



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:29 AM UTC

PDB ID : 7RIE / pdb_00007rie
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)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

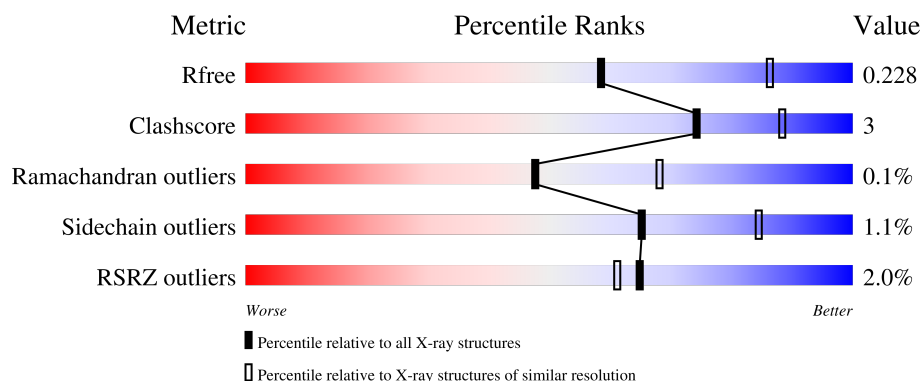
1 Overall quality at a glance

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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% 86% 11%
1	C	527	2% 89% 9%
1	D	527	93% 5%
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%5%.
1	H	527	5%87%10%..
1	I	527	2%92%6%.
1	J	527	2%91%6%..
1	K	527	%91%6%.
1	L	527	2%87%9%.

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

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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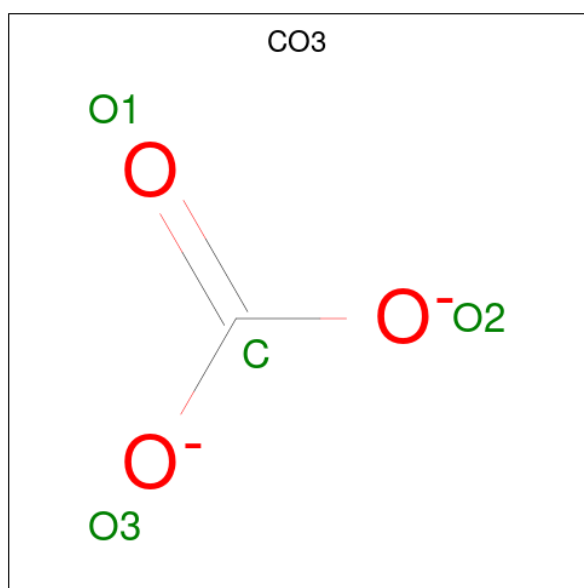
Chain	Residue	Modelled	Actual	Comment	Reference
F	546	GLN	ASN	conflict	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression tag	UNP 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 (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	1	3		
2	B	1	Total	C	O	0	0
			4	1	3		

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

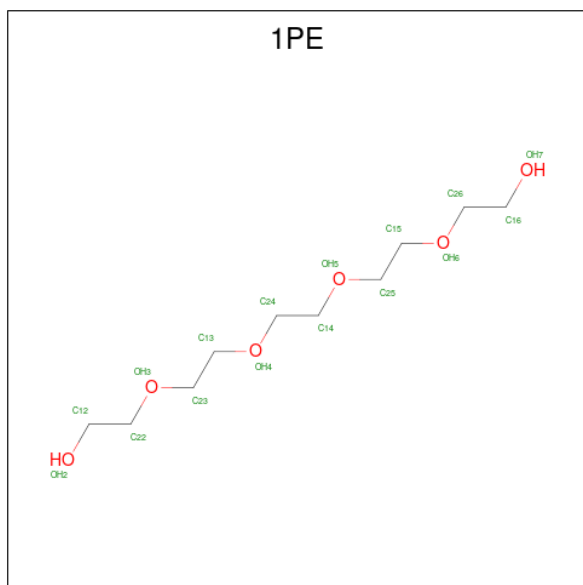
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0

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

- Molecule 4 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



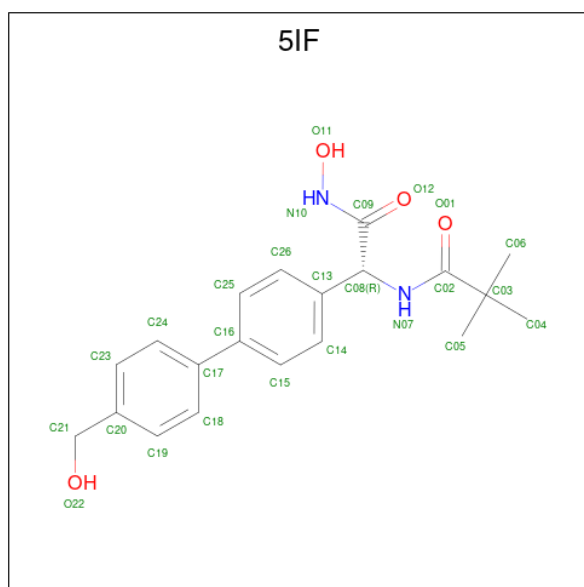
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			8	5	3		
4	C	1	Total	C	O	0	0
			8	5	3		
4	E	1	Total	C	O	0	0
			10	6	4		
4	I	1	Total	C	O	0	0
			10	6	4		
4	J	1	Total	C	O	0	0
			10	6	4		
4	K	1	Total	C	O	0	0
			13	8	5		

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

- Molecule 5 is N-{(1R)-2-(hydroxyamino)-1-[4'-(hydroxymethyl)[1,1'-biphenyl]-4-yl]-2-oxoethyl}-2,2-dimethylpropanamide (CCD ID: 5IF) (formula: C₂₀H₂₄N₂O₄) (labeled as "Ligand of Interest" by depositor).



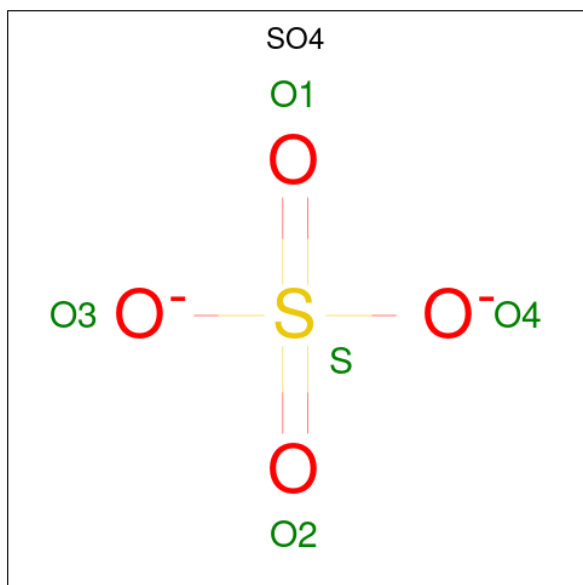
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			26	20	2	4		
5	B	1	Total	C	N	O	0	0
			26	20	2	4		
5	C	1	Total	C	N	O	0	0
			26	20	2	4		
5	D	1	Total	C	N	O	0	0
			26	20	2	4		
5	E	1	Total	C	N	O	0	0
			26	20	2	4		
5	F	1	Total	C	N	O	0	0
			26	20	2	4		
5	G	1	Total	C	N	O	0	0
			26	20	2	4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

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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 (CCD ID: SO4) (formula: O₄S).



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	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		

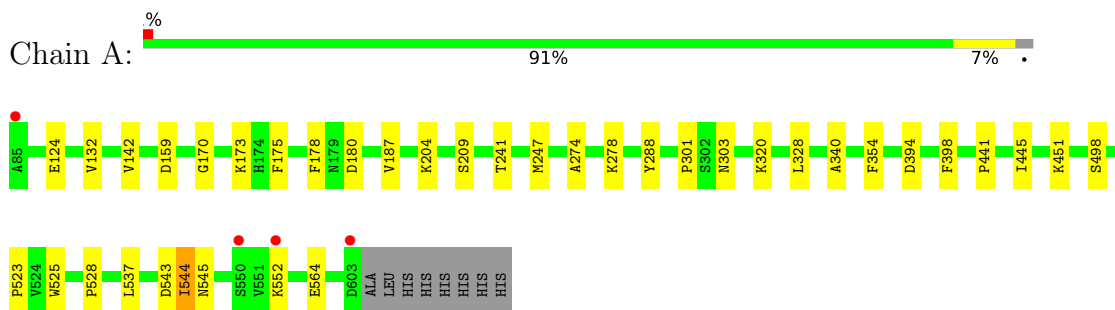
- Molecule 7 is water.

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

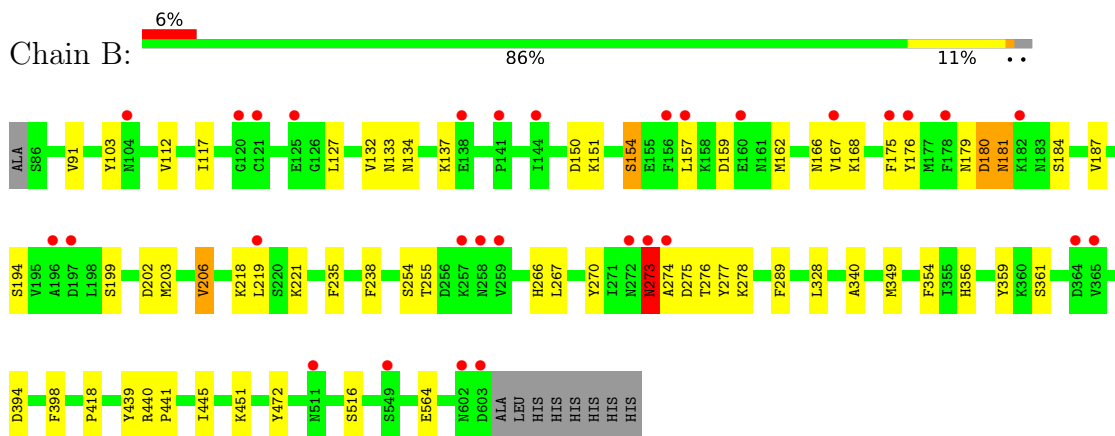
3 Residue-property plots [i](#)

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.

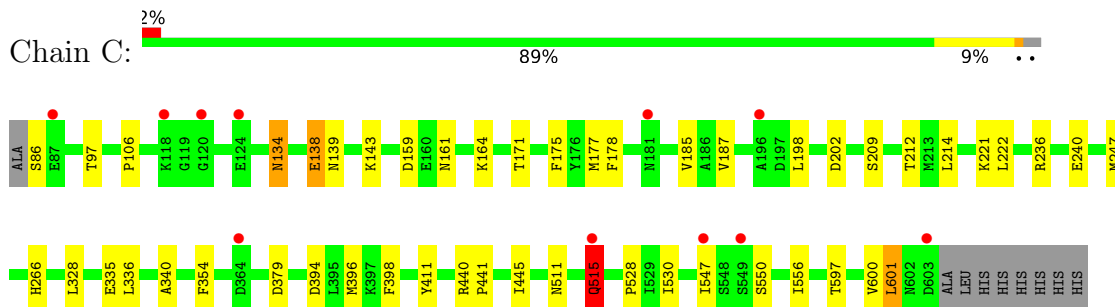
- Molecule 1: M17 leucyl aminopeptidase



- Molecule 1: M17 leucyl aminopeptidase

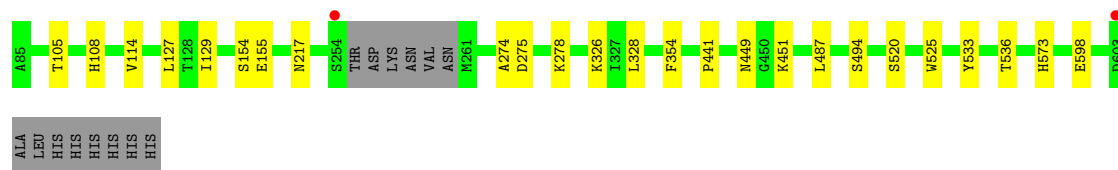


- Molecule 1: M17 leucyl aminopeptidase



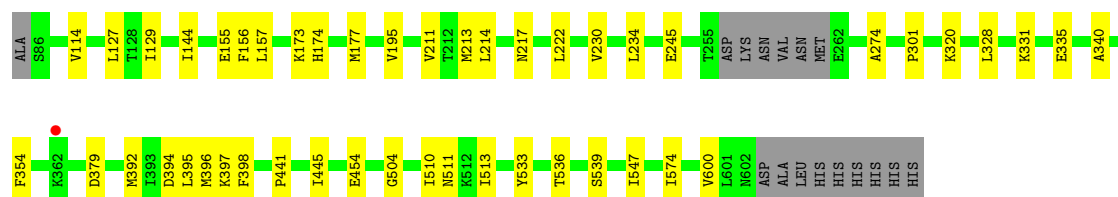
- Molecule 1: M17 leucyl aminopeptidase

Chain D:  93% 5% .



