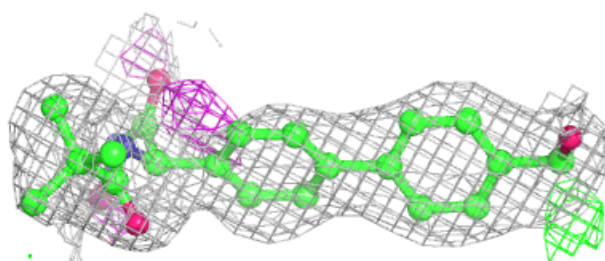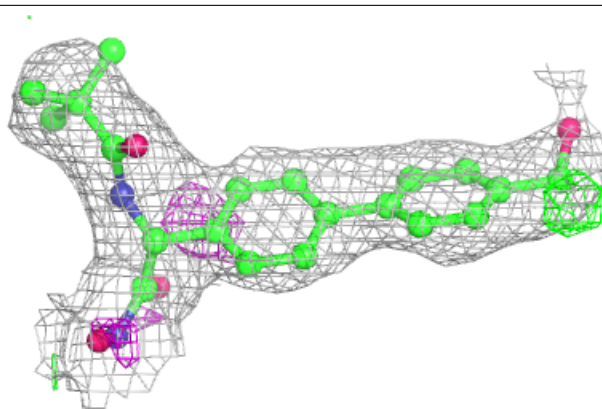
Electron density around 5IF C 707:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
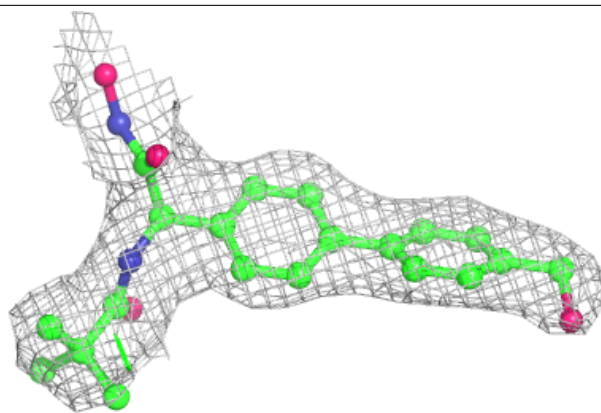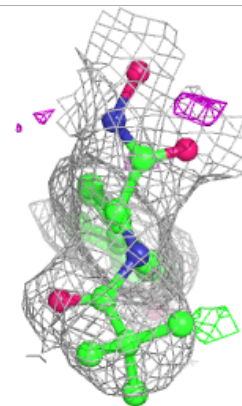and green (positive)
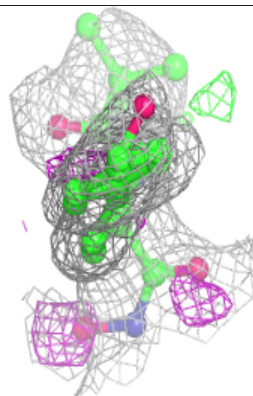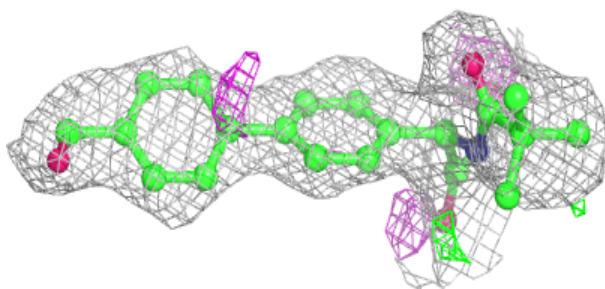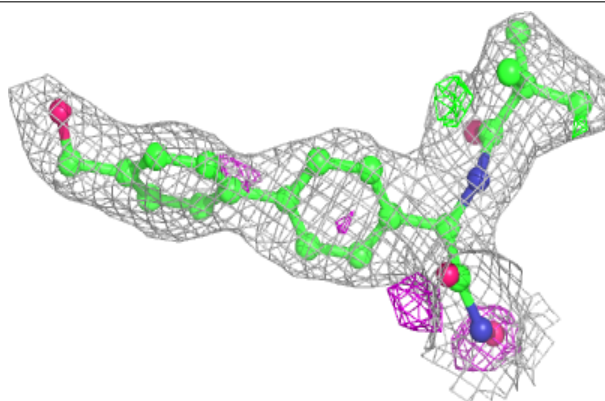
Electron density around 5IF I 705:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
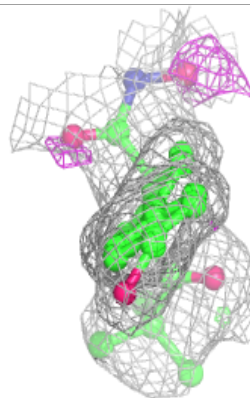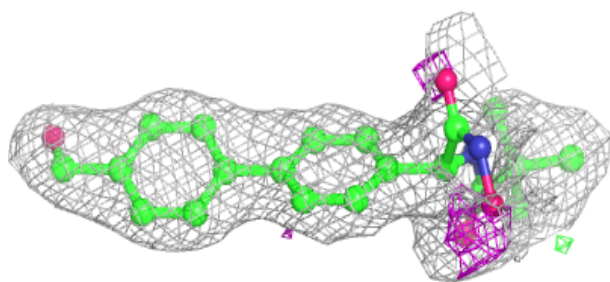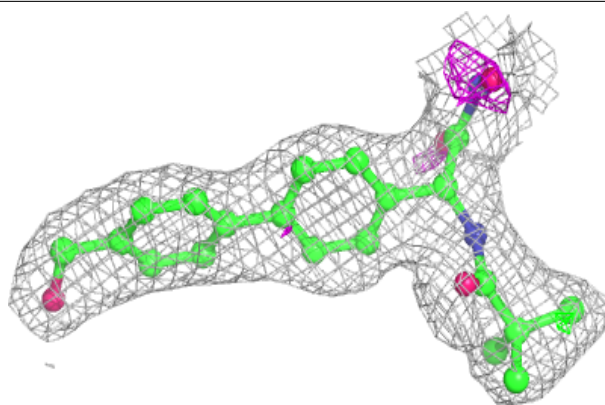
Electron density around 5IF F 705:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
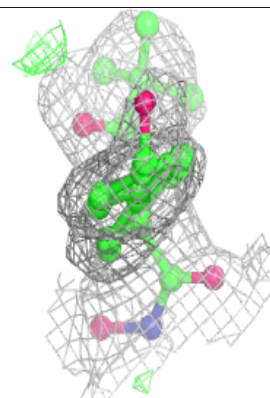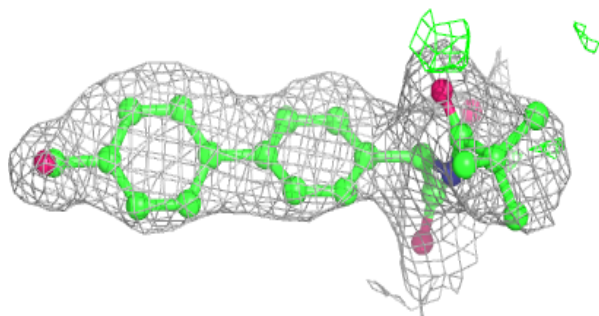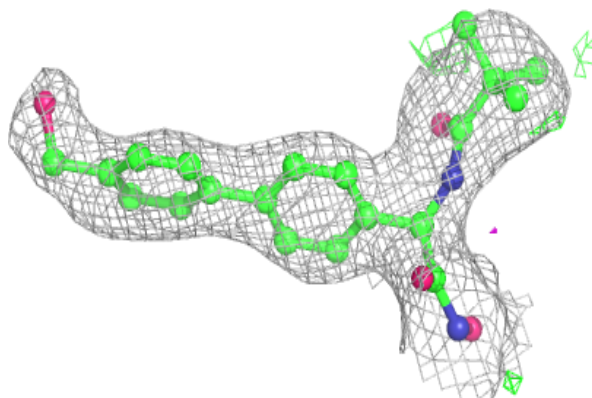
Electron density around 5IF B 706:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
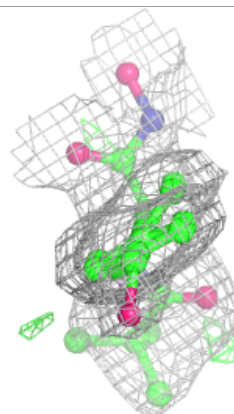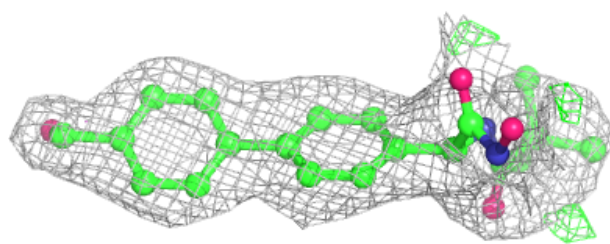
Electron density around 5IF D 704:

