



Full wwPDB X-ray Structure Validation Report i

Apr 15, 2024 – 05:54 PM EDT

PDB ID : 8SVM
Title : Plasmodium falciparum M17 aminopeptidase bound to MMV1557817
Authors : McGowan, S.; Drinkwater, N.
Deposited on : 2023-05-17
Resolution : 2.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>
with specific help available everywhere you see the i symbol.

The types of validation reports are described at
<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) 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 : 2.36.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.1

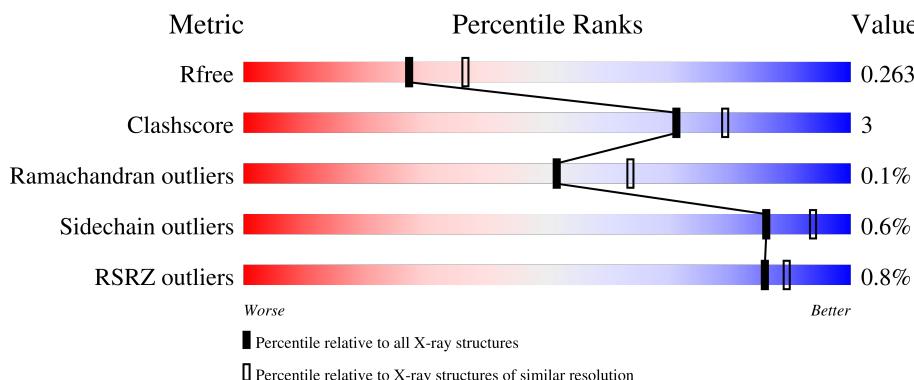
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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.



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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	1PE	L	705	-	-	-	X
5	1PE	L	706	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 50860 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 Leucine aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
1	A	519	Total	C 3962	N 2544	O 637	S 761	20	0	1	0
1	B	517	Total	C 3913	N 2511	O 636	S 746	20	0	1	0
1	C	516	Total	C 3961	N 2543	O 639	S 758	21	0	1	0
1	D	514	Total	C 3917	N 2521	O 634	S 742	20	0	0	0
1	E	509	Total	C 3904	N 2509	O 631	S 745	19	0	0	0
1	F	512	Total	C 3869	N 2487	O 622	S 740	20	0	1	0
1	G	519	Total	C 3971	N 2549	O 640	S 762	20	0	1	0
1	H	517	Total	C 3910	N 2513	O 635	S 742	20	0	1	0
1	I	518	Total	C 3964	N 2548	O 638	S 756	22	0	2	0
1	J	514	Total	C 3945	N 2537	O 637	S 751	20	0	0	0
1	K	509	Total	C 3894	N 2508	O 626	S 741	19	0	0	0
1	L	512	Total	C 3861	N 2479	O 624	S 739	19	0	0	0

There are 108 discrepancies between the modelled and reference sequences:

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

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

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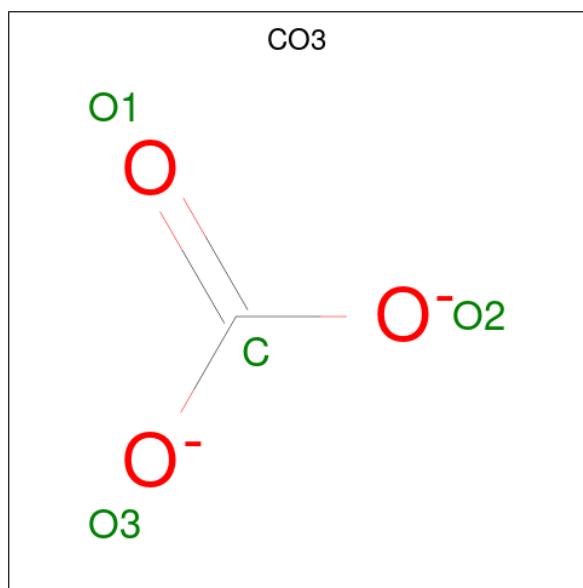
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F	546	GLN	ASN	engineered mutation	UNP Q8IL11
F	606	HIS	-	expression tag	UNP Q8IL11
F	607	HIS	-	expression tag	UNP Q8IL11
F	608	HIS	-	expression tag	UNP Q8IL11
F	609	HIS	-	expression tag	UNP Q8IL11
F	610	HIS	-	expression tag	UNP Q8IL11
F	611	HIS	-	expression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

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

- Molecule 2 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

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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 (three-letter code: ZN) (formula: Zn).

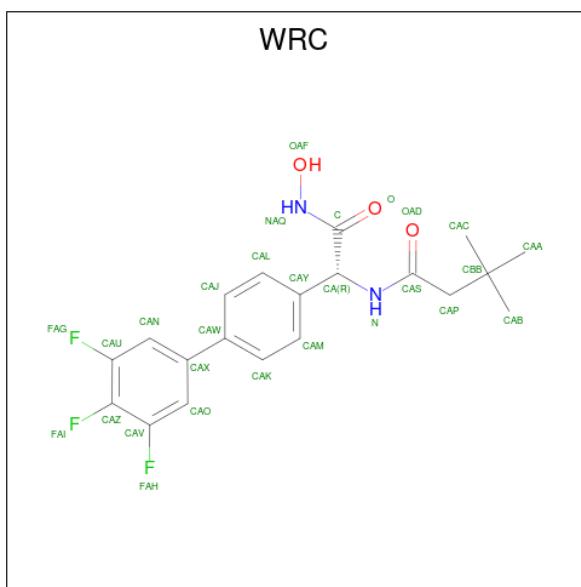
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Zn 2 2	0	0
3	B	2	Total Zn 2 2	0	0
3	C	2	Total Zn 2 2	0	0
3	D	2	Total Zn 2 2	0	0
3	E	2	Total Zn 2 2	0	0
3	F	2	Total Zn 2 2	0	0
3	G	2	Total Zn 2 2	0	0
3	H	2	Total Zn 2 2	0	0
3	I	2	Total Zn 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	2	Total 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 N-[(1R)-2-(hydroxyamino)-2-oxo-1-(3',4',5'-trifluoro[1,1'-biphenyl]-4-yl)ethyl]-3,3-dimethylbutanamide (three-letter code: WRC) (formula: C₂₀H₂₁F₃N₂O₃) (labeled as "Ligand of Interest" by depositor).



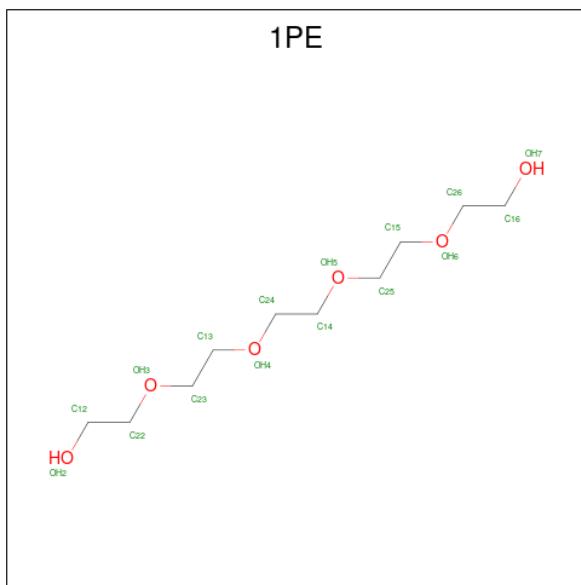
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 28	C 20	F 3	N 2	O 3	0
4	B	1	Total 28	C 20	F 3	N 2	O 3	0
4	C	1	Total 28	C 20	F 3	N 2	O 3	0
4	D	1	Total 28	C 20	F 3	N 2	O 3	0
4	E	1	Total 28	C 20	F 3	N 2	O 3	0
4	F	1	Total 28	C 20	F 3	N 2	O 3	0
4	G	1	Total 28	C 20	F 3	N 2	O 3	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	H	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	I	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	J	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	K	1	Total	C	F	N	O	0	0
			28	20	3	2	3		
4	L	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

- Molecule 5 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			9	6	3		
5	A	1	Total	C	O	0	0
			6	4	2		
5	A	1	Total	C	O	0	0
			15	10	5		
5	B	1	Total	C	O	0	0
			10	7	3		
5	B	1	Total	C	O	0	0
			10	7	3		
5	C	1	Total	C	O	0	0
			15	10	5		

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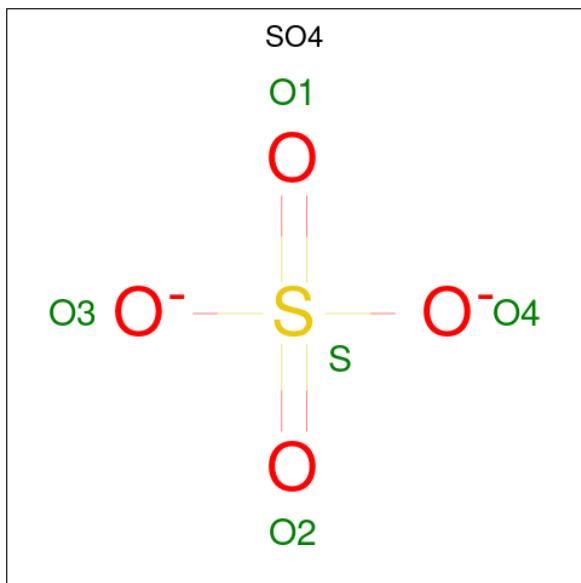
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 11 8 3	0	0
5	C	1	Total C O 7 5 2	0	0
5	D	1	Total C O 11 7 4	0	0
5	D	1	Total C O 10 6 4	0	0
5	E	1	Total C O 10 6 4	0	0
5	E	1	Total C O 12 8 4	0	0
5	E	1	Total C O 6 4 2	0	0
5	F	1	Total C O 10 6 4	0	0
5	F	1	Total C O 12 8 4	0	0
5	G	1	Total C O 9 6 3	0	0
5	G	1	Total C O 12 8 4	0	0
5	H	1	Total C O 10 7 3	0	0
5	H	1	Total C O 10 7 3	0	0
5	I	1	Total C O 13 9 4	0	0
5	I	1	Total C O 9 6 3	0	0
5	I	1	Total C O 9 6 3	0	0
5	J	1	Total C O 10 7 3	0	0
5	J	1	Total C O 10 7 3	0	0
5	K	1	Total C O 12 8 4	0	0
5	L	1	Total C O 10 6 4	0	0
5	L	1	Total C O 10 6 4	0	0