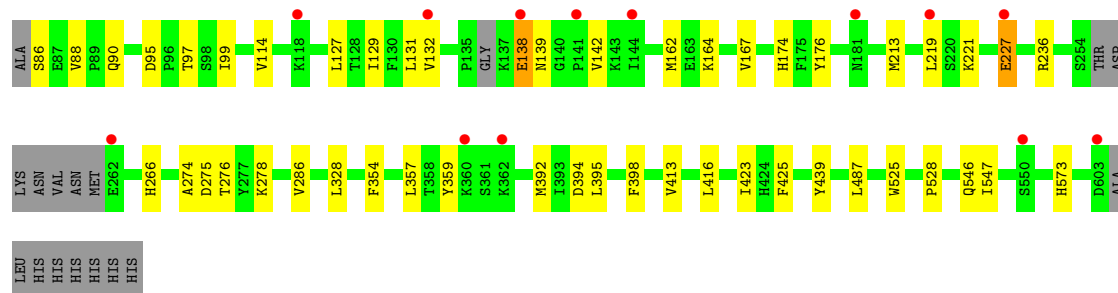
- Molecule 1: M17 leucyl aminopeptidase

Chain E:  88% 9% .



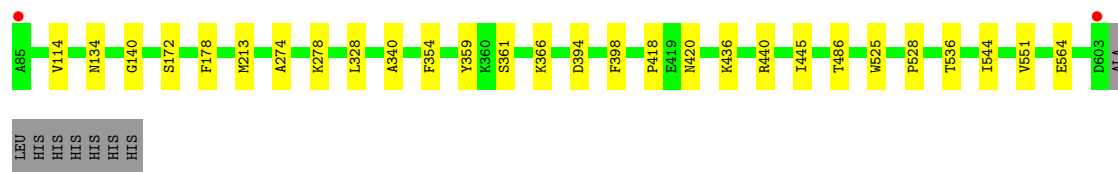
- Molecule 1: M17 leucyl aminopeptidase

Chain F:  87% 9% .



- Molecule 1: M17 leucyl aminopeptidase

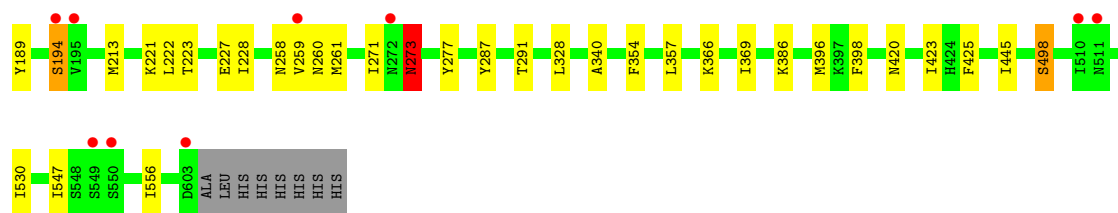
Chain G:  93% 5% .



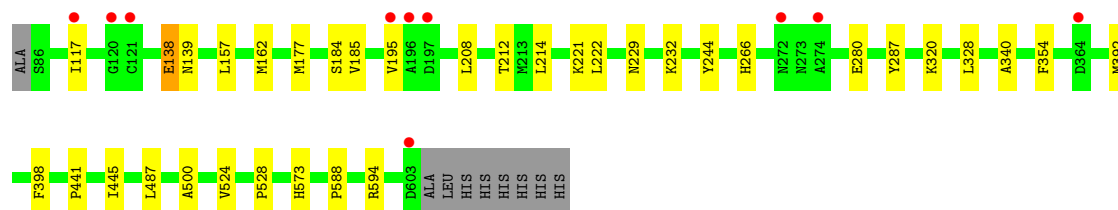
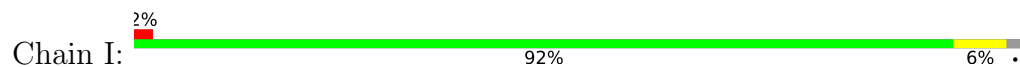
- Molecule 1: M17 leucyl aminopeptidase

Chain H:  87% 10% ..

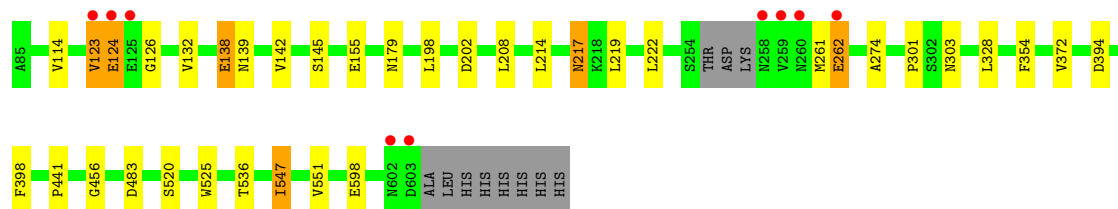
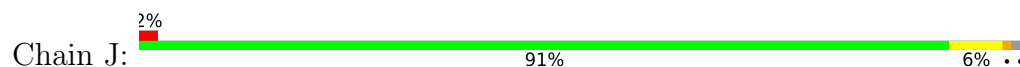




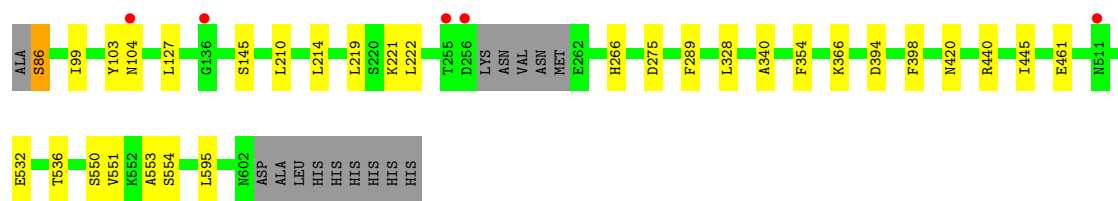
• Molecule 1: M17 leucyl aminopeptidase



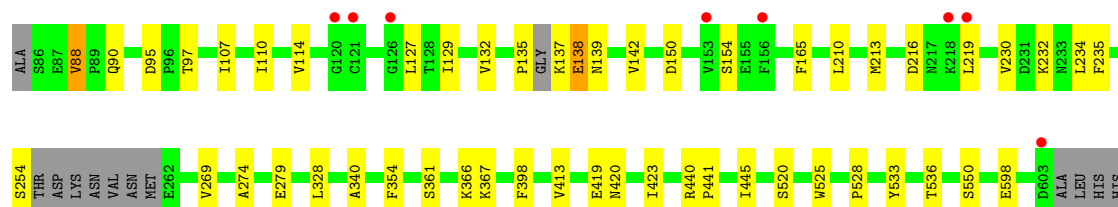
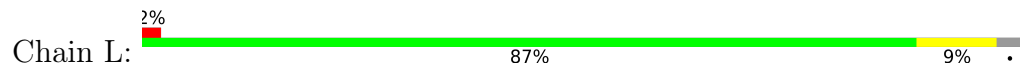
• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



• Molecule 1: M17 leucyl aminopeptidase



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 48.75 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.75-2.49) 92.8 (48.75-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.32 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.195 , 0.229 0.195 , 0.228	Depositor DCC
R_{free} test set	12437 reflections (4.94%)	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 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: ZN, SO4, 1PE, 5IF, 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	0.19	1/4071 (0.0%)	0.35	2/5521 (0.0%)
1	B	0.17	0/3970	0.38	3/5398 (0.1%)
1	C	0.25	1/4020 (0.0%)	0.41	3/5459 (0.1%)
1	D	0.08	0/3993	0.26	0/5416
1	E	0.12	0/3962	0.27	0/5382
1	F	0.21	1/3915 (0.0%)	0.35	3/5325 (0.1%)
1	G	0.10	0/4068	0.28	0/5518
1	H	0.21	1/3978 (0.0%)	0.34	1/5407 (0.0%)
1	I	0.18	1/4029 (0.0%)	0.31	0/5467
1	J	0.22	1/4021 (0.0%)	0.58	8/5451 (0.1%)
1	K	0.20	1/3985 (0.0%)	0.33	3/5411 (0.1%)
1	L	0.09	0/3935	0.27	0/5348
All	All	0.18	7/47947 (0.0%)	0.35	23/65103 (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	A	124	GLU	N-CA	7.76	1.51	1.46
1	C	515	GLN	CD-NE2	7.30	1.48	1.33
1	H	273	ASN	CG-OD1	7.30	1.37	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	99	ILE	CA-C	-6.51	1.48	1.53
1	K	99	ILE	N-CA	5.98	1.50	1.46
1	I	229	ASN	CG-OD1	5.55	1.34	1.23
1	J	124	GLU	CD-OE2	5.11	1.35	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	123	VAL	CA-C-N	-22.21	88.10	122.08
1	J	123	VAL	C-N-CA	-22.21	88.10	122.08
1	J	262	GLU	CB-CA-C	8.46	122.18	110.34
1	F	227	GLU	CA-CB-CG	8.12	130.34	114.10
1	J	124	GLU	CG-CD-OE1	-7.28	101.66	118.40
1	B	181	ASN	CA-C-N	6.64	132.02	122.40
1	B	181	ASN	C-N-CA	6.64	132.02	122.40
1	C	515	GLN	N-CA-CB	-6.53	100.50	110.16
1	A	552	LYS	N-CA-CB	6.49	119.89	110.47
1	C	515	GLN	CB-CA-C	6.45	121.81	110.85
1	A	552	LYS	CB-CG-CD	6.15	125.44	111.30
1	F	99	ILE	CA-C-O	6.14	122.77	119.15
1	B	273	ASN	CB-CG-ND2	-5.88	107.58	116.40
1	J	261	MET	CA-C-N	5.81	131.00	121.58
1	J	261	MET	C-N-CA	5.81	131.00	121.58
1	K	104	ASN	OD1-CG-ND2	5.80	128.40	122.60
1	C	335	GLU	CA-CB-CG	-5.58	102.94	114.10
1	J	262	GLU	CA-CB-CG	5.52	125.14	114.10
1	F	227	GLU	CB-CG-CD	-5.35	103.50	112.60
1	J	124	GLU	N-CA-CB	5.26	118.00	111.00
1	K	104	ASN	N-CA-CB	-5.20	102.84	110.49
1	H	273	ASN	CB-CG-ND2	-5.02	108.87	116.40
1	K	99	ILE	CA-C-O	5.01	122.11	119.15