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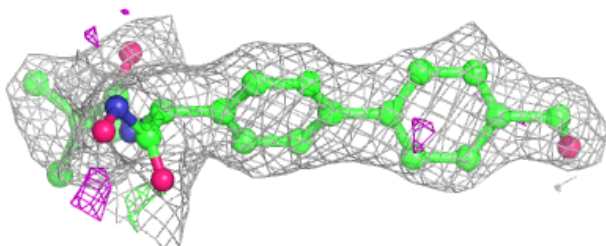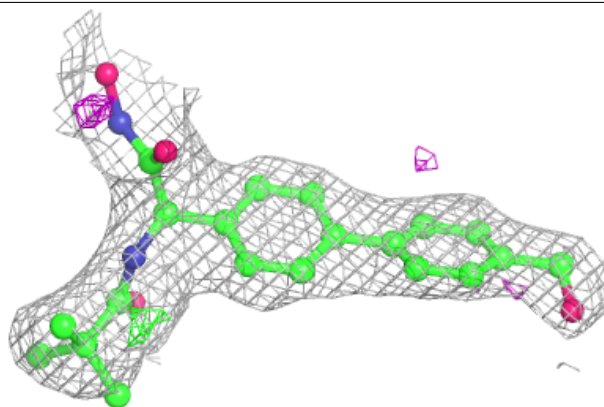and green (positive)

Electron density around 5IF L 706:

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 5IF G 707:

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 5IF A 705:

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

Electron density around 5IF J 705:

$2mF_o$-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.