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	F	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	J	1	Total O S 5 4 1	0	0

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

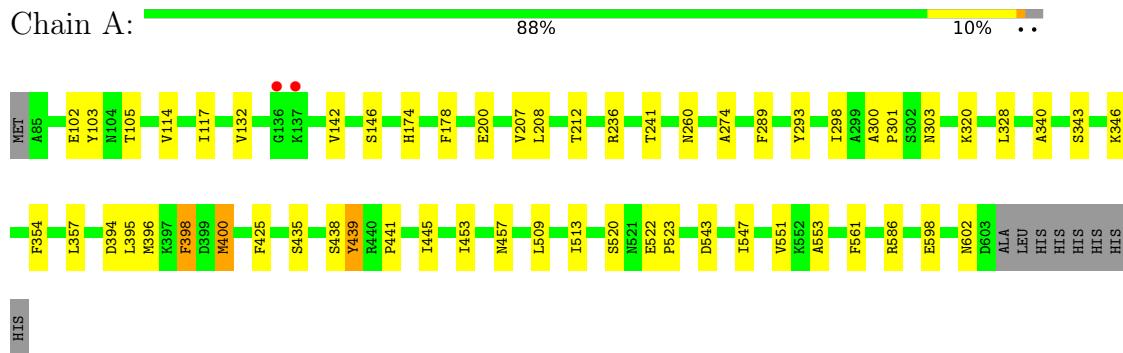
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	282	Total O 282 282	0	0
7	B	229	Total O 229 229	0	0
7	C	254	Total O 254 254	0	0
7	D	246	Total O 246 246	0	0
7	E	281	Total O 281 281	0	0
7	F	225	Total O 225 225	0	0
7	G	270	Total O 270 270	0	0
7	H	219	Total O 219 219	0	0
7	I	281	Total O 281 281	0	0
7	J	271	Total O 271 271	0	0
7	K	254	Total O 254 254	0	0
7	L	221	Total O 221 221	0	0

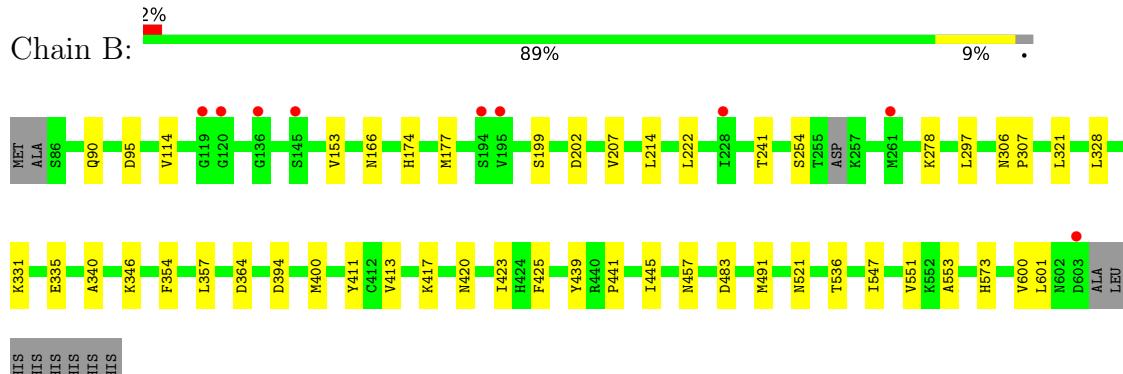
3 Residue-property plots [i](#)

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.

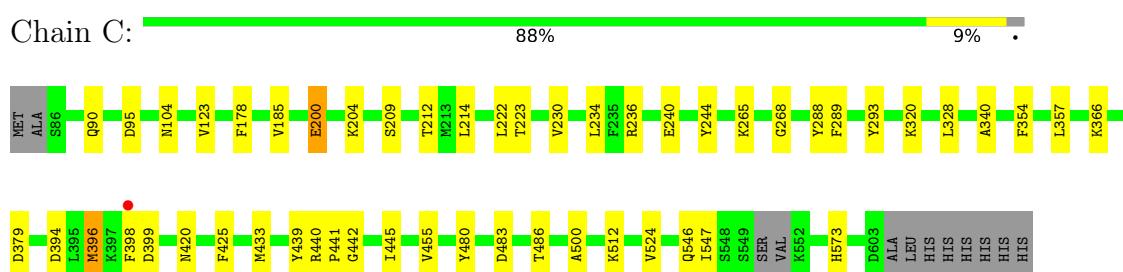
- Molecule 1: Leucine aminopeptidase

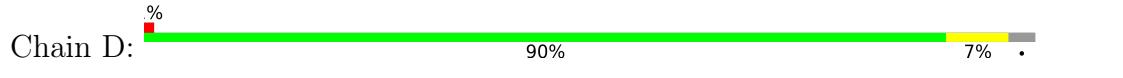


- Molecule 1: Leucine aminopeptidase



- #### • Molecule 1: Leucine aminopeptidase

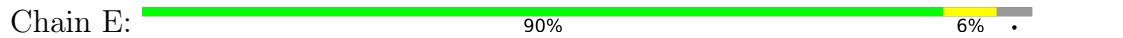




The diagram illustrates the SARS-CoV-2 spike protein structure. It consists of two main domains: S1 and S2. S1 is primarily green and contains the RBD (Receptor-Binding Domain), which is highly conserved. S2 is primarily yellow and contains the FP (Fusion Peptide). A cleavage site (C) is indicated between the two domains. Several mutations are shown as colored bars above the protein:

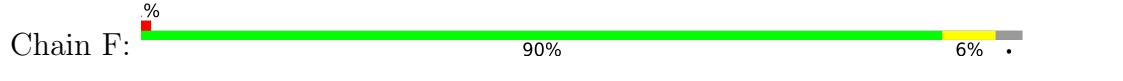
- MET**: Located at the N-terminus of S1.
- A85**: Located in the S1 domain.
- V114**: Located in the S1 domain.
- E124**: Located in the S1 domain.
- V132**: Located in the S1 domain.
- G136**: Located in the S1 domain.
- V142**: Located in the S1 domain.
- K143**: Located in the S1 domain.
- D150**: Located in the S1 domain.
- I144**: Located in the S1 domain.
- E155**: Located in the S1 domain.
- F156**: Located in the S1 domain.
- L157**: Located in the S1 domain.
- K164**: Located in the S1 domain.
- F175**: Located in the S1 domain.
- N179**: Located in the S1 domain.
- V195**: Located in the S1 domain.
- V207**: Located in the S1 domain.
- T241**: Located in the S1 domain.
- S264**: Located in the S2 domain.
- Y309**: Located in the S1 domain.
- L440**: Located in the S1 domain.
- F425**: Located in the S1 domain.
- P441**: Located in the S1 domain.
- I445**: Located in the S1 domain.
- T486**: Located in the S1 domain.
- S494**: Located in the S1 domain.
- L495**: Located in the S1 domain.
- I513**: Located in the S1 domain.
- S520**: Located in the S1 domain.
- Y533**: Located in the S1 domain.
- T536**: Located in the S1 domain.
- V551**: Located in the S1 domain.
- E598**: Located in the S1 domain.
- D603**: Located in the S1 domain.
- A614**: Located in the S1 domain.
- L615**: Located in the S1 domain.
- H617**: Located in the S1 domain.
- H618**: Located in the S1 domain.
- V620**: Located in the S1 domain.
- H620**: Located in the S1 domain.
- M621**: Located in the S1 domain.
- A274**: Located in the S2 domain.
- I298**: Located in the S2 domain.
- A399**: Located in the S2 domain.
- A300**: Located in the S2 domain.
- P301**: Located in the S2 domain.
- R320**: Located in the S2 domain.
- L328**: Located in the S2 domain.
- A340**: Located in the S2 domain.
- F354**: Located in the S2 domain.
- L357**: Located in the S2 domain.
- D394**: Located in the S2 domain.

- Molecule 1: Leucine aminopeptidase



Detailed description: This figure is a horizontal bar chart representing the SARS-CoV-2 genome. The genome is divided into segments by vertical lines. Each segment's color corresponds to a specific amino acid change (mutation). Yellow segments represent mutations R, P, I, D, T, S, Q, H, E, and N. Green segments represent mutations V, K, A, and M. Red segments represent mutation F. Blue segments represent mutation G. A single red dot is positioned at the 1547th position from the start of the genome.

- Molecule 1: Leucine aminopeptidase

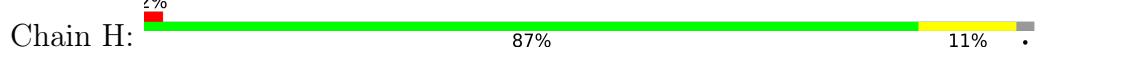


The diagram illustrates the structure of the human complement C1q domain. The domain is composed of 23 alpha-helices, labeled A1 to A23 from left to right. Several mutations are highlighted: V123 (red dot), K137 (red dot), E138 (red dot), F175 (red dot), A196 (red dot), H213 (red dot), L214 (red dot), N217 (red dot), I222 (red dot), T255 (green bar), and E262 (green bar). Below the helices, a color-coded scale indicates hydrophilicity: orange for hydrophobic, yellow for hydrophilic, and grey for intermediate. A large grey box covers the region between helices A196 and E262.

- Molecule 1: Leucine aminopeptidase



- Molecule 1: Leucine aminopeptidase

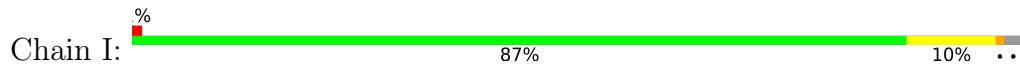


The diagram illustrates the human MET gene structure with various mutations marked by red dots. The gene is represented by a green horizontal bar with exons as vertical tick marks. Mutations are indicated by red dots at specific positions: L94, I110, I117, V132, E138, V142, K143, I144, S146, Q152, D159, K164, H174, F178, N179, D180, S194, V195, L198, L214, L222, V230, L234, Y244, S254, T255, ASP, K257, N273, T276, and K283.