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	38	0
1	C	3942	0	3842	34	0
1	D	3916	0	3855	14	0
1	E	3885	0	3783	28	0
1	F	3839	0	3707	30	0
1	G	3987	0	3913	17	1
1	H	3900	0	3786	32	0
1	I	3951	0	3878	17	0
1	J	3944	0	3889	24	0
1	K	3908	0	3815	15	0
1	L	3859	0	3745	32	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	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	4	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	1	0
All	All	49071	0	46010	287	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 (287) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:ASN:OD1	1:B:134:ASN:N	2.34	0.60
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: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:F:127:LEU:HD21	1:F:213:MET:HE2	1.84	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:B:150:ASP:O	1:B:154:SER:OG	2.23	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:B:203:MET:HE2	1:B:238:PHE:HD1	1.70	0.56
1:E:511:ASN:ND2	7:E:803:HOH:O	2.37	0.56
1:F:129:ILE:HD11	1:F:213:MET:HE1	1.87	0.56
1:K:366:LYS:HG3	1:K:420:ASN:HB3	1.87	0.56
1:L:210:LEU:HA	1:L:213:MET:HE2	1.86	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:I:157:LEU:HA	1:I:162:MET:HE3	1.88	0.55
1:H:157:LEU:HD23	1:H:162:MET:HE2	1.88	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:B:359:TYR:OH	1:B:418:PRO:O	2.21	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: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:J:126:GLY:C	1:J:219:LEU:HD13	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:HIS:HB3	1:F:213:MET:HE3	1.92	0.52
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.92	0.52
1:J:124:GLU:CD	1:J:179:ASN:HD22	2.07	0.52
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
1:J:126:GLY:HA2	1:J:219:LEU:HD22	1.91	0.51
1:H:129:ILE:HD11	1:H:213:MET:HE1	1.90	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: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: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:A:170:GLY:O	1:A:209:SER:OG	2.25	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:J:456:GLY:HA3	1:J:547:ILE:HD11	1.96	0.48
1:C:106:PRO:HD2	1:C:247:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H:258:ASN:HD22	1:H:261:MET:HE2	1.80	0.47
1:K:214:LEU:HD21	1:K:222:LEU:HD22	1.97	0.47
1:B:91:VAL:HG23	1:B:349:MET:HE1	1.95	0.47
1:B:451:LYS:NZ	1:B:564:GLU:O	2.46	0.47
1:L:413:VAL:HG11	1:L:423:ILE:HD13	1.96	0.47
1:E:392:MET:HE2	1:E:395:LEU:HB2	1.97	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
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:F:174:HIS:CG	1:F:213:MET:HE3	2.51	0.46
1:K:103:TYR:HA	1:K:289:PHE:CZ	2.50	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: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: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:392:MET:HE2	1:F:395:LEU:HB2	1.97	0.46
1:F:413:VAL:HG11	1:F:423:ILE:HD13	1.98	0.46
1:E:156:PHE:CG	1:E:177:MET:HE1	2.51	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:E:173:LYS:NZ	7:E:811:HOH:O	2.49	0.45
1:L:138:GLU:O	1:L:139:ASN:HB2	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:GLU:O	1:C:139:ASN:HB2	2.16	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
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: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:H:162:MET:HE1	1:H:175:PHE:CE2	2.52	0.44
1:I:232:LYS:NZ	1:I:280:GLU:OE2	2.36	0.44
1:G:394:ASP:HA	1:I:441:PRO:HB2	1.98	0.44
1:H:129:ILE:HD11	1:H:213:MET:CE	2.48	0.44
1:B:356:HIS:ND1	1:B:472:TYR:OH	2.45	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:B:179:ASN:C	1:B:181:ASN:H	2.26	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:OD1	1:A:159:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:ASP:O	1:E:396:MET:HG3	2.18	0.43
1:E:392:MET:HE2	1:E:392:MET:HB3	1.75	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: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:L:150:ASP:O	1:L:154:SER:OG	2.33	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
1:B:203:MET:HE3	1:B:206:VAL:HG13	2.00	0.42
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:162:MET:HE2	1:F:162:MET:HA	2.01	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:L:213:MET:HE3	1:L:213:MET:HB2	1.89	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:E:174:HIS:HB3	1:E:213:MET:HE3	2.02	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:172:SER:HB2	1:G:213:MET:HE3	2.02	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:I:320:LYS:NZ	7:I:809:HOH:O	2.48	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:C:177:MET:HE2	1:C:177:MET:HB3	1.90	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: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
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:G:359:TYR:OH	1:G:418:PRO:O	2.33	0.41
1:H:166:ASN:OD1	1:H:166:ASN:C	2.63	0.41
1:B:157:LEU:HA	1:B:162:MET:HE3	2.03	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:E:320:LYS:NZ	7:E:814:HOH:O	2.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:138:GLU:HA	1:H:194:SER:CB	2.52	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	518/527 (98%)	501 (97%)	17 (3%)	0	100	100
1	B	516/527 (98%)	498 (96%)	17 (3%)	1 (0%)	43	63
1	C	516/527 (98%)	501 (97%)	14 (3%)	1 (0%)	43	63
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%)	43	63
1	G	518/527 (98%)	502 (97%)	16 (3%)	0	100	100
1	H	516/527 (98%)	493 (96%)	20 (4%)	3 (1%)	21	38
1	I	516/527 (98%)	503 (98%)	12 (2%)	1 (0%)	43	63
1	J	512/527 (97%)	496 (97%)	15 (3%)	1 (0%)	43	63
1	K	508/527 (96%)	495 (97%)	13 (3%)	0	100	100
1	L	504/527 (96%)	491 (97%)	12 (2%)	1 (0%)	43	63
All	All	6144/6324 (97%)	5964 (97%)	171 (3%)	9 (0%)	48	68

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 ⓘ

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%)	425 (100%)	2 (0%)	81	92
1	B	403/454 (89%)	396 (98%)	7 (2%)	53	78
1	C	417/454 (92%)	410 (98%)	7 (2%)	53	78
1	D	415/454 (91%)	412 (99%)	3 (1%)	76	89
1	E	410/454 (90%)	407 (99%)	3 (1%)	76	89
1	F	400/454 (88%)	395 (99%)	5 (1%)	61	82
1	G	427/454 (94%)	426 (100%)	1 (0%)	87	95
1	H	405/454 (89%)	397 (98%)	8 (2%)	48	75
1	I	419/454 (92%)	414 (99%)	5 (1%)	63	83
1	J	418/454 (92%)	412 (99%)	6 (1%)	59	81
1	K	415/454 (91%)	408 (98%)	7 (2%)	53	78
1	L	406/454 (89%)	403 (99%)	3 (1%)	76	89
All	All	4962/5448 (91%)	4905 (99%)	57 (1%)	65	84

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	398	PHE
1	A	544	ILE

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Mol	Chain	Res	Type
1	B	154	SER
1	B	194	SER
1	B	206	VAL
1	B	361	SER
1	B	398	PHE
1	B	439	TYR
1	B	516	SER
1	C	134	ASN
1	C	171	THR
1	C	398	PHE
1	C	515	GLN
1	C	550	SER
1	C	600	VAL
1	C	601	LEU
1	D	154	SER
1	D	217	ASN
1	D	494	SER
1	E	398	PHE
1	E	547	ILE
1	E	600	VAL
1	F	86	SER
1	F	219	LEU
1	F	276	THR
1	F	398	PHE
1	F	439	TYR
1	G	398	PHE
1	H	86	SER
1	H	146	SER
1	H	154	SER
1	H	184	SER
1	H	194	SER
1	H	398	PHE
1	H	498	SER
1	H	547	ILE
1	I	117	ILE
1	I	184	SER
1	I	195	VAL
1	I	392	MET
1	I	398	PHE
1	J	145	SER
1	J	208	LEU
1	J	217	ASN

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Mol	Chain	Res	Type
1	J	262	GLU
1	J	398	PHE
1	J	547	ILE
1	K	86	SER
1	K	145	SER
1	K	275	ASP
1	K	398	PHE
1	K	550	SER
1	K	554	SER
1	K	595	LEU
1	L	88	VAL
1	L	398	PHE
1	L	550	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	ASN
1	A	273	ASN
1	A	567	GLN
1	B	139	ASN
1	B	273	ASN
1	C	134	ASN
1	C	272	ASN
1	C	273	ASN
1	C	420	ASN
1	C	515	GLN
1	D	108	HIS
1	D	139	ASN
1	D	272	ASN
1	D	273	ASN
1	D	515	GLN
1	E	567	GLN
1	F	179	ASN
1	G	521	ASN
1	H	113	GLN
1	H	134	ASN
1	H	217	ASN
1	H	260	ASN
1	H	515	GLN
1	I	104	ASN
1	I	515	GLN

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Mol	Chain	Res	Type
1	K	149	ASN
1	K	515	GLN
1	L	161	ASN
1	L	166	ASN
1	L	174	HIS
1	L	420	ASN
1	L	531	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	1PE	J	704	-	9,9,15	0.09	0	8,8,14	0.17	0
6	SO4	B	704	-	4,4,4	0.23	0	6,6,6	0.09	0
4	1PE	K	705	-	12,12,15	0.10	0	11,11,14	0.12	0
2	CO3	J	701	-	3,3,3	0.83	0	2,3,3	0.11	0
5	5IF	J	705	3	26,27,27	1.36	3 (11%)	36,38,38	1.01	0
6	SO4	H	704	-	4,4,4	0.22	0	6,6,6	0.09	0
4	1PE	I	704	-	9,9,15	0.10	0	8,8,14	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5IF	D	704	3	26,27,27	1.38	3 (11%)	36,38,38	0.94	0
5	5IF	E	707	3	26,27,27	1.38	3 (11%)	36,38,38	1.01	1 (2%)
6	SO4	K	704	-	4,4,4	0.25	0	6,6,6	0.08	0
2	CO3	B	701	-	3,3,3	0.82	0	2,3,3	0.14	0
2	CO3	G	701	-	3,3,3	0.85	0	2,3,3	0.16	0
4	1PE	E	706	-	9,9,15	0.09	0	8,8,14	0.17	0
6	SO4	G	705	-	4,4,4	0.25	0	6,6,6	0.09	0
5	5IF	C	707	3	26,27,27	1.37	3 (11%)	36,38,38	0.99	1 (2%)
4	1PE	C	705	-	7,7,15	0.15	0	6,6,14	0.14	0
4	1PE	L	705	-	9,9,15	0.11	0	8,8,14	0.17	0
6	SO4	E	705	-	4,4,4	0.24	0	6,6,6	0.07	0
6	SO4	G	704	-	4,4,4	0.23	0	6,6,6	0.07	0
5	5IF	L	706	3	26,27,27	1.37	3 (11%)	36,38,38	1.03	0
4	1PE	B	705	-	9,9,15	0.11	0	8,8,14	0.13	0
6	SO4	F	704	-	4,4,4	0.23	0	6,6,6	0.07	0
2	CO3	E	701	-	3,3,3	0.80	0	2,3,3	0.16	0
5	5IF	I	705	3	26,27,27	1.37	3 (11%)	36,38,38	1.03	1 (2%)
2	CO3	L	701	-	3,3,3	0.83	0	2,3,3	0.14	0
2	CO3	F	701	-	3,3,3	0.81	0	2,3,3	0.15	0
6	SO4	L	704	-	4,4,4	0.24	0	6,6,6	0.10	0
2	CO3	I	701	-	3,3,3	0.84	0	2,3,3	0.19	0
5	5IF	H	705	3	26,27,27	1.39	3 (11%)	36,38,38	1.06	1 (2%)
6	SO4	E	704	-	4,4,4	0.23	0	6,6,6	0.08	0
5	5IF	K	706	3	26,27,27	1.38	3 (11%)	36,38,38	0.99	0
5	5IF	B	706	3	26,27,27	1.37	3 (11%)	36,38,38	0.96	0
2	CO3	H	701	-	3,3,3	0.82	0	2,3,3	0.10	0
6	SO4	C	704	-	4,4,4	0.24	0	6,6,6	0.08	0
2	CO3	K	701	-	3,3,3	0.81	0	2,3,3	0.17	0
2	CO3	A	701	-	3,3,3	0.82	0	2,3,3	0.11	0
2	CO3	D	701	-	3,3,3	0.83	0	2,3,3	0.14	0
2	CO3	C	701	-	3,3,3	0.80	0	2,3,3	0.21	0
4	1PE	A	704	-	9,9,15	0.09	0	8,8,14	0.16	0
5	5IF	F	705	3	26,27,27	1.39	3 (11%)	36,38,38	1.01	0
4	1PE	C	706	-	7,7,15	0.15	0	6,6,14	0.13	0
5	5IF	G	707	3	26,27,27	1.37	3 (11%)	36,38,38	0.95	0
6	SO4	G	706	-	4,4,4	0.23	0	6,6,6	0.11	0
5	5IF	A	705	3	26,27,27	1.37	3 (11%)	36,38,38	1.03	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
4	1PE	J	704	-	-	1/7/7/13	-
4	1PE	K	705	-	-	3/10/10/13	-
5	5IF	J	705	3	-	3/26/26/26	0/2/2/2
4	1PE	I	704	-	-	2/7/7/13	-
5	5IF	D	704	3	-	4/26/26/26	0/2/2/2
5	5IF	E	707	3	-	4/26/26/26	0/2/2/2
4	1PE	E	706	-	-	3/7/7/13	-
5	5IF	C	707	3	-	3/26/26/26	0/2/2/2
4	1PE	C	705	-	-	3/5/5/13	-
4	1PE	L	705	-	-	5/7/7/13	-
5	5IF	L	706	3	-	2/26/26/26	0/2/2/2
4	1PE	B	705	-	-	2/7/7/13	-
5	5IF	I	705	3	-	2/26/26/26	0/2/2/2
5	5IF	H	705	3	-	4/26/26/26	0/2/2/2
5	5IF	K	706	3	-	4/26/26/26	0/2/2/2
5	5IF	B	706	3	-	2/26/26/26	0/2/2/2
4	1PE	A	704	-	-	2/7/7/13	-
5	5IF	F	705	3	-	4/26/26/26	0/2/2/2
4	1PE	C	706	-	-	3/5/5/13	-
5	5IF	G	707	3	-	2/26/26/26	0/2/2/2
5	5IF	A	705	3	-	2/26/26/26	0/2/2/2

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	705	5IF	C02-N07	5.92	1.45	1.34
5	F	705	5IF	C02-N07	5.91	1.45	1.34
5	K	706	5IF	C02-N07	5.87	1.45	1.34
5	G	707	5IF	C02-N07	5.86	1.45	1.34
5	D	704	5IF	C02-N07	5.86	1.45	1.34
5	A	705	5IF	C02-N07	5.83	1.45	1.34
5	C	707	5IF	C02-N07	5.83	1.45	1.34
5	L	706	5IF	C02-N07	5.82	1.45	1.34
5	B	706	5IF	C02-N07	5.81	1.45	1.34
5	E	707	5IF	C02-N07	5.81	1.45	1.34
5	I	705	5IF	C02-N07	5.80	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	705	5IF	C02-N07	5.76	1.45	1.34
5	I	705	5IF	O12-C09	-2.51	1.18	1.23
5	C	707	5IF	O12-C09	-2.47	1.18	1.23
5	K	706	5IF	O12-C09	-2.45	1.18	1.23
5	E	707	5IF	O12-C09	-2.45	1.18	1.23
5	F	705	5IF	O12-C09	-2.44	1.18	1.23
5	J	705	5IF	O12-C09	-2.43	1.18	1.23
5	E	707	5IF	O01-C02	-2.43	1.18	1.22
5	H	705	5IF	O12-C09	-2.43	1.18	1.23
5	B	706	5IF	O12-C09	-2.43	1.18	1.23
5	L	706	5IF	O12-C09	-2.42	1.18	1.23
5	D	704	5IF	O12-C09	-2.40	1.18	1.23
5	H	705	5IF	O01-C02	-2.40	1.18	1.22
5	A	705	5IF	O12-C09	-2.40	1.18	1.23
5	B	706	5IF	O01-C02	-2.38	1.18	1.22
5	L	706	5IF	O01-C02	-2.37	1.18	1.22
5	K	706	5IF	O01-C02	-2.36	1.18	1.22
5	D	704	5IF	O01-C02	-2.36	1.18	1.22
5	F	705	5IF	O01-C02	-2.35	1.18	1.22
5	G	707	5IF	O12-C09	-2.34	1.18	1.23
5	A	705	5IF	O01-C02	-2.34	1.18	1.22
5	J	705	5IF	O01-C02	-2.34	1.18	1.22
5	G	707	5IF	O01-C02	-2.34	1.18	1.22
5	I	705	5IF	O01-C02	-2.30	1.18	1.22
5	C	707	5IF	O01-C02	-2.24	1.19	1.22

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	705	5IF	C08-C09-N10	2.26	122.63	116.84
5	E	707	5IF	C08-C09-N10	2.21	122.51	116.84
5	H	705	5IF	C13-C08-N07	2.03	117.86	112.75
5	C	707	5IF	C08-C09-N10	2.00	121.96	116.84

There are no chirality outliers.

All (60) 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

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

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

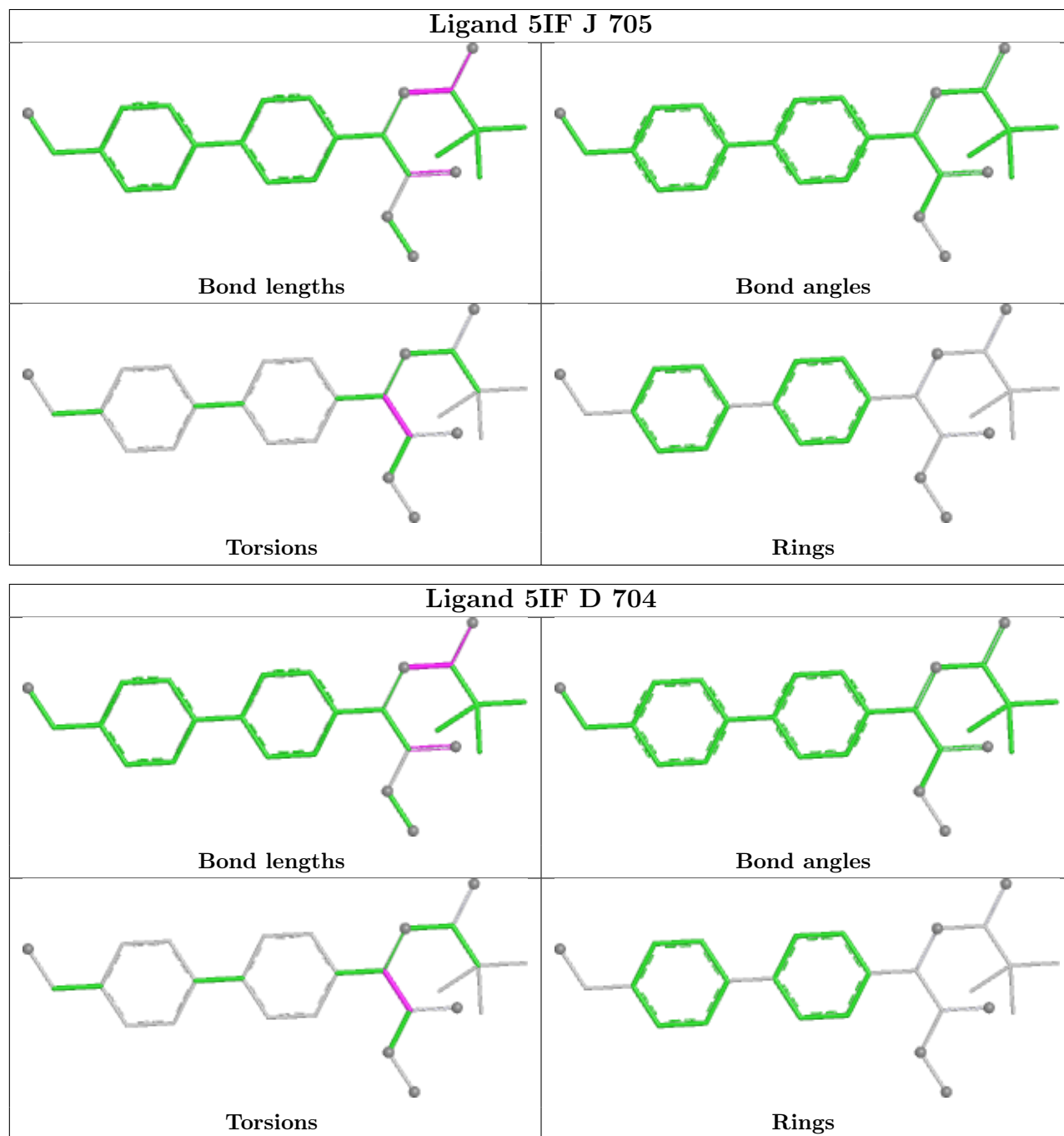
There are no ring outliers.

17 monomers are involved in 11 short contacts:

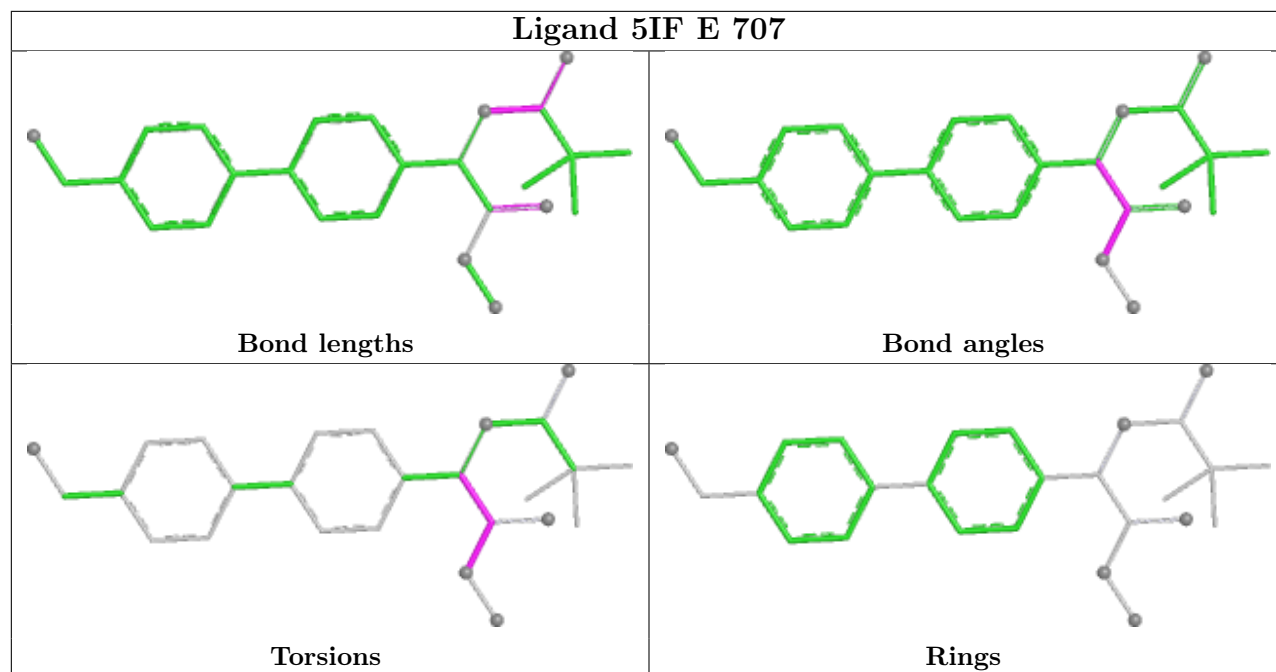
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	704	SO4	1	0
4	I	704	1PE	1	0
5	E	707	5IF	1	0
4	E	706	1PE	1	0
5	C	707	5IF	1	0
4	C	705	1PE	1	0
2	E	701	CO3	1	0
5	I	705	5IF	1	0
2	F	701	CO3	1	0
2	I	701	CO3	1	0
5	H	705	5IF	1	0
5	K	706	5IF	1	0
2	H	701	CO3	1	0
2	K	701	CO3	1	0
2	C	701	CO3	1	0
4	A	704	1PE	1	0
5	F	705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

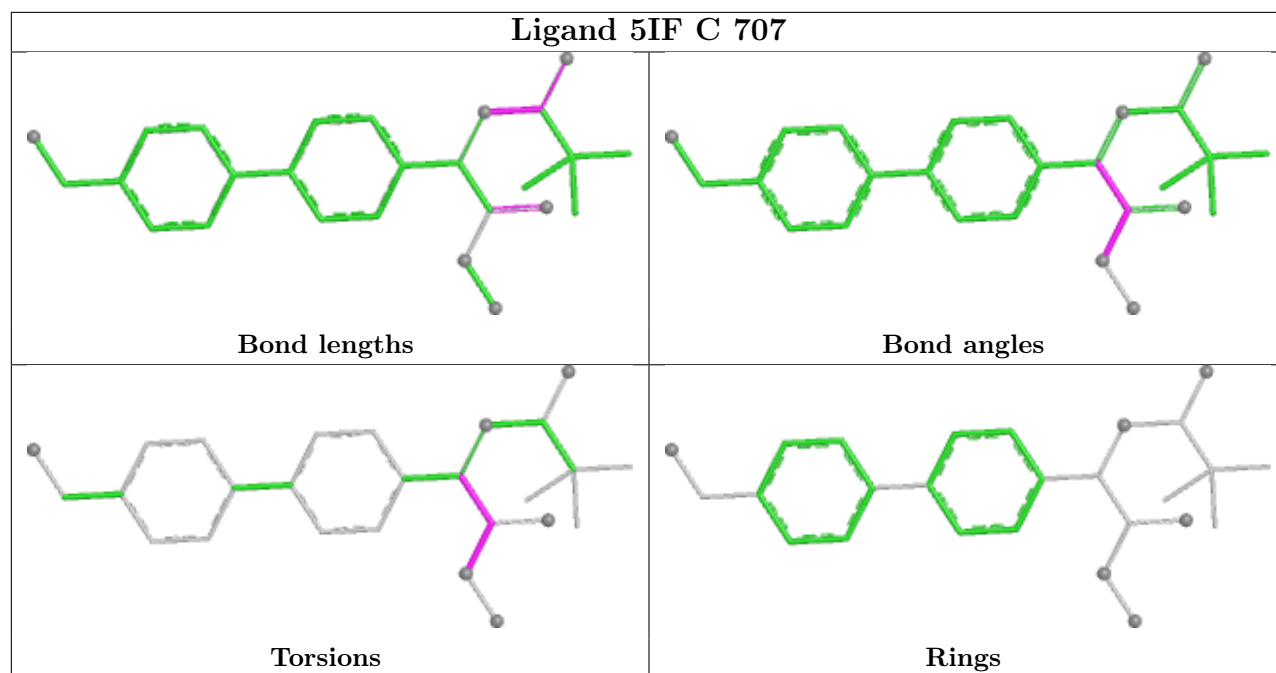
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