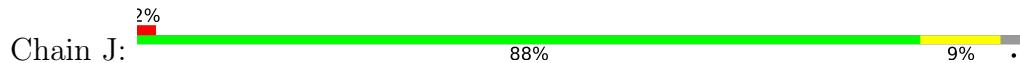
L601 N602 D603 ALA LEU HIS HIS HIS HIS HIS HIS HIS

- Molecule 1: Leucine aminopeptidase



L333 A340 F354

- Molecule 1: Leucine aminopeptidase



SIH

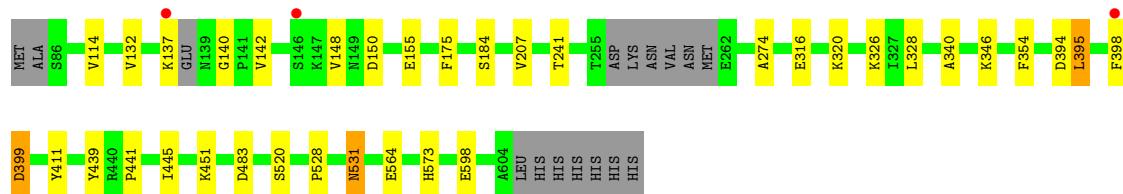
- Molecule 1: Leucine aminopeptidase



A340
Y341
F354

- Molecule 1: Leucine aminopeptidase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	174.20 Å 177.93 Å 229.76 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.30 49.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.00-2.30) 97.5 (49.02-2.30)	Depositor EDS
R_{merge}	0.33	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	2.02 (at 2.29 Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R , R_{free}	0.204 , 0.252 0.217 , 0.263	Depositor DCC
R_{free} test set	15208 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.0	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	50860	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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 42.85 % 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 1.9207e-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 i

5.1 Standard geometry i

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

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	0.26	1/4043 (0.0%)	0.38	0/5490
1	B	0.26	0/3993	0.39	0/5426
1	C	0.31	2/4041 (0.0%)	0.41	0/5480
1	D	0.27	1/3994 (0.0%)	0.40	0/5419
1	E	0.25	0/3980	0.39	0/5398
1	F	0.26	0/3949	0.41	1/5369 (0.0%)
1	G	0.26	0/4052	0.39	0/5498
1	H	0.37	3/3990 (0.1%)	0.44	1/5421 (0.0%)
1	I	0.32	2/4048 (0.0%)	0.41	0/5492
1	J	0.26	0/4022	0.39	0/5453
1	K	0.25	0/3970	0.39	0/5385
1	L	0.34	0/3937	0.45	1/5354 (0.0%)
All	All	0.29	9/48019 (0.0%)	0.40	3/65185 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	461	GLU	CD-OE2	-8.34	1.16	1.25
1	H	438	SER	CB-OG	-6.04	1.34	1.42
1	I	396[A]	MET	CA-C	5.79	1.68	1.52
1	I	396[B]	MET	CA-C	5.79	1.68	1.52
1	C	396[A]	MET	CA-C	5.46	1.67	1.52
1	C	396[B]	MET	CA-C	5.46	1.67	1.52
1	A	439	TYR	CZ-OH	-5.28	1.28	1.37
1	D	439	TYR	CE1-CZ	-5.03	1.32	1.38
1	H	461	GLU	CD-OE1	-5.01	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	440	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	F	137	LYS	CB-CA-C	-7.08	96.24	110.40
1	L	399	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3962	0	3865	35	0
1	B	3913	0	3789	29	0
1	C	3961	0	3893	31	0
1	D	3917	0	3840	22	0
1	E	3904	0	3836	20	0
1	F	3869	0	3733	22	0
1	G	3971	0	3881	31	0
1	H	3910	0	3791	34	0
1	I	3964	0	3888	44	0
1	J	3945	0	3893	30	0
1	K	3894	0	3828	29	0
1	L	3861	0	3721	24	0
2	A	4	0	0	0	0
2	B	4	0	0	0	0
2	C	4	0	0	0	0
2	D	4	0	0	0	0
2	E	4	0	0	0	0
2	F	4	0	0	0	0
2	G	4	0	0	0	0
2	H	4	0	0	0	0
2	I	4	0	0	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	28	0	0	0	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	28	0	0	0	0
4	E	28	0	0	0	0
4	F	28	0	0	1	0
4	G	28	0	0	1	0
4	H	28	0	0	0	0
4	I	28	0	0	0	0
4	J	28	0	0	0	0
4	K	28	0	0	0	0
4	L	28	0	0	0	0
5	A	30	0	33	2	0
5	B	20	0	20	0	0
5	C	33	0	37	1	0
5	D	21	0	26	1	0
5	E	28	0	30	2	0
5	F	22	0	27	3	0
5	G	21	0	22	3	0
5	H	20	0	20	2	0
5	I	31	0	34	4	0
5	J	20	0	20	1	0
5	K	12	0	14	1	0
5	L	30	0	39	2	0
6	A	10	0	0	1	0
6	C	10	0	0	1	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	G	15	0	0	1	0
6	J	5	0	0	0	0
6	K	5	0	0	0	0
6	L	5	0	0	0	0
7	A	282	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	229	0	0	5	0
7	C	254	0	0	3	0
7	D	246	0	0	1	0
7	E	281	0	0	1	0
7	F	225	0	0	1	0
7	G	270	0	0	4	0
7	H	219	0	0	1	0
7	I	281	0	0	1	0
7	J	271	0	0	3	0
7	K	254	0	0	1	0
7	L	221	0	0	0	0
All	All	50860	0	46280	325	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (325) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:396[B]:MET:CE	1:I:398:PHE:HE2	1.68	1.06
1:I:396[B]:MET:HE1	1:I:398:PHE:HE2	1.22	1.01
1:I:396[B]:MET:CE	1:I:398:PHE:CE2	2.54	0.88
1:I:396[B]:MET:HE1	1:I:398:PHE:CE2	2.12	0.83
1:K:272:ASN:C	1:K:273:ASN:HD22	1.81	0.82
1:I:396[B]:MET:HE3	1:I:398:PHE:CE2	2.15	0.82
1:J:328:LEU:HB2	1:J:354:PHE:HB3	1.63	0.78
1:H:328:LEU:HB2	1:H:354:PHE:HB3	1.68	0.76
1:F:328:LEU:HB2	1:F:354:PHE:HB3	1.68	0.75
1:L:328:LEU:HB2	1:L:354:PHE:HB3	1.71	0.73
1:K:273:ASN:HD22	1:K:273:ASN:N	1.86	0.72
1:G:178:PHE:HZ	1:J:155:GLU:HG2	1.55	0.71
1:C:366:LYS:HG3	1:C:420:ASN:HB3	1.73	0.70
1:C:200:GLU:OE2	1:C:204:LYS:NZ	2.25	0.69
1:L:451:LYS:NZ	1:L:564:GLU:O	2.24	0.69
1:A:328:LEU:HB2	1:A:354:PHE:HB3	1.75	0.68
1:K:328:LEU:HB2	1:K:354:PHE:HB3	1.75	0.68
1:I:328:LEU:HB2	1:I:354:PHE:HB3	1.76	0.68
1:C:433:MET:O	7:C:801:HOH:O	2.12	0.66
1:B:328:LEU:HB2	1:B:354:PHE:HB3	1.79	0.65
1:B:491:MET:SD	7:B:820:HOH:O	2.54	0.65
1:G:328:LEU:HB2	1:G:354:PHE:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:LEU:HB2	1:E:354:PHE:HB3	1.78	0.64
1:A:298:ILE:HA	1:A:400[A]:MET:HE1	1.81	0.63
1:H:152:GLN:OE1	1:H:180:ASP:N	2.32	0.63
1:E:214:LEU:HD21	1:E:222:LEU:HD22	1.81	0.63
1:H:110:ILE:O	1:H:285:ARG:NH2	2.22	0.62
1:L:132:VAL:HG21	1:L:142:VAL:HG13	1.81	0.62
1:F:451:LYS:NZ	1:F:564:GLU:O	2.30	0.62
1:I:320:LYS:HB3	5:I:706:1PE:H142	1.82	0.62
1:I:366:LYS:HG3	1:I:420:ASN:HB3	1.82	0.61
1:H:178:PHE:HZ	1:L:155:GLU:HG2	1.65	0.61
1:I:298:ILE:HA	1:I:400[B]:MET:HE1	1.83	0.61
1:L:114:VAL:HG12	1:L:274:ALA:HB1	1.82	0.61
1:B:153:VAL:HA	1:B:177:MET:HE1	1.82	0.60
1:L:326:LYS:HE3	1:L:328:LEU:HD11	1.84	0.60
1:F:214:LEU:HD21	1:F:222:LEU:HD22	1.84	0.59
1:H:132:VAL:HG21	1:H:142:VAL:HG13	1.85	0.59
1:L:451:LYS:HG3	5:L:707:1PE:H251	1.83	0.59
1:C:340:ALA:HA	1:C:445:ILE:HD12	1.84	0.59
1:G:117:ILE:HG22	1:G:270:TYR:HB3	1.85	0.59
1:I:90:GLN:NE2	1:I:95:ASP:O	2.36	0.59
1:L:137:LYS:CB	1:L:140:GLY:H	2.16	0.59
1:E:114:VAL:HG12	1:E:274:ALA:HB1	1.84	0.59
1:F:298:ILE:HA	1:F:400[B]:MET:HE1	1.83	0.59
1:J:229:ASN:OD1	7:J:801:HOH:O	2.17	0.58
1:C:328:LEU:HB2	1:C:354:PHE:HB3	1.85	0.58
1:I:396[B]:MET:HE3	1:I:398:PHE:CD2	2.38	0.58
1:F:451:LYS:HE3	5:F:706:1PE:H241	1.85	0.58
1:B:521:ASN:ND2	7:B:807:HOH:O	2.37	0.58
1:H:536:THR:HG21	1:H:551:VAL:HG23	1.86	0.57
1:E:483:ASP:OD1	1:E:573:HIS:ND1	2.32	0.57
1:L:340:ALA:HA	1:L:445:ILE:HD12	1.85	0.56
1:A:394:ASP:HA	1:C:441:PRO:HB2	1.85	0.56
1:H:273:ASN:O	1:H:276:THR:OG1	2.22	0.56
1:B:166:ASN:ND2	7:B:810:HOH:O	2.38	0.56
1:G:340:ALA:HA	1:G:445:ILE:HD12	1.87	0.56
1:J:321:LEU:HD11	1:J:411:TYR:HA	1.87	0.56
1:L:148:VAL:HG12	1:L:150:ASP:H	1.70	0.56
1:L:395:LEU:O	1:L:395:LEU:HG	2.04	0.56
1:G:320:LYS:HB3	5:G:705:1PE:H242	1.88	0.56
1:J:441:PRO:HB2	1:K:394:ASP:HA	1.87	0.56
1:C:483:ASP:OD1	1:C:573:HIS:ND1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:298:ILE:HA	1:G:400[A]:MET:HE1	1.86	0.56
1:L:531:ASN:HD22	1:L:531:ASN:H	1.52	0.56
1:J:340:ALA:HA	1:J:445:ILE:HD12	1.87	0.56
1:K:520:SER:HB3	1:K:598:GLU:HG3	1.88	0.56
1:G:520:SER:HB3	1:G:598:GLU:HG3	1.88	0.55
1:I:357:LEU:HB2	1:I:425:PHE:HB2	1.88	0.55
1:A:178:PHE:HZ	1:D:155:GLU:HG2	1.71	0.55
1:A:236:ARG:NH1	7:A:816:HOH:O	2.36	0.55
1:E:520:SER:HB3	1:E:598:GLU:HG3	1.87	0.55
1:C:480:TYR:OH	1:C:512:LYS:NZ	2.39	0.55
1:I:520:SER:HB3	1:I:598:GLU:HG3	1.89	0.55
1:B:357:LEU:HB2	1:B:425:PHE:HB2	1.89	0.54
1:D:520:SER:HB3	1:D:598:GLU:HG3	1.88	0.54
1:K:273:ASN:N	1:K:273:ASN:ND2	2.52	0.54
1:K:364:ASP:O	1:K:420:ASN:HA	2.08	0.54
1:H:357:LEU:HB2	1:H:425:PHE:HB2	1.89	0.54
1:J:132:VAL:HG21	1:J:144:ILE:HD13	1.89	0.54
1:G:400[A]:MET:H	1:G:400[A]:MET:HE2	1.73	0.54
1:I:112:VAL:HG22	1:I:267:LEU:HB3	1.90	0.54
1:A:357:LEU:HB2	1:A:425:PHE:HB2	1.88	0.54
1:D:357:LEU:HB2	1:D:425:PHE:HB2	1.89	0.54
1:H:230:VAL:HG12	1:H:234:LEU:HD23	1.89	0.54
1:C:357:LEU:HB2	1:C:425:PHE:HB2	1.89	0.53
1:E:320:LYS:NZ	5:E:705:1PE:OH3	2.40	0.53
1:K:144:ILE:HG13	1:K:157:LEU:HD22	1.91	0.53
1:K:272:ASN:OD1	1:K:273:ASN:ND2	2.41	0.53
1:I:198:LEU:HD22	1:I:202:ASP:HB3	1.91	0.53
1:J:144:ILE:HG13	1:J:157:LEU:HD22	1.90	0.53
1:I:298:ILE:HG12	1:I:400[B]:MET:HE3	1.91	0.53
1:J:229:ASN:ND2	7:J:822:HOH:O	2.41	0.53
1:J:520:SER:HB3	1:J:598:GLU:HG3	1.91	0.53
1:D:132:VAL:HG21	1:D:142:VAL:HG13	1.90	0.52
1:F:400[B]:MET:H	1:F:400[B]:MET:HE2	1.72	0.52
1:K:340:ALA:HA	1:K:445:ILE:HD12	1.90	0.52
1:G:521:ASN:ND2	7:G:818:HOH:O	2.38	0.52
1:A:551:VAL:HG12	1:A:553:ALA:H	1.74	0.52
1:D:164:LYS:NZ	7:D:815:HOH:O	2.42	0.52
1:I:100:PRO:O	1:I:251:ARG:NH1	2.39	0.52
1:J:232:LYS:NZ	1:J:276:THR:O	2.42	0.52
1:E:96:PRO:HA	5:E:707:1PE:H241	1.92	0.52
1:K:374:LYS:NZ	1:K:486:THR:O	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:483:ASP:OD1	1:K:573:HIS:ND1	2.34	0.52
1:A:520:SER:HB3	1:A:598:GLU:HG3	1.92	0.52
1:I:503:PHE:O	1:I:573:HIS:N	2.32	0.52
1:K:230:VAL:HG13	1:K:234:LEU:HB3	1.92	0.51
1:G:103:TYR:N	6:G:707:SO4:O4	2.41	0.51
1:B:331:LYS:O	1:B:335:GLU:HG3	2.11	0.51
1:H:164:LYS:NZ	1:L:184:SER:OG	2.44	0.51
1:E:340:ALA:HA	1:E:445:ILE:HD12	1.92	0.51
1:K:463:ARG:N	2:K:701:CO3:O3	2.32	0.51
1:K:441:PRO:HB2	1:L:394:ASP:HA	1.92	0.51
1:G:345:GLY:O	7:G:801:HOH:O	2.20	0.51
1:B:346:LYS:NZ	7:B:818:HOH:O	2.45	0.50
1:F:88:VAL:HG21	1:F:97:THR:HA	1.93	0.50
1:F:515:GLN:NE2	7:F:813:HOH:O	2.34	0.50
1:G:320:LYS:HZ1	5:G:706:1PE:H152	1.76	0.50
1:G:298:ILE:HG12	1:G:400[A]:MET:HE3	1.93	0.50
1:I:396[B]:MET:HE3	1:I:396[B]:MET:HA	1.92	0.50
1:A:114:VAL:HG12	1:A:274:ALA:HB1	1.93	0.50
1:H:413:VAL:HG11	1:H:423:ILE:HD13	1.92	0.50
1:B:214:LEU:HD21	1:B:222:LEU:HD22	1.93	0.50
1:A:340:ALA:HA	1:A:445:ILE:HD12	1.94	0.50
1:G:174:HIS:HB3	1:J:175:PHE:CD2	2.46	0.50
1:A:400[A]:MET:HE2	1:A:400[A]:MET:H	1.77	0.50
1:C:104:ASN:N	6:C:708:SO4:O2	2.39	0.50
1:J:366:LYS:HG3	1:J:420:ASN:HB3	1.94	0.49
1:D:144:ILE:HG13	1:D:157:LEU:HD22	1.94	0.49
1:H:340:ALA:HA	1:H:445:ILE:HD12	1.94	0.49
1:B:174:HIS:HB3	1:F:175:PHE:CD1	2.47	0.49
1:F:480:TYR:OH	1:F:512:LYS:NZ	2.38	0.49
1:L:520:SER:HB3	1:L:598:GLU:HG3	1.93	0.49