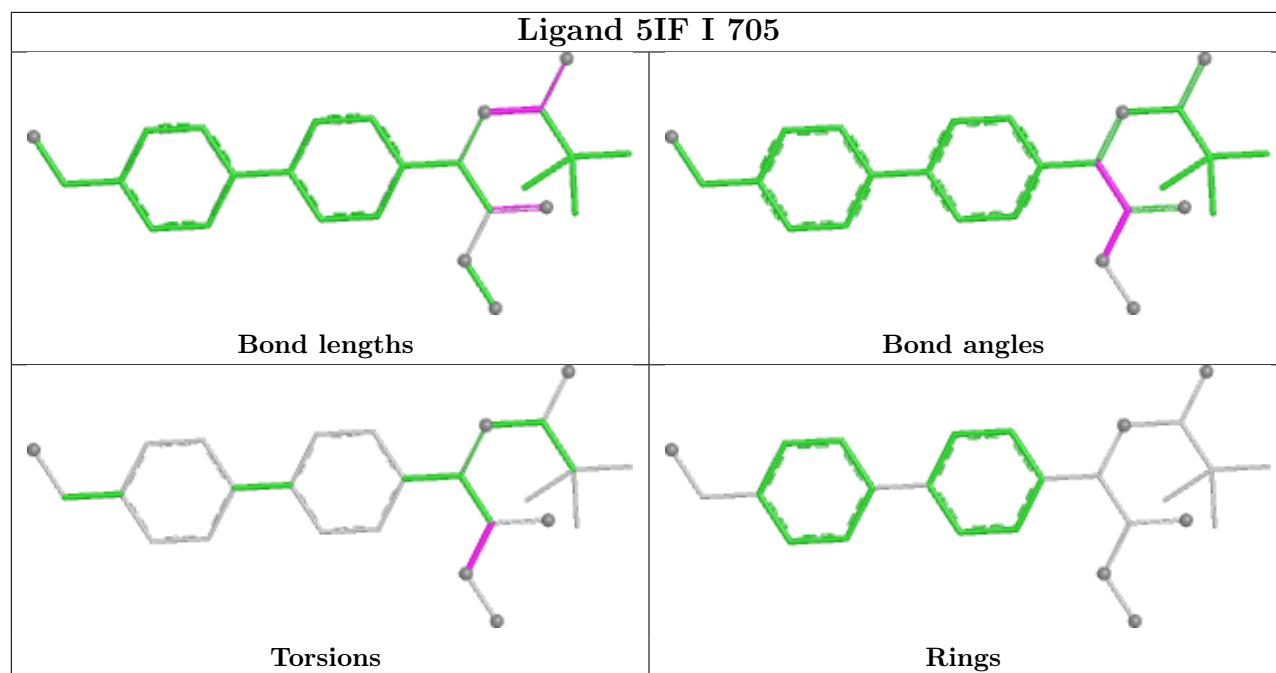
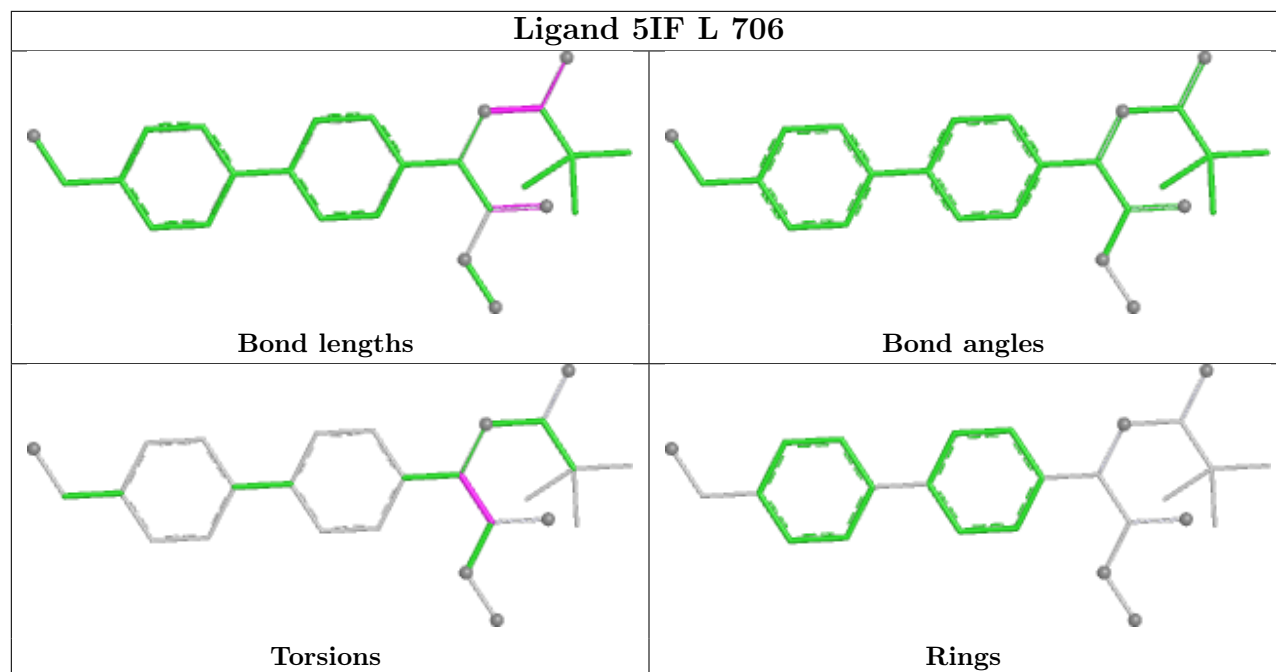