1:D:441:PRO:HB2	1:E:394:ASP:HA	1.93	0.49
1:E:399:ASP:OD1	1:E:486:THR:OG1	2.30	0.49
1:J:413:VAL:HG11	1:J:423:ILE:HD12	1.95	0.49
1:G:441:PRO:HB2	1:H:394:ASP:HA	1.95	0.49
1:A:441:PRO:HB2	1:B:394:ASP:HA	1.94	0.49
1:J:103:TYR:HB3	5:J:705:1PE:H241	1.95	0.49
1:D:399:ASP:OD1	1:D:486:THR:OG1	2.18	0.48
1:E:551:VAL:HG12	1:E:553:ALA:H	1.78	0.48
1:B:340:ALA:HA	1:B:445:ILE:HD12	1.95	0.48
1:E:357:LEU:HB2	1:E:425:PHE:HB2	1.95	0.48
1:F:492:LEU:HD11	4:F:704:WRC:CAZ	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:MET:O	1:F:217:ASN:ND2	2.42	0.48
1:H:417:LYS:NZ	7:H:816:HOH:O	2.46	0.48
1:B:199:SER:OG	1:B:202:ASP:OD2	2.23	0.48
1:H:138:GLU:O	1:H:194:SER:OG	2.31	0.48
1:A:174:HIS:HB3	1:D:175:PHE:CD2	2.49	0.48
1:C:178:PHE:HZ	1:E:155:GLU:HG2	1.78	0.48
1:E:546:GLN:HG2	1:E:547:ILE:HG23	1.95	0.48
1:K:320:LYS:HB3	5:K:705:1PE:H142	1.96	0.48
1:A:132:VAL:HG21	1:A:142:VAL:HG13	1.95	0.48
1:B:413:VAL:HG11	1:B:423:ILE:HD12	1.96	0.48
1:K:440:ARG:NH2	7:K:826:HOH:O	2.44	0.47
1:I:534:ARG:NH2	7:I:820:HOH:O	2.43	0.47
1:H:460:ALA:O	1:H:546:GLN:NE2	2.47	0.47
1:I:321:LEU:HD11	1:I:411:TYR:HA	1.97	0.47
1:F:340:ALA:HA	1:F:445:ILE:HD12	1.96	0.47
1:G:114:VAL:HG12	1:G:274:ALA:HB1	1.95	0.47
1:J:329:GLY:N	1:J:332:GLU:OE1	2.38	0.47
1:F:320:LYS:HB3	5:F:705:1PE:H162	1.97	0.47
1:H:320:LYS:HZ1	5:H:706:1PE:H131	1.79	0.47
1:J:394:ASP:HA	1:L:441:PRO:HB2	1.96	0.47
1:E:441:PRO:HB2	1:F:394:ASP:HA	1.97	0.47
1:H:441:PRO:HB2	1:I:394:ASP:HA	1.97	0.47
1:J:396:MET:SD	1:J:398:PHE:HE2	2.38	0.47
1:L:483:ASP:OD2	1:L:573:HIS:ND1	2.38	0.47
1:C:230:VAL:HG12	1:C:234:LEU:HD23	1.97	0.47
1:G:357:LEU:HB2	1:G:425:PHE:HB2	1.97	0.47
1:I:174:HIS:HB3	1:K:175:PHE:CD2	2.50	0.47
1:A:103:TYR:N	6:A:708:SO4:O3	2.48	0.46
1:H:320:LYS:HZ1	5:H:706:1PE:H142	1.79	0.46
1:I:173:LYS:HB2	1:I:189:TYR:CE1	2.51	0.46
1:H:174:HIS:HB3	1:L:175:PHE:CD1	2.50	0.46
1:I:400[B]:MET:HE2	1:I:400[B]:MET:H	1.80	0.46
1:H:321:LEU:HD11	1:H:411:TYR:HA	1.97	0.46
1:B:321:LEU:HD11	1:B:411:TYR:HA	1.97	0.46
1:H:214:LEU:HD21	1:H:222:LEU:HD22	1.98	0.46
1:G:440:ARG:NH1	7:G:820:HOH:O	2.48	0.46
1:L:316:GLU:O	1:L:320:LYS:HG3	2.16	0.46
1:B:364:ASP:O	1:B:420:ASN:HA	2.16	0.46
1:D:320:LYS:NZ	5:D:706:1PE:H142	2.31	0.46
1:H:152:GLN:HE22	1:H:180:ASP:HA	1.79	0.46
1:K:135:PRO:O	1:K:137:LYS:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:ASN:HB2	1:B:547:ILE:HD13	1.98	0.46
1:C:379:ASP:HB3	1:C:396[B]:MET:HE2	1.98	0.46
1:G:417:LYS:NZ	7:G:826:HOH:O	2.44	0.46
1:I:340:ALA:HA	1:I:445:ILE:HD12	1.98	0.46
1:E:440:ARG:NH2	7:E:827:HOH:O	2.49	0.45
1:C:123:VAL:HG12	1:C:185:VAL:HG21	1.98	0.45
1:I:550:SER:OG	1:I:551:VAL:N	2.49	0.45
1:D:340:ALA:HA	1:D:445:ILE:HD12	1.97	0.45
1:F:132:VAL:HG21	1:F:142:VAL:HG13	1.98	0.45
1:C:244:TYR:HA	1:C:288:TYR:HE1	1.82	0.45
1:I:377:THR:HA	1:I:400[B]:MET:HG2	1.97	0.45
1:J:453:ILE:HD13	1:J:561:PHE:HZ	1.82	0.45
1:B:536:THR:HG21	1:B:551:VAL:HG23	1.99	0.45
1:D:533:TYR:O	1:D:536:THR:HG22	2.16	0.45
1:C:209:SER:O	1:C:212:THR:OG1	2.31	0.45
1:C:440:ARG:NH2	7:C:836:HOH:O	2.49	0.45
1:B:417:LYS:NZ	7:B:825:HOH:O	2.49	0.44
1:H:546:GLN:HG2	1:H:547:ILE:HG23	1.99	0.44
1:J:483:ASP:OD1	1:J:573:HIS:ND1	2.44	0.44
1:A:602:ASN:ND2	7:A:841:HOH:O	2.51	0.44
1:E:230:VAL:HG22	1:E:234:LEU:HD23	1.99	0.44
1:J:91:VAL:HB	1:L:346:LYS:HE3	1.99	0.44
1:J:326:LYS:HE3	1:J:328:LEU:HD11	1.99	0.44
1:C:90:GLN:HB3	1:C:95:ASP:HB2	1.99	0.44
1:D:509:LEU:O	1:D:513:ILE:HG12	2.17	0.44
1:G:395:LEU:HD11	1:G:581:TRP:CE2	2.51	0.44
1:A:208:LEU:O	1:A:212:THR:HG23	2.17	0.44
1:C:546:GLN:HG2	1:C:547:ILE:HG23	1.99	0.44
1:J:114:VAL:HG12	1:J:274:ALA:HB1	1.99	0.44
1:K:150:ASP:OD1	1:K:179:ASN:HB2	2.18	0.44
1:J:214:LEU:HD21	1:J:222:LEU:HD22	2.00	0.44
1:H:117:ILE:HD11	1:H:146:SER:OG	2.18	0.44
1:I:230:VAL:HG12	1:I:234:LEU:HD23	2.00	0.44
1:B:551:VAL:HG12	1:B:553:ALA:H	1.82	0.44
1:C:265:LYS:NZ	7:C:839:HOH:O	2.51	0.44
1:F:451:LYS:HG2	5:F:706:1PE:H131	2.00	0.44
1:G:509:LEU:O	1:G:513:ILE:HG12	2.17	0.44
1:I:149:ASN:ND2	5:I:707:1PE:H242	2.33	0.44
1:I:483:ASP:OD2	1:I:573:HIS:ND1	2.39	0.44
1:B:114:VAL:HB	1:B:278:LYS:HG2	2.00	0.43
1:D:328:LEU:HB2	1:D:354:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:411:TYR:CE1	5:L:705:1PE:H251	2.53	0.43
1:A:117:ILE:HD11	1:A:146:SER:OG	2.18	0.43
1:E:160:GLU:OE1	1:E:160:GLU:N	2.50	0.43
1:A:102:GLU:HG2	1:A:105:THR:HG22	2.00	0.43
1:A:457:ASN:HB2	1:A:547:ILE:HD13	1.99	0.43
1:C:500:ALA:HB3	1:C:524:VAL:HG22	1.99	0.43
1:D:114:VAL:HG12	1:D:274:ALA:HB1	1.99	0.43
1:I:114:VAL:HG12	1:I:274:ALA:HB1	2.00	0.43
1:I:509:LEU:O	1:I:513:ILE:HG12	2.18	0.43
1:L:207:VAL:HG11	1:L:241:THR:HG22	1.99	0.43
1:J:371:LEU:HD22	1:J:596:LEU:HD22	2.00	0.43
5:A:705:1PE:H132	5:A:707:1PE:H161	2.00	0.43
1:D:150:ASP:OD1	1:D:179:ASN:HB2	2.18	0.43
1:H:440:ARG:HG2	1:I:378:PHE:CE2	2.54	0.43
1:I:300:ALA:HA	1:I:301:PRO:HD3	1.83	0.43
1:B:90:GLN:NE2	1:B:95:ASP:O	2.49	0.43
1:I:232:LYS:NZ	1:I:279:GLU:OE2	2.49	0.43
1:A:301:PRO:HB2	1:A:303:ASN:OD1	2.18	0.43
1:A:543:ASP:OD2	1:B:254:SER:OG	2.30	0.43
1:G:337:LYS:HA	1:H:94:LEU:HD11	2.00	0.43
1:C:204:LYS:HB2	1:C:204:LYS:HE2	1.81	0.43
1:G:525:TRP:CZ3	1:L:528:PRO:HB3	2.53	0.43
1:B:483:ASP:OD1	1:B:573:HIS:ND1	2.39	0.43
1:F:383:TYR:HE2	1:F:438:SER:HB2	1.84	0.43
1:G:321:LEU:HD11	1:G:411:TYR:HA	2.00	0.43
1:D:124:GLU:HA	1:D:179:ASN:HD22	1.84	0.42
1:H:283:LYS:HE2	1:H:287:TYR:CZ	2.54	0.42
1:A:289:PHE:O	1:A:293:TYR:N	2.39	0.42
1:B:207:VAL:HG11	1:B:241:THR:HG22	2.00	0.42
1:J:417:LYS:NZ	7:J:838:HOH:O	2.52	0.42
1:F:300:ALA:HA	1:F:301:PRO:HD3	1.88	0.42
1:H:504:GLY:HA3	1:H:510:ILE:HD11	2.01	0.42
1:J:457:ASN:HB2	1:J:547:ILE:HD13	2.00	0.42
1:J:510:ILE:HD13	1:J:526:TRP:NE1	2.34	0.42
1:K:341:TYR:HD1	1:K:465:THR:HG22	1.83	0.42
1:A:435:SER:N	1:A:438:SER:OG	2.52	0.42
1:B:297:LEU:HB3	1:B:400:MET:HE1	2.01	0.42
1:C:236:ARG:NE	1:C:240:GLU:OE2	2.41	0.42
1:E:307:PRO:HD3	1:E:377:THR:OG1	2.18	0.42
1:G:135:PRO:HA	1:G:194:SER:O	2.20	0.42
1:G:244:TYR:OH	1:G:588:PRO:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:132:VAL:HG11	1:J:142:VAL:HG13	2.02	0.42
1:A:522:GLU:HA	1:A:523:PRO:HD3	1.82	0.42
1:C:214:LEU:HD21	1:C:222:LEU:HD22	2.01	0.42
1:C:289:PHE:O	1:C:293:TYR:N	2.41	0.42
1:G:320:LYS:NZ	5:G:706:1PE:H152	2.35	0.42
1:I:115:TYR:CZ	5:I:707:1PE:H221	2.54	0.42
1:A:200:GLU:OE1	1:A:200:GLU:N	2.53	0.42
1:A:586:ARG:NH1	7:A:839:HOH:O	2.50	0.42
1:E:150:ASP:OD1	1:E:179:ASN:HB2	2.20	0.42
1:G:394:ASP:HA	1:I:441:PRO:HB2	2.01	0.42
1:H:300:ALA:HA	1:H:301:PRO:HD3	1.83	0.42
1:I:330:VAL:HA	1:I:333:LEU:HD12	2.02	0.42
1:D:394:ASP:HA	1:F:441:PRO:HB2	2.01	0.42
1:G:386:LYS:NZ	4:G:704:WRC:O	2.46	0.42
1:C:223:THR:HG22	1:C:268:GLY:HA3	2.02	0.41
1:I:448:SER:HB2	1:I:471:VAL:HG11	2.01	0.41
1:K:331:LYS:O	1:K:335:GLU:HG2	2.20	0.41
1:K:509:LEU:O	1:K:513:ILE:HD12	2.20	0.41
1:C:320:LYS:NZ	5:C:705:1PE:OH6	2.50	0.41
1:I:273:ASN:O	1:I:276:THR:OG1	2.36	0.41
1:C:442:GLY:N	1:C:455:VAL:O	2.50	0.41
1:D:207:VAL:HG11	1:D:241:THR:HG22	2.01	0.41
1:H:301:PRO:HB2	1:H:303:ASN:OD1	2.21	0.41
1:K:214:LEU:HD21	1:K:222:LEU:HD22	2.01	0.41
1:K:132:VAL:HG11	1:K:142:VAL:HG13	2.01	0.41
1:A:300:ALA:HA	1:A:301:PRO:HD3	1.86	0.41
1:A:509:LEU:O	1:A:513:ILE:HG12	2.21	0.41
1:D:298:ILE:HA	1:D:400:MET:SD	2.61	0.41
1:D:494:SER:OG	1:D:495:LEU:N	2.53	0.41
1:G:342:LEU:O	1:G:346:LYS:HG3	2.21	0.41
1:J:300:ALA:HA	1:J:301:PRO:HD3	1.81	0.41
1:K:300:ALA:HA	1:K:301:PRO:HD3	1.91	0.41
1:A:320:LYS:HD3	5:A:707:1PE:H261	2.02	0.41
1:H:244:TYR:OH	1:H:588:PRO:O	2.37	0.41
1:K:165:PHE:CD2	1:K:173:LYS:HG3	2.56	0.41
1:A:207:VAL:HG11	1:A:241:THR:HG22	2.02	0.41
1:A:343:SER:HA	1:A:346:LYS:HD3	2.03	0.41
1:B:600:VAL:HG12	1:B:601:LEU:HD12	2.03	0.41
1:C:399:ASP:OD1	1:C:486:THR:OG1	2.29	0.41
1:F:520:SER:HB3	1:F:598:GLU:HG3	2.03	0.41
1:B:441:PRO:HB2	1:C:394:ASP:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:300:ALA:HA	1:D:301:PRO:HD3	1.85	0.41
1:I:306:ASN:HB2	1:I:307:PRO:HD2	2.03	0.41
1:A:396:MET:SD	1:A:398:PHE:HE2	2.43	0.40
1:B:306:ASN:HB2	1:B:307:PRO:HD2	2.02	0.40
1:I:320:LYS:NZ	5:I:705:1PE:H132	2.36	0.40
1:K:114:VAL:HG12	1:K:274:ALA:HB1	2.03	0.40
1:K:395:LEU:HD23	1:K:398:PHE:CD2	2.56	0.40
1:C:244:TYR:HA	1:C:288:TYR:CE1	2.57	0.40
1:F:357:LEU:HB2	1:F:425:PHE:HB2	2.02	0.40
1:H:416:LEU:HD13	1:H:601:LEU:HD21	2.02	0.40
1:G:350:TYR:HA	1:G:351:PRO:HD3	1.93	0.40
1:L:531:ASN:HD22	1:L:531:ASN:N	2.19	0.40
1:A:260:ASN:ND2	7:A:808:HOH:O	2.31	0.40
1:A:453:ILE:HD13	1:A:561:PHE:HZ	1.86	0.40
1:H:488:THR:HG21	1:H:555:SER:HA	2.02	0.40
1:I:298:ILE:HA	1:I:400[B]:MET:CE	2.50	0.40