Ligand 5IF E 707

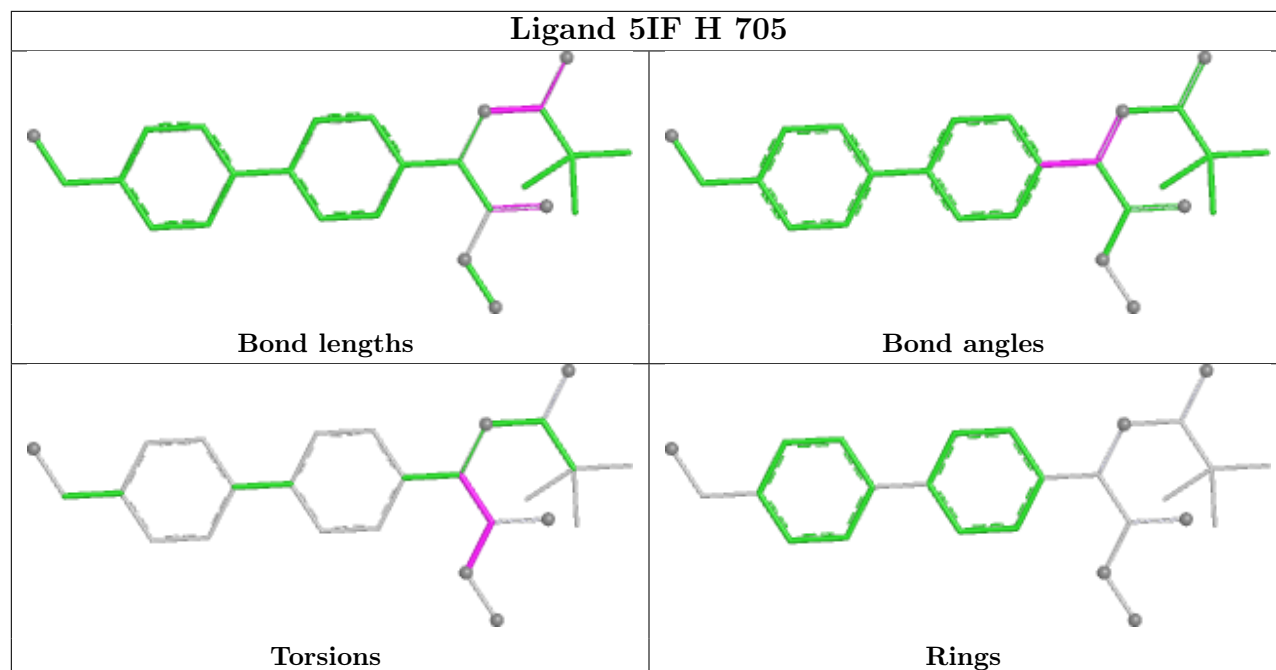


Ligand 5IF C 707

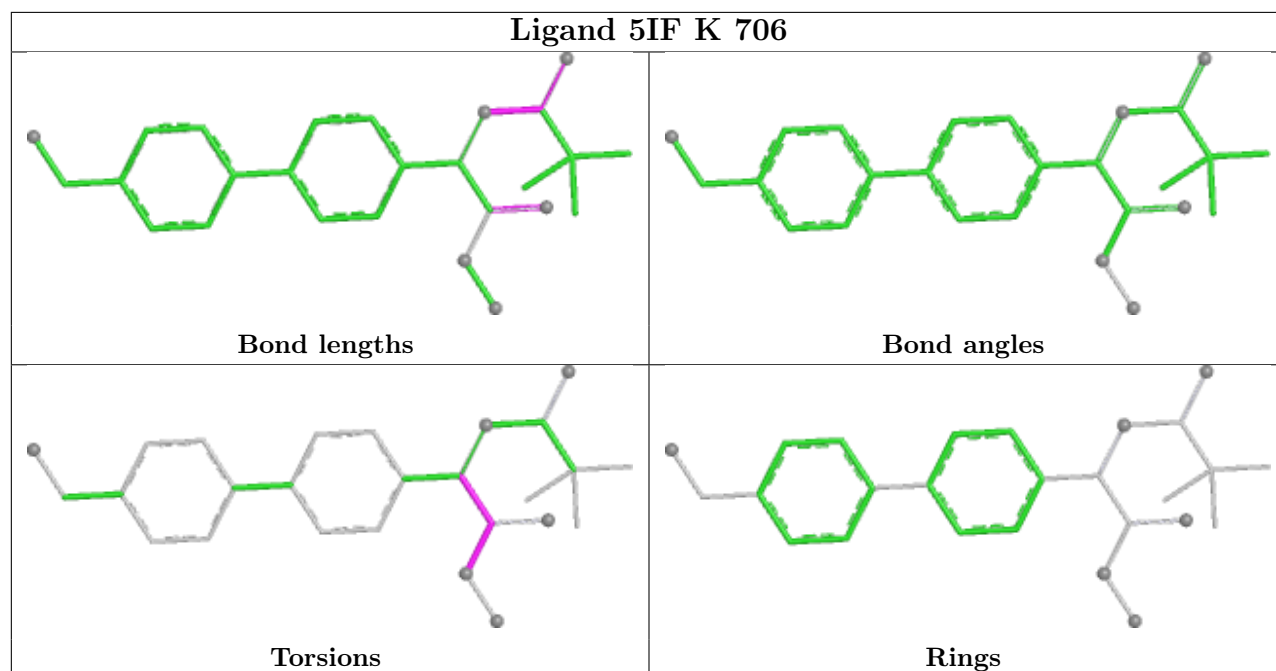


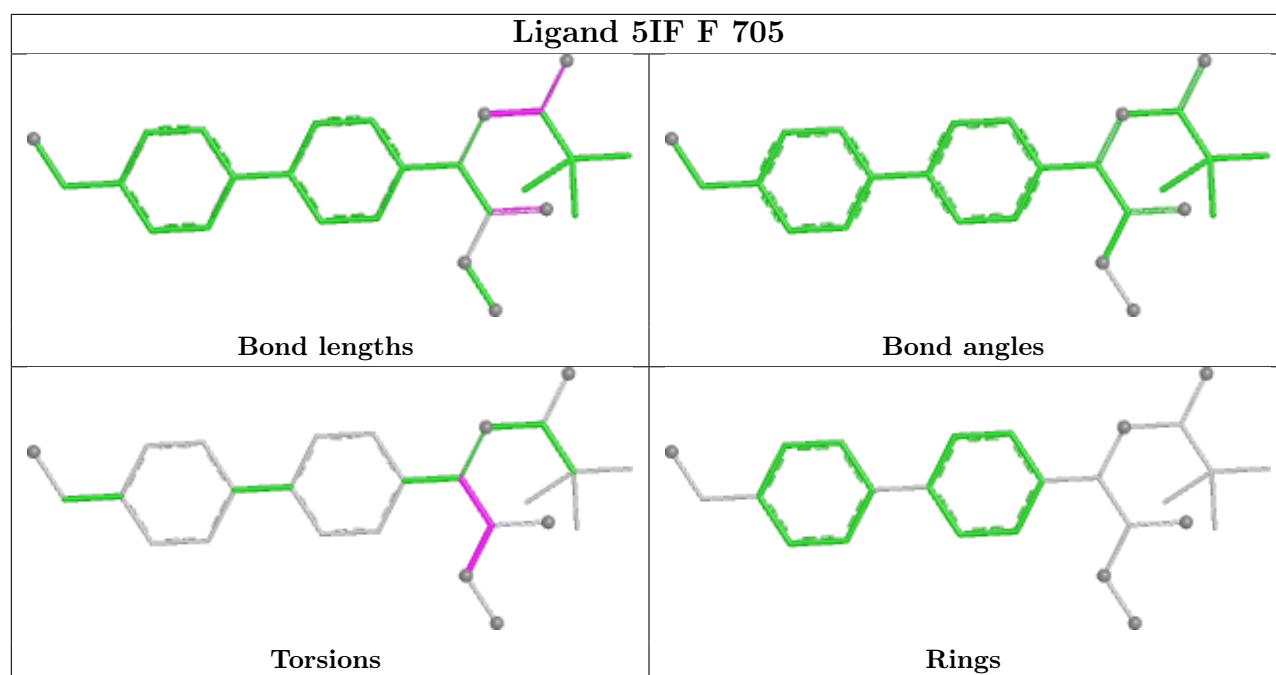
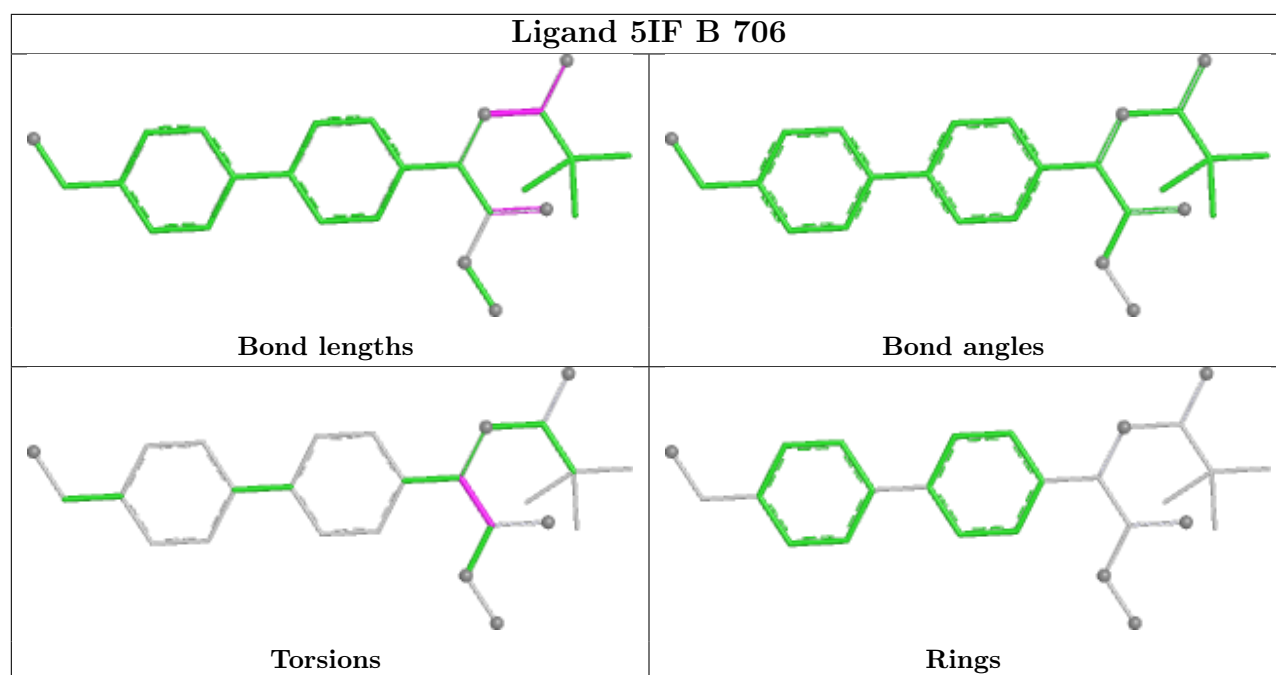


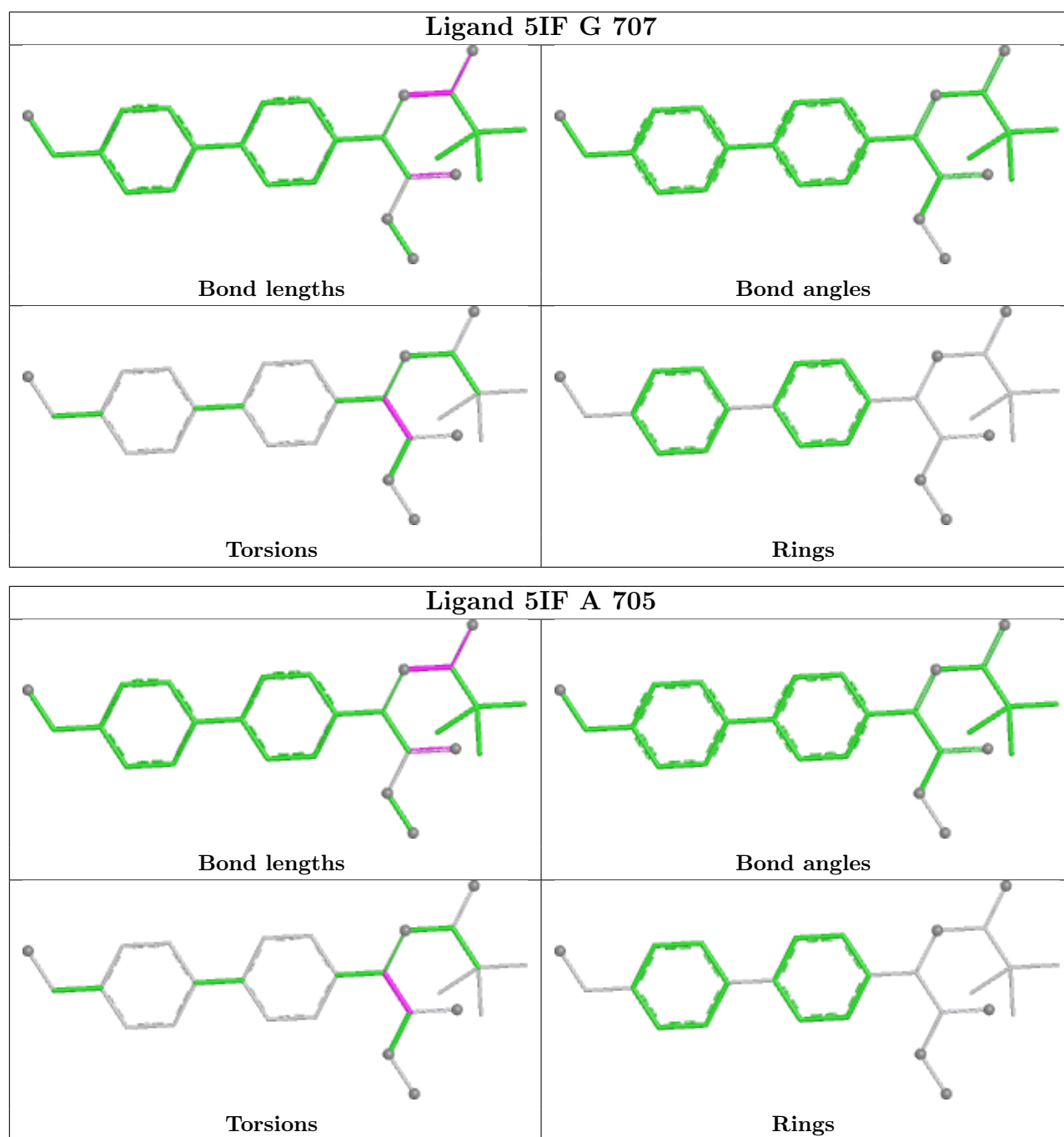
Ligand 5IF H 705



Ligand 5IF K 706







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	519/527 (98%)	-0.16	4 (0%)	82 80	23, 39, 57, 71	1 (0%)
1	B	518/527 (98%)	0.38	30 (5%)	29 25	27, 46, 90, 99	0
1	C	518/527 (98%)	-0.01	11 (2%)	63 59	27, 40, 64, 86	0
1	D	513/527 (97%)	-0.15	2 (0%)	88 86	29, 39, 55, 74	0
1	E	511/527 (96%)	-0.08	1 (0%)	91 89	32, 40, 55, 81	0
1	F	510/527 (96%)	0.27	13 (2%)	58 54	32, 45, 78, 96	0
1	G	519/527 (98%)	-0.19	2 (0%)	88 86	25, 37, 59, 74	1 (0%)
1	H	518/527 (98%)	0.15	28 (5%)	31 27	26, 39, 82, 94	0
1	I	518/527 (98%)	-0.07	10 (1%)	66 62	24, 37, 67, 83	0
1	J	516/527 (97%)	-0.17	9 (1%)	69 65	28, 36, 52, 98	0
1	K	512/527 (97%)	-0.12	5 (0%)	79 76	27, 38, 53, 69	0
1	L	510/527 (96%)	0.16	8 (1%)	70 67	29, 43, 73, 86	0
All	All	6182/6324 (97%)	0.00	123 (1%)	65 61	23, 40, 71, 99	2 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	603	ASP	5.6
1	J	260	ASN	5.4
1	H	549	SER	5.3
1	J	603	ASP	4.2
1	C	603	ASP	3.9
1	J	124	GLU	3.8
1	H	259	VAL	3.8
1	B	272	ASN	3.8
1	L	219	LEU	3.7
1	B	104	ASN	3.6
1	G	603	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	H	272	ASN	3.5
1	J	123	VAL	3.5
1	I	196	ALA	3.5
1	J	259	VAL	3.4
1	H	167	VAL	3.4
1	F	227	GLU	3.3
1	L	603	ASP	3.2
1	K	511	ASN	3.1
1	B	259	VAL	3.1
1	I	603	ASP	3.1
1	B	258	ASN	3.1
1	H	510	ILE	3.1
1	K	104	ASN	3.0
1	I	364	ASP	3.0
1	B	274	ALA	2.9
1	G	85	ALA	2.9
1	K	256	ASP	2.9
1	H	157	LEU	2.9
1	L	121	CYS	2.9
1	C	196	ALA	2.9
1	A	603	ASP	2.9
1	I	274	ALA	2.8
1	F	603	ASP	2.8
1	H	603	ASP	2.8
1	B	273	ASN	2.8
1	J	258	ASN	2.8
1	B	121	CYS	2.8
1	K	255	THR	2.7
1	B	197	ASP	2.7
1	I	195	VAL	2.7
1	H	118	LYS	2.7
1	J	262	GLU	2.7
1	F	181	ASN	2.7
1	F	362	LYS	2.6
1	B	157	LEU	2.6
1	F	219	LEU	2.6
1	I	121	CYS	2.6
1	L	153	VAL	2.6
1	B	603	ASP	2.6
1	C	547	ILE	2.6
1	B	175	PHE	2.5
1	L	156	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	118	LYS	2.5
1	B	549	SER	2.5
1	H	178	PHE	2.5
1	F	144	ILE	2.5
1	C	549	SER	2.5
1	C	87	GLU	2.4
1	H	125	GLU	2.4
1	H	138	GLU	2.4
1	J	125	GLU	2.4
1	B	167	VAL	2.4
1	B	141	PRO	2.4
1	H	156	PHE	2.4
1	C	120	GLY	2.4
1	B	178	PHE	2.4
1	B	511	ASN	2.4
1	A	552	LYS	2.4
1	E	362	LYS	2.4
1	H	550	SER	2.3
1	C	118	LYS	2.3
1	H	133	ASN	2.3
1	C	124	GLU	2.3
1	H	152	GLN	2.3
1	C	364	ASP	2.3
1	B	257	LYS	2.3
1	F	360	LYS	2.3
1	B	196	ALA	2.3
1	H	181	ASN	2.3
1	I	120	GLY	2.3
1	H	122	ASN	2.2
1	F	550	SER	2.2
1	B	602	ASN	2.2
1	B	125	GLU	2.2
1	B	160	GLU	2.2
1	H	175	PHE	2.2
1	B	219	LEU	2.2
1	A	85	ALA	2.2
1	I	272	ASN	2.2
1	B	120	GLY	2.2
1	I	117	ILE	2.2
1	A	550	SER	2.2
1	H	124	GLU	2.2
1	B	182	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	365	VAL	2.1
1	C	181	ASN	2.1
1	H	511	ASN	2.1
1	B	144	ILE	2.1
1	H	160	GLU	2.1
1	F	141	PRO	2.1
1	L	218	LYS	2.1
1	B	156	PHE	2.1
1	C	515	GLN	2.1
1	H	134	ASN	2.1
1	K	136	GLY	2.1
1	F	138	GLU	2.1
1	H	141	PRO	2.1
1	B	176	TYR	2.1
1	H	120	GLY	2.1
1	L	126	GLY	2.1
1	H	155	GLU	2.1
1	H	176	TYR	2.1
1	I	197	ASP	2.1
1	H	194	SER	2.1
1	H	195	VAL	2.0
1	F	262	GLU	2.0
1	B	364	ASP	2.0
1	F	132	VAL	2.0
1	B	138	GLU	2.0
1	J	602	ASN	2.0
1	L	120	GLY	2.0
1	D	254	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
6	SO4	E	705	5/5	0.68	0.13	77,81,89,92	0
6	SO4	C	704	5/5	0.71	0.10	87,87,97,100	0
4	1PE	L	705	10/16	0.74	0.16	55,62,69,72	0
4	1PE	C	706	8/16	0.78	0.16	46,53,64,66	0
6	SO4	G	705	5/5	0.82	0.17	59,60,75,83	0
6	SO4	G	706	5/5	0.82	0.30	51,56,74,76	0
4	1PE	C	705	8/16	0.83	0.16	46,54,58,65	0
6	SO4	K	704	5/5	0.86	0.20	51,58,70,72	0
4	1PE	B	705	10/16	0.87	0.13	54,62,67,68	0
4	1PE	I	704	10/16	0.87	0.12	39,46,55,56	0
6	SO4	F	704	5/5	0.88	0.21	59,63,72,73	0
4	1PE	K	705	13/16	0.90	0.10	41,50,58,59	0
4	1PE	A	704	10/16	0.90	0.11	39,48,54,55	0
5	5IF	H	705	26/26	0.91	0.10	28,34,46,49	0
5	5IF	K	706	26/26	0.91	0.11	31,36,44,54	0
5	5IF	C	707	26/26	0.91	0.10	28,35,41,46	0
5	5IF	E	707	26/26	0.91	0.11	27,39,48,59	0
5	5IF	I	705	26/26	0.92	0.09	26,32,44,46	0
4	1PE	E	706	10/16	0.92	0.09	42,52,57,64	0
2	CO3	E	701	4/4	0.93	0.12	34,36,39,43	0
4	1PE	J	704	10/16	0.93	0.09	43,47,55,62	0
5	5IF	F	705	26/26	0.93	0.09	32,37,51,53	0
5	5IF	D	704	26/26	0.94	0.08	28,33,42,53	0
5	5IF	B	706	26/26	0.94	0.09	28,37,42,51	0
2	CO3	L	701	4/4	0.94	0.08	31,31,33,36	0
5	5IF	L	706	26/26	0.94	0.09	25,35,43,48	0
5	5IF	G	707	26/26	0.94	0.09	26,33,40,47	0
2	CO3	C	701	4/4	0.95	0.07	32,34,37,37	0
6	SO4	G	704	5/5	0.95	0.11	39,42,44,51	5
2	CO3	A	701	4/4	0.95	0.11	33,36,40,45	0
2	CO3	K	701	4/4	0.95	0.08	32,34,36,38	0
5	5IF	J	705	26/26	0.95	0.08	27,31,39,50	0
2	CO3	I	701	4/4	0.96	0.07	30,31,31,32	0
2	CO3	G	701	4/4	0.96	0.06	31,32,34,36	0
5	5IF	A	705	26/26	0.96	0.07	29,36,44,53	0
2	CO3	B	701	4/4	0.97	0.06	34,35,35,39	0
2	CO3	J	701	4/4	0.97	0.09	31,33,34,36	0
2	CO3	F	701	4/4	0.97	0.06	33,36,36,38	0
2	CO3	D	701	4/4	0.97	0.04	33,35,36,37	0
6	SO4	B	704	5/5	0.98	0.05	28,31,37,37	0
2	CO3	H	701	4/4	0.98	0.04	29,33,34,35	0