There are no symmetry-related clashes.

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	518/528 (98%)	501 (97%)	17 (3%)	0	100 100
1	B	514/528 (97%)	497 (97%)	17 (3%)	0	100 100
1	C	513/528 (97%)	495 (96%)	18 (4%)	0	100 100
1	D	510/528 (97%)	495 (97%)	14 (3%)	1 (0%)	47 58
1	E	503/528 (95%)	487 (97%)	16 (3%)	0	100 100
1	F	509/528 (96%)	489 (96%)	19 (4%)	1 (0%)	47 58
1	G	518/528 (98%)	502 (97%)	16 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	H	514/528 (97%)	496 (96%)	16 (3%)	2 (0%)	34 42
1	I	518/528 (98%)	501 (97%)	16 (3%)	1 (0%)	47 58
1	J	510/528 (97%)	497 (98%)	13 (2%)	0	100 100
1	K	503/528 (95%)	489 (97%)	14 (3%)	0	100 100
1	L	506/528 (96%)	491 (97%)	14 (3%)	1 (0%)	47 58
All	All	6136/6336 (97%)	5940 (97%)	190 (3%)	6 (0%)	51 64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	392	MET
1	H	552	LYS
1	I	550	SER
1	L	531	ASN
1	H	254	SER
1	D	551	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	420/455 (92%)	415 (99%)	5 (1%)	71 84
1	B	410/455 (90%)	409 (100%)	1 (0%)	93 97
1	C	425/455 (93%)	422 (99%)	3 (1%)	84 92
1	D	413/455 (91%)	410 (99%)	3 (1%)	84 92
1	E	418/455 (92%)	418 (100%)	0	100 100
1	F	404/455 (89%)	401 (99%)	3 (1%)	84 92
1	G	421/455 (92%)	417 (99%)	4 (1%)	76 87
1	H	408/455 (90%)	406 (100%)	2 (0%)	88 95
1	I	422/455 (93%)	418 (99%)	4 (1%)	78 89
1	J	422/455 (93%)	421 (100%)	1 (0%)	93 97

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	K	415/455 (91%)	413 (100%)	2 (0%)	88 95
1	L	403/455 (89%)	399 (99%)	4 (1%)	76 87
All	All	4981/5460 (91%)	4949 (99%)	32 (1%)	86 94