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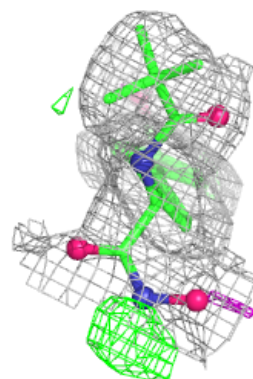
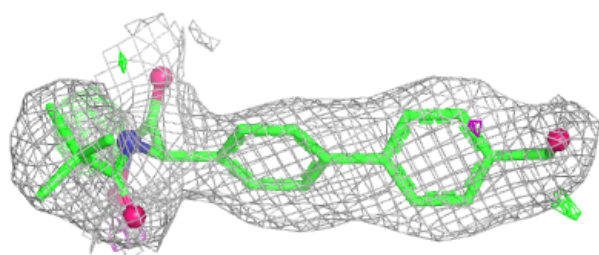
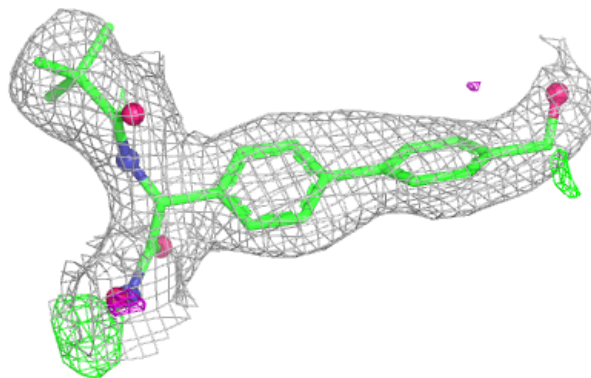
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	SO4	E	704	5/5	0.98	0.06	35,39,41,49	0
6	SO4	L	704	5/5	0.98	0.05	29,35,42,42	0
3	ZN	K	702	1/1	0.99	0.02	38,38,38,38	0
3	ZN	K	703	1/1	0.99	0.03	38,38,38,38	0
3	ZN	A	702	1/1	0.99	0.02	39,39,39,39	0
3	ZN	B	703	1/1	0.99	0.02	38,38,38,38	0
3	ZN	C	702	1/1	0.99	0.03	37,37,37,37	0
3	ZN	E	702	1/1	0.99	0.03	41,41,41,41	0
3	ZN	E	703	1/1	0.99	0.02	39,39,39,39	0
3	ZN	G	702	1/1	0.99	0.02	39,39,39,39	0
3	ZN	H	702	1/1	0.99	0.03	36,36,36,36	0
6	SO4	H	704	5/5	0.99	0.05	30,30,32,35	0
3	ZN	H	703	1/1	0.99	0.02	35,35,35,35	0
3	ZN	J	703	1/1	0.99	0.02	32,32,32,32	0
3	ZN	I	703	1/1	1.00	0.01	31,31,31,31	0
3	ZN	J	702	1/1	1.00	0.01	34,34,34,34	0
3	ZN	A	703	1/1	1.00	0.01	36,36,36,36	0
3	ZN	B	702	1/1	1.00	0.02	39,39,39,39	0
3	ZN	F	702	1/1	1.00	0.02	38,38,38,38	0
3	ZN	L	702	1/1	1.00	0.02	37,37,37,37	0
3	ZN	L	703	1/1	1.00	0.02	34,34,34,34	0
3	ZN	F	703	1/1	1.00	0.01	35,35,35,35	0
3	ZN	C	703	1/1	1.00	0.01	34,34,34,34	0
3	ZN	G	703	1/1	1.00	0.01	31,31,31,31	0
3	ZN	D	702	1/1	1.00	0.02	38,38,38,38	0
3	ZN	D	703	1/1	1.00	0.01	38,38,38,38	0
3	ZN	I	702	1/1	1.00	0.02	35,35,35,35	0

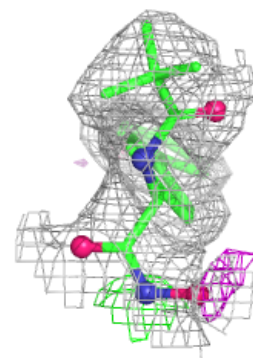
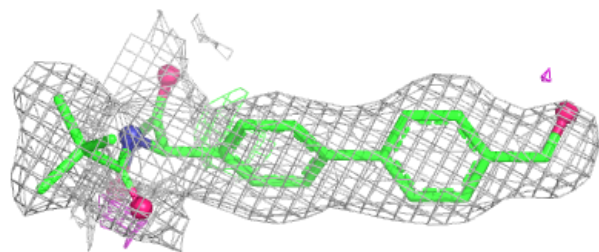
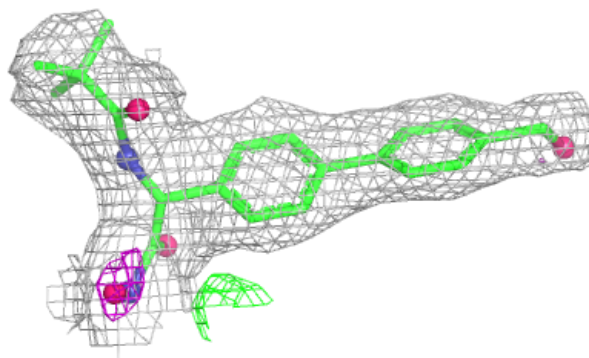
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5IF H 705:

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

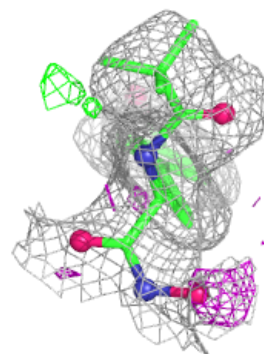
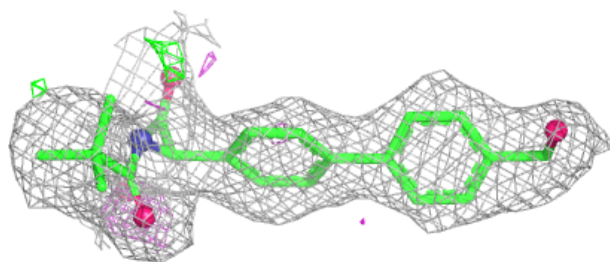
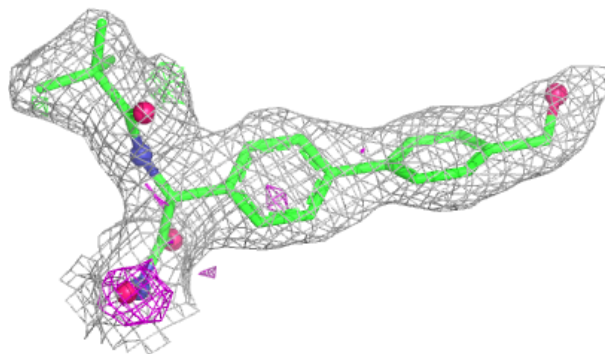
**Electron density around 5IF K 706:**

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

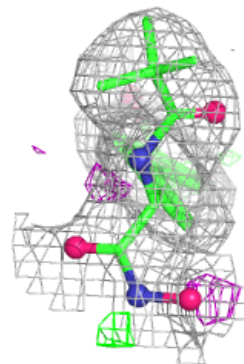
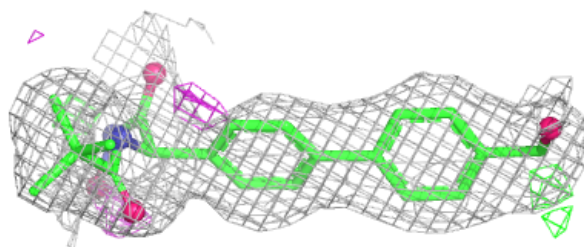
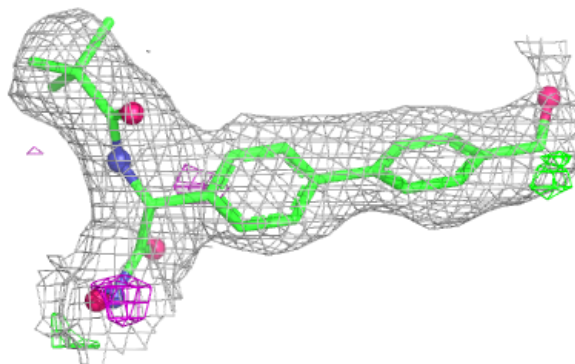


Electron density around 5IF C 707:

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

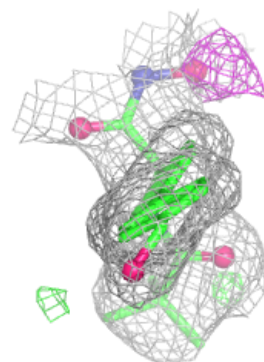
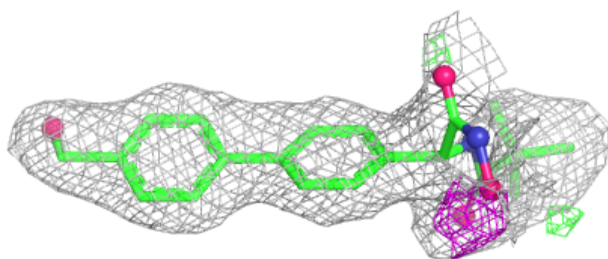
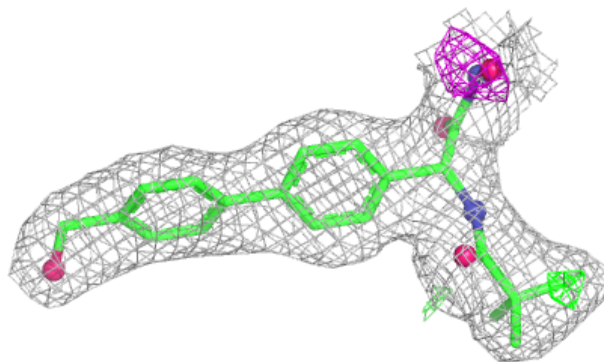
**Electron density around 5IF E 707:**

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

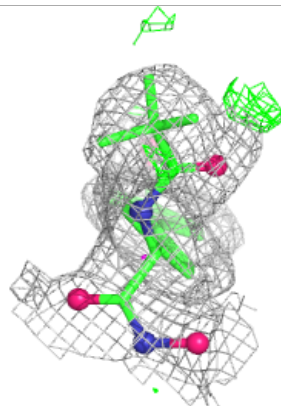
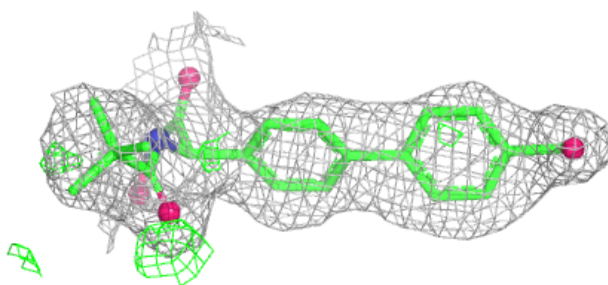
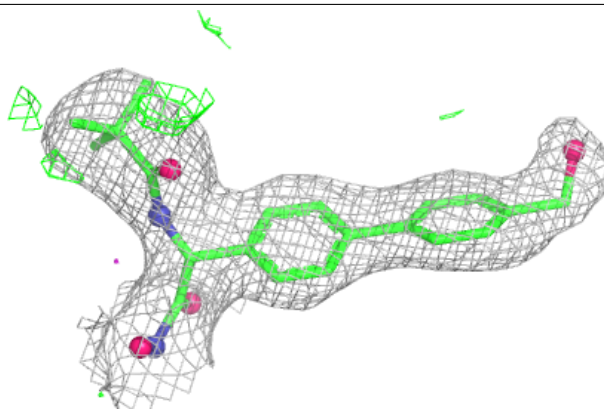


Electron density around 5IF I 705:

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

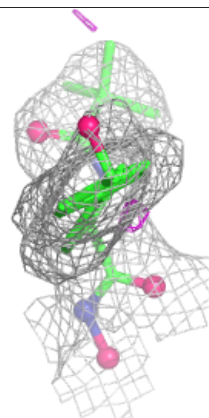
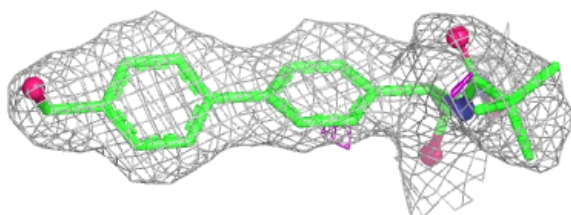
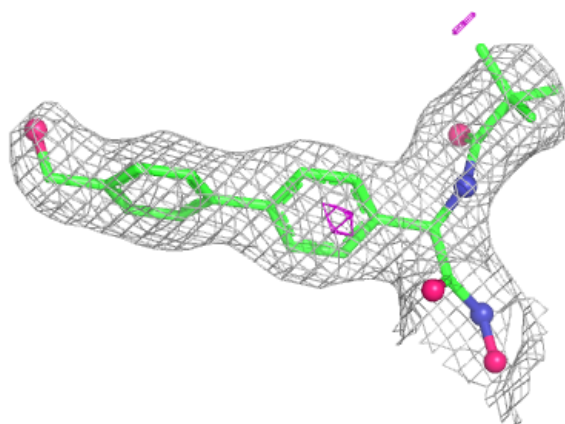
**Electron density around 5IF F 705:**

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

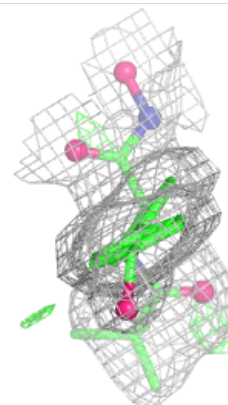
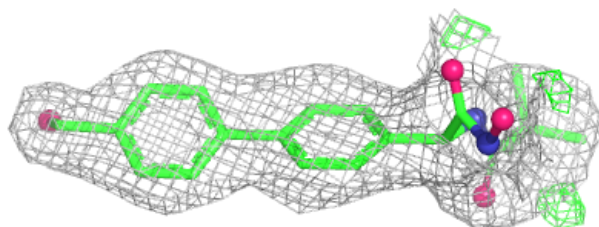
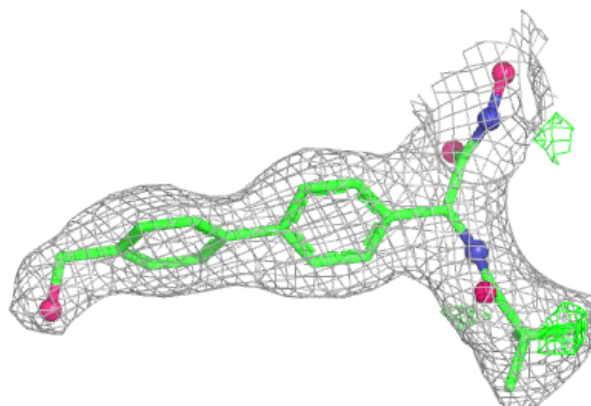


Electron density around 5IF D 704:

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

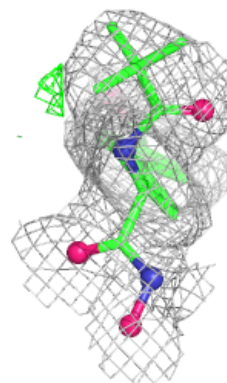
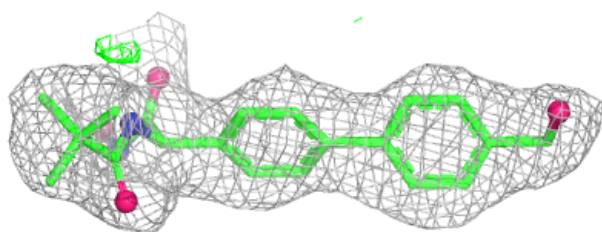
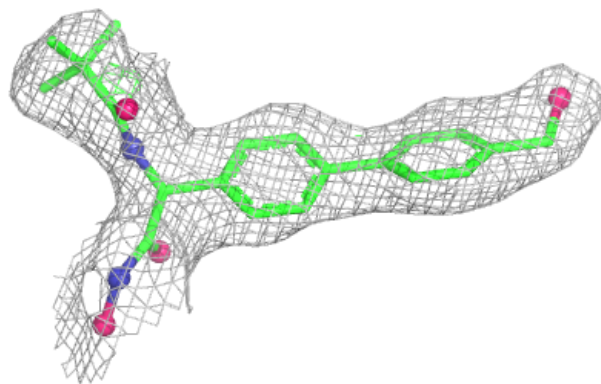
**Electron density around 5IF B 706:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

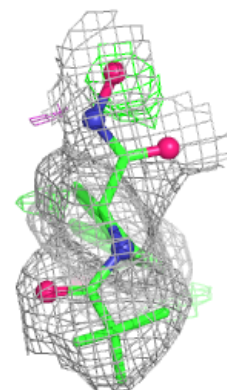
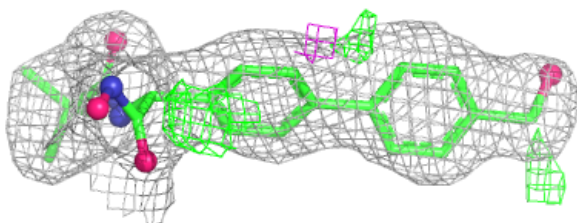
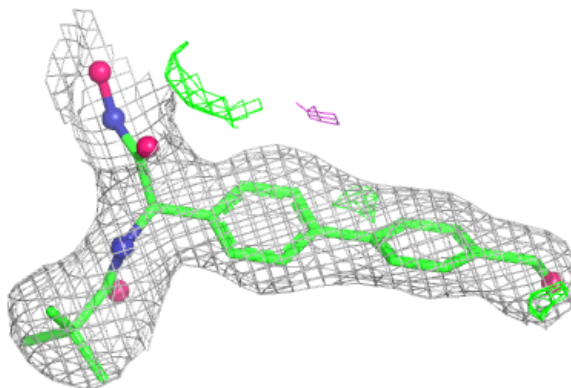


Electron density around 5IF L 706:

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

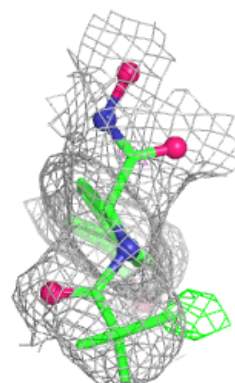
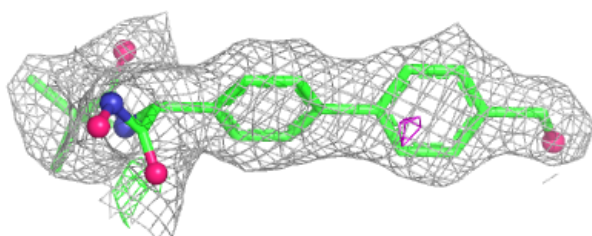
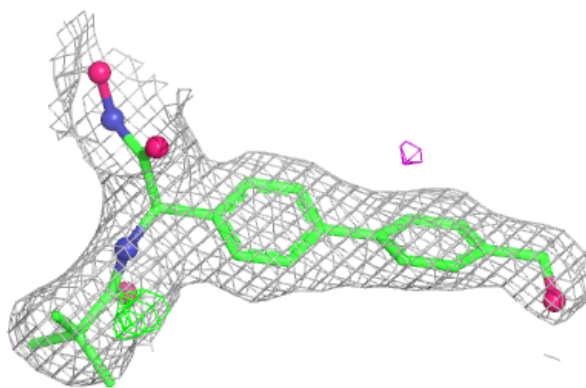
**Electron density around 5IF G 707:**

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

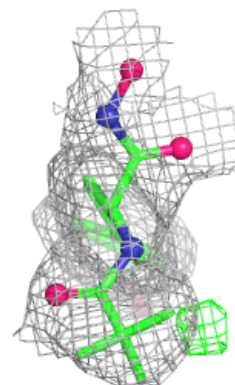
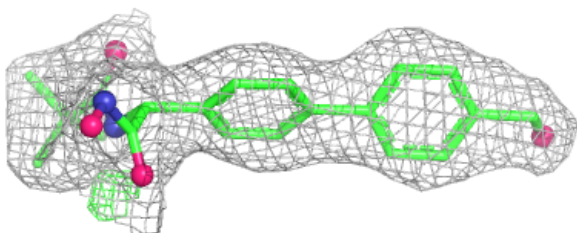
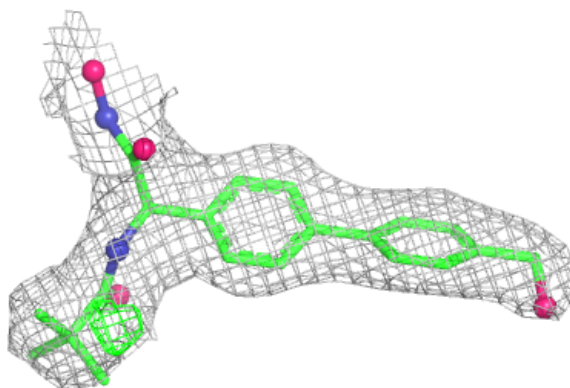


Electron density around 5IF J 705:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.