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	LEU
1	A	398	PHE
1	A	400[A]	MET
1	A	400[B]	MET
1	A	439	TYR
1	B	439	TYR
1	C	200	GLU
1	C	398	PHE
1	C	439	TYR
1	D	395	LEU
1	D	399	ASP
1	D	439	TYR
1	F	400[A]	MET
1	F	400[B]	MET
1	F	439	TYR
1	G	398	PHE
1	G	400[A]	MET
1	G	400[B]	MET
1	G	439	TYR
1	H	343	SER
1	H	439	TYR
1	I	398	PHE
1	I	400[A]	MET
1	I	400[B]	MET
1	I	439	TYR
1	J	439	TYR
1	K	273	ASN
1	K	439	TYR
1	L	395	LEU
1	L	398	PHE
1	L	399	ASP
1	L	439	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	K	272	ASN
1	K	273	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 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	1PE	A	705	-	8,8,15	0.67	0	7,7,14	0.17	0
5	1PE	K	705	-	11,11,15	0.68	0	10,10,14	0.24	0
5	1PE	I	706	-	8,8,15	0.68	0	7,7,14	0.22	0
6	SO4	K	706	-	4,4,4	0.14	0	6,6,6	0.04	0
5	1PE	H	705	-	9,9,15	0.66	0	8,8,14	0.23	0
5	1PE	H	706	-	9,9,15	0.68	0	8,8,14	0.19	0
6	SO4	G	708	-	4,4,4	0.14	0	6,6,6	0.06	0
2	CO3	F	701	-	2,3,3	0.40	0	2,3,3	0.19	0
5	1PE	G	705	-	8,8,15	0.69	0	7,7,14	0.24	0
5	1PE	F	706	-	11,11,15	0.69	0	10,10,14	0.23	0
6	SO4	F	707	-	4,4,4	0.15	0	6,6,6	0.07	0
5	1PE	F	705	-	9,9,15	0.63	0	8,8,14	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	D	707	-	4,4,4	0.14	0	6,6,6	0.05	0
4	WRC	E	704	3	29,29,29	1.74	2 (6%)	40,42,42	0.88	1 (2%)
5	1PE	J	706	-	9,9,15	0.67	0	8,8,14	0.20	0
5	1PE	L	706	-	9,9,15	0.65	0	8,8,14	0.30	0
4	WRC	B	704	3	29,29,29	1.75	3 (10%)	40,42,42	0.85	0
4	WRC	C	704	3	29,29,29	1.72	2 (6%)	40,42,42	0.91	1 (2%)
5	1PE	B	706	-	9,9,15	0.67	0	8,8,14	0.20	0
5	1PE	L	705	-	9,9,15	0.62	0	8,8,14	0.28	0
4	WRC	D	704	3	29,29,29	1.80	2 (6%)	40,42,42	0.88	0
6	SO4	A	709	-	4,4,4	0.15	0	6,6,6	0.06	0
6	SO4	L	708	-	4,4,4	0.14	0	6,6,6	0.06	0
2	CO3	L	701	-	2,3,3	0.42	0	2,3,3	0.25	0
5	1PE	L	707	-	9,9,15	0.63	0	8,8,14	0.24	0
5	1PE	A	706	-	5,5,15	0.63	0	4,4,14	0.30	0
5	1PE	C	706	-	10,10,15	0.71	0	9,9,14	0.20	0
2	CO3	E	701	-	2,3,3	0.42	0	2,3,3	0.22	0
5	1PE	D	705	-	10,10,15	0.63	0	9,9,14	0.23	0
6	SO4	A	708	-	4,4,4	0.15	0	6,6,6	0.05	0
5	1PE	C	707	-	6,6,15	0.70	0	5,5,14	0.20	0
5	1PE	I	707	-	8,8,15	0.68	0	7,7,14	0.27	0
2	CO3	A	701	-	2,3,3	0.42	0	2,3,3	0.24	0
4	WRC	G	704	3	29,29,29	1.78	3 (10%)	40,42,42	0.92	1 (2%)
2	CO3	H	701	-	2,3,3	0.40	0	2,3,3	0.11	0
2	CO3	I	701	-	2,3,3	0.42	0	2,3,3	0.30	0
5	1PE	G	706	-	11,11,15	0.67	0	10,10,14	0.17	0
4	WRC	L	704	3	29,29,29	1.79	2 (6%)	40,42,42	0.88	1 (2%)
4	WRC	H	704	3	29,29,29	1.75	2 (6%)	40,42,42	0.84	0
2	CO3	G	701	-	2,3,3	0.41	0	2,3,3	0.14	0
6	SO4	G	709	-	4,4,4	0.15	0	6,6,6	0.06	0
4	WRC	I	704	3	29,29,29	1.81	2 (6%)	40,42,42	0.93	1 (2%)
5	1PE	E	705	-	9,9,15	0.69	0	8,8,14	0.23	0
2	CO3	J	701	-	2,3,3	0.39	0	2,3,3	0.12	0
4	WRC	F	704	3	29,29,29	1.85	2 (6%)	40,42,42	1.03	3 (7%)
4	WRC	J	704	3	29,29,29	1.80	3 (10%)	40,42,42	0.91	0
5	1PE	I	705	-	12,12,15	0.68	0	11,11,14	0.19	0
4	WRC	K	704	3	29,29,29	1.82	2 (6%)	40,42,42	0.93	0
6	SO4	J	707	-	4,4,4	0.15	0	6,6,6	0.05	0
2	CO3	D	701	-	2,3,3	0.42	0	2,3,3	0.22	0
5	1PE	B	705	-	9,9,15	0.66	0	8,8,14	0.24	0
4	WRC	A	704	3	29,29,29	1.80	3 (10%)	40,42,42	0.93	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	CO3	B	701	-	2,3,3	0.39	0	2,3,3	0.08	0
5	1PE	E	707	-	5,5,15	0.62	0	4,4,14	0.19	0
5	1PE	D	706	-	9,9,15	0.63	0	8,8,14	0.23	0
5	1PE	J	705	-	9,9,15	0.67	0	8,8,14	0.19	0
2	CO3	K	701	-	2,3,3	0.42	0	2,3,3	0.26	0
6	SO4	C	708	-	4,4,4	0.14	0	6,6,6	0.06	0
2	CO3	C	701	-	2,3,3	0.41	0	2,3,3	0.23	0
6	SO4	C	709	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	C	705	-	14,14,15	0.66	0	13,13,14	0.23	0
5	1PE	E	706	-	11,11,15	0.67	0	10,10,14	0.23	0
6	SO4	G	707	-	4,4,4	0.14	0	6,6,6	0.05	0
5	1PE	A	707	-	14,14,15	0.67	0	13,13,14	0.18	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	A	705	-	-	3/6/6/13	-
5	1PE	K	705	-	-	4/9/9/13	-
5	1PE	I	706	-	-	5/6/6/13	-
5	1PE	H	705	-	-	3/7/7/13	-
5	1PE	H	706	-	-	6/7/7/13	-
5	1PE	G	705	-	-	2/6/6/13	-
5	1PE	F	706	-	-	5/9/9/13	-
5	1PE	F	705	-	-	4/7/7/13	-
4	WRC	E	704	3	-	0/23/23/23	0/2/2/2
5	1PE	J	706	-	-	3/7/7/13	-
5	1PE	L	706	-	-	3/7/7/13	-
4	WRC	B	704	3	-	0/23/23/23	0/2/2/2
4	WRC	C	704	3	-	0/23/23/23	0/2/2/2
5	1PE	B	706	-	-	2/7/7/13	-
5	1PE	L	705	-	-	5/7/7/13	-
4	WRC	D	704	3	-	0/23/23/23	0/2/2/2
5	1PE	L	707	-	-	4/7/7/13	-
5	1PE	A	706	-	-	3/3/3/13	-
5	1PE	C	706	-	-	5/8/8/13	-
5	1PE	D	705	-	-	7/8/8/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	1PE	C	707	-	-	2/4/4/13	-
5	1PE	I	707	-	-	3/6/6/13	-
4	WRC	G	704	3	-	0/23/23/23	0/2/2/2
5	1PE	G	706	-	-	5/9/9/13	-
4	WRC	L	704	3	-	0/23/23/23	0/2/2/2
4	WRC	H	704	3	-	0/23/23/23	0/2/2/2
4	WRC	I	704	3	-	0/23/23/23	0/2/2/2
5	1PE	E	705	-	-	4/7/7/13	-
4	WRC	F	704	3	-	0/23/23/23	0/2/2/2
4	WRC	J	704	3	-	1/23/23/23	0/2/2/2
5	1PE	I	705	-	-	7/10/10/13	-
4	WRC	K	704	3	-	0/23/23/23	0/2/2/2
5	1PE	B	705	-	-	4/7/7/13	-
4	WRC	A	704	3	-	0/23/23/23	0/2/2/2
5	1PE	E	707	-	-	1/3/3/13	-
5	1PE	D	706	-	-	4/7/7/13	-
5	1PE	J	705	-	-	4/7/7/13	-
5	1PE	C	705	-	-	6/12/12/13	-
5	1PE	E	706	-	-	1/9/9/13	-
5	1PE	A	707	-	-	3/12/12/13	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	704	WRC	CAY-CA	-8.56	1.38	1.52
4	K	704	WRC	CAY-CA	-8.26	1.39	1.52
4	L	704	WRC	CAY-CA	-8.15	1.39	1.52
4	D	704	WRC	CAY-CA	-8.13	1.39	1.52
4	I	704	WRC	CAY-CA	-8.10	1.39	1.52
4	J	704	WRC	CAY-CA	-7.93	1.39	1.52
4	B	704	WRC	CAY-CA	-7.92	1.39	1.52
4	H	704	WRC	CAY-CA	-7.88	1.39	1.52
4	E	704	WRC	CAY-CA	-7.83	1.39	1.52
4	A	704	WRC	CAY-CA	-7.82	1.39	1.52
4	G	704	WRC	CAY-CA	-7.74	1.40	1.52
4	C	704	WRC	CAY-CA	-7.73	1.40	1.52
4	F	704	WRC	CAX-CAW	-4.00	1.39	1.49
4	K	704	WRC	CAX-CAW	-3.98	1.39	1.49
4	D	704	WRC	CAX-CAW	-3.97	1.39	1.49
4	A	704	WRC	CAX-CAW	-3.93	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	704	WRC	CAX-CAW	-3.91	1.39	1.49
4	G	704	WRC	CAX-CAW	-3.88	1.39	1.49
4	L	704	WRC	CAX-CAW	-3.87	1.39	1.49
4	J	704	WRC	CAX-CAW	-3.86	1.39	1.49
4	B	704	WRC	CAX-CAW	-3.84	1.39	1.49
4	E	704	WRC	CAX-CAW	-3.83	1.39	1.49
4	H	704	WRC	CAX-CAW	-3.82	1.39	1.49
4	C	704	WRC	CAX-CAW	-3.81	1.39	1.49
4	G	704	WRC	FAI-CAZ	-2.53	1.31	1.35
4	J	704	WRC	OAF-NAQ	2.17	1.45	1.40
4	B	704	WRC	CAP-CAS	2.07	1.54	1.51
4	A	704	WRC	FAI-CAZ	-2.06	1.31	1.35

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	704	WRC	CBB-CAP-CAS	-2.49	111.07	114.64
4	I	704	WRC	CBB-CAP-CAS	-2.48	111.08	114.64
4	E	704	WRC	CBB-CAP-CAS	-2.42	111.17	114.64
4	A	704	WRC	CBB-CAP-CAS	-2.34	111.28	114.64
4	L	704	WRC	CBB-CAP-CAS	-2.33	111.30	114.64
4	C	704	WRC	CBB-CAP-CAS	-2.22	111.45	114.64
4	F	704	WRC	CAJ-CAL-CAY	-2.13	119.05	121.20
4	F	704	WRC	CBB-CAP-CAS	-2.09	111.64	114.64
4	F	704	WRC	CAL-CAY-CAM	2.01	120.80	118.29

There are no chirality outliers.

All (109) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	L	705	1PE	C16-C26-OH6-C15
5	L	707	1PE	OH7-C16-C26-OH6
5	C	706	1PE	OH4-C13-C23-OH3
5	A	705	1PE	OH4-C13-C23-OH3
5	G	706	1PE	OH4-C13-C23-OH3
5	G	706	1PE	OH6-C15-C25-OH5
5	C	705	1PE	OH5-C14-C24-OH4
5	I	706	1PE	OH4-C13-C23-OH3
5	J	705	1PE	OH4-C13-C23-OH3
5	L	707	1PE	OH6-C15-C25-OH5
5	I	707	1PE	OH4-C13-C23-OH3
5	L	706	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
5	E	705	1PE	OH5-C14-C24-OH4
5	B	706	1PE	OH4-C13-C23-OH3
5	D	705	1PE	OH5-C14-C24-OH4
5	J	705	1PE	OH5-C14-C24-OH4
5	E	705	1PE	OH6-C15-C25-OH5
5	L	706	1PE	OH7-C16-C26-OH6
5	D	706	1PE	OH6-C15-C25-OH5
5	I	705	1PE	OH5-C14-C24-OH4
5	C	706	1PE	C24-C14-OH5-C25
5	D	706	1PE	OH7-C16-C26-OH6
5	E	706	1PE	OH6-C15-C25-OH5
5	F	705	1PE	OH5-C14-C24-OH4
5	I	705	1PE	OH4-C13-C23-OH3
5	H	706	1PE	OH4-C13-C23-OH3
5	A	706	1PE	OH6-C15-C25-OH5
5	I	706	1PE	OH5-C14-C24-OH4
5	I	705	1PE	C13-C23-OH3-C22
5	H	705	1PE	C12-C22-OH3-C23
5	I	707	1PE	C12-C22-OH3-C23
5	I	705	1PE	C14-C24-OH4-C13
5	F	705	1PE	OH7-C16-C26-OH6
5	I	707	1PE	OH5-C14-C24-OH4
5	C	706	1PE	OH5-C14-C24-OH4
5	L	705	1PE	OH6-C15-C25-OH5
5	J	706	1PE	OH5-C14-C24-OH4
5	B	706	1PE	C12-C22-OH3-C23
5	F	706	1PE	C12-C22-OH3-C23
5	I	706	1PE	C12-C22-OH3-C23
5	J	706	1PE	C12-C22-OH3-C23
5	H	705	1PE	OH4-C13-C23-OH3
5	D	706	1PE	C15-C25-OH5-C14
5	F	706	1PE	C13-C23-OH3-C22
5	F	706	1PE	OH4-C13-C23-OH3
5	D	705	1PE	OH6-C15-C25-OH5
5	I	705	1PE	OH6-C15-C25-OH5
5	G	705	1PE	OH4-C13-C23-OH3
5	L	705	1PE	OH7-C16-C26-OH6
5	D	705	1PE	C15-C25-OH5-C14
5	H	706	1PE	C13-C23-OH3-C22
5	C	706	1PE	C23-C13-OH4-C24
5	A	705	1PE	C13-C23-OH3-C22
5	J	705	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
5	I	705	1PE	C23-C13-OH4-C24
5	L	707	1PE	C15-C25-OH5-C14
5	G	706	1PE	C14-C24-OH4-C13
5	K	705	1PE	C15-C25-OH5-C14
5	I	706	1PE	C23-C13-OH4-C24
5	D	705	1PE	OH7-C16-C26-OH6
5	K	705	1PE	C14-C24-OH4-C13
5	K	705	1PE	OH6-C15-C25-OH5
5	L	705	1PE	OH5-C14-C24-OH4
5	D	705	1PE	C24-C14-OH5-C25
5	C	707	1PE	C14-C24-OH4-C13
5	H	706	1PE	OH5-C14-C24-OH4
5	L	706	1PE	C15-C25-OH5-C14
5	B	705	1PE	OH5-C14-C24-OH4
5	D	705	1PE	C25-C15-OH6-C26
5	G	706	1PE	C13-C23-OH3-C22
5	A	707	1PE	C25-C15-OH6-C26
5	L	707	1PE	OH5-C14-C24-OH4
5	E	705	1PE	C15-C25-OH5-C14
5	A	707	1PE	C13-C23-OH3-C22
5	C	705	1PE	C12-C22-OH3-C23
5	H	705	1PE	C14-C24-OH4-C13
5	A	705	1PE	OH5-C14-C24-OH4
5	H	706	1PE	C24-C14-OH5-C25
5	G	705	1PE	OH5-C14-C24-OH4
5	C	705	1PE	C15-C25-OH5-C14
5	F	706	1PE	C15-C25-OH5-C14
5	C	706	1PE	C12-C22-OH3-C23
5	C	705	1PE	C14-C24-OH4-C13
5	H	706	1PE	C14-C24-OH4-C13
5	F	705	1PE	C16-C26-OH6-C15
5	F	705	1PE	C24-C14-OH5-C25
5	B	705	1PE	C23-C13-OH4-C24
5	C	707	1PE	C15-C25-OH5-C14
5	J	706	1PE	C13-C23-OH3-C22
5	I	706	1PE	C14-C24-OH4-C13
5	F	706	1PE	C23-C13-OH4-C24
5	H	706	1PE	C12-C22-OH3-C23
4	J	704	WRC	NAQ-C-CA-N
5	J	705	1PE	C13-C23-OH3-C22
5	A	707	1PE	C12-C22-OH3-C23
5	G	706	1PE	OH5-C14-C24-OH4

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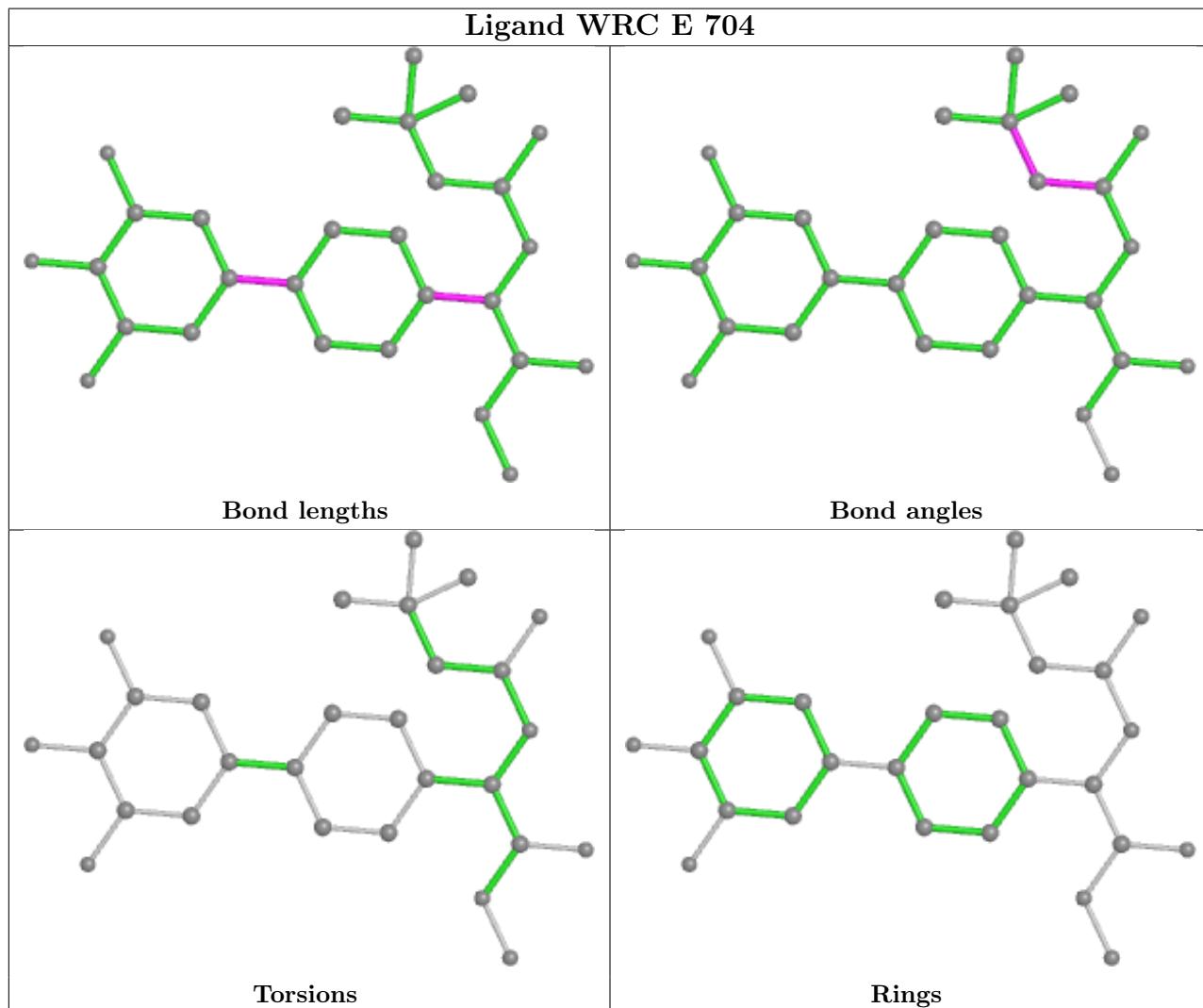
Mol	Chain	Res	Type	Atoms
5	A	706	1PE	C24-C14-OH5-C25
5	K	705	1PE	C12-C22-OH3-C23
5	C	705	1PE	OH4-C13-C23-OH3
5	E	705	1PE	C24-C14-OH5-C25
5	A	706	1PE	C15-C25-OH5-C14
5	D	705	1PE	C14-C24-OH4-C13
5	E	707	1PE	OH5-C14-C24-OH4
5	B	705	1PE	C13-C23-OH3-C22
5	L	705	1PE	C15-C25-OH5-C14
5	D	706	1PE	C16-C26-OH6-C15
5	C	705	1PE	C13-C23-OH3-C22
5	I	705	1PE	C15-C25-OH5-C14
5	B	705	1PE	C14-C24-OH4-C13

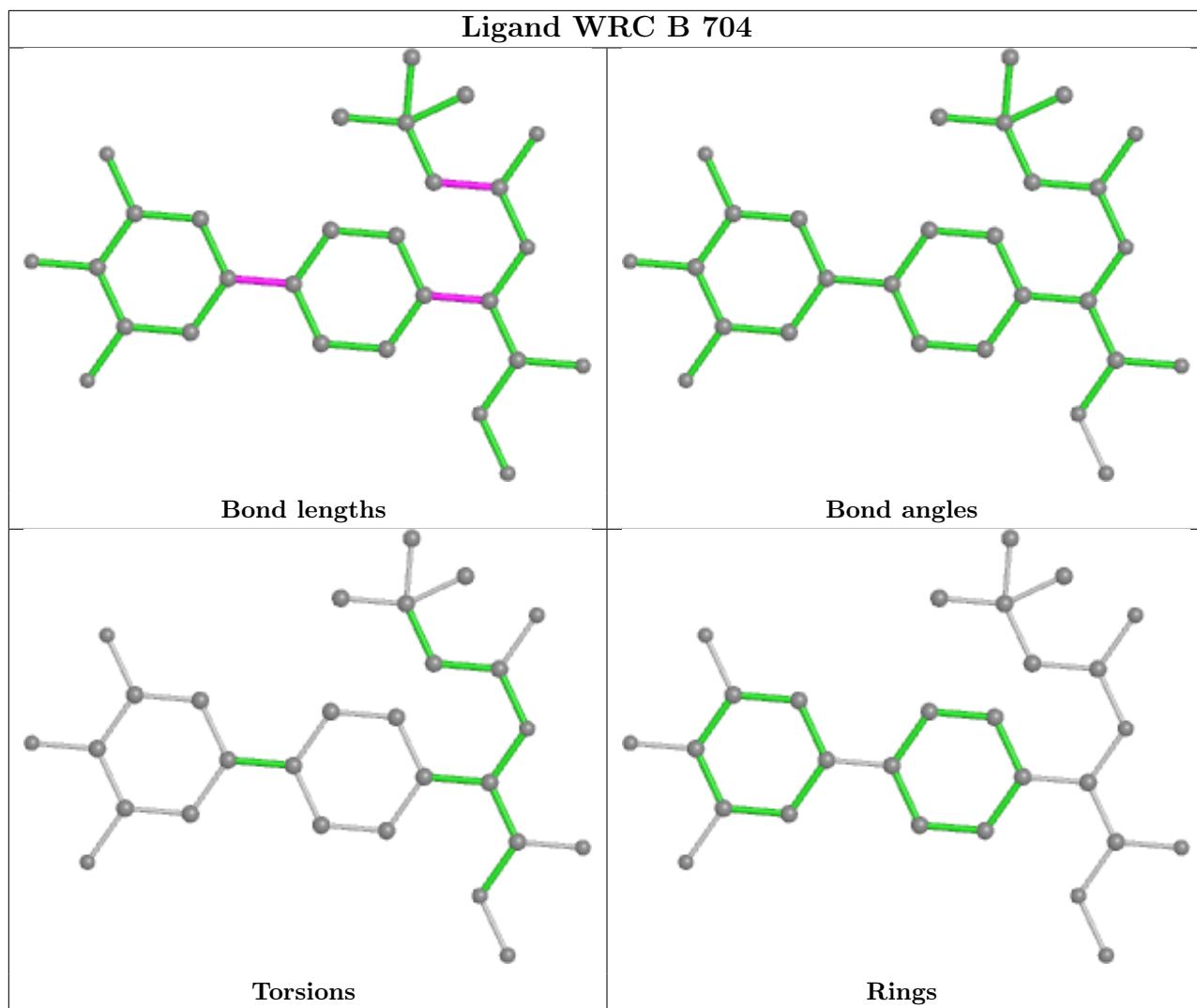
There are no ring outliers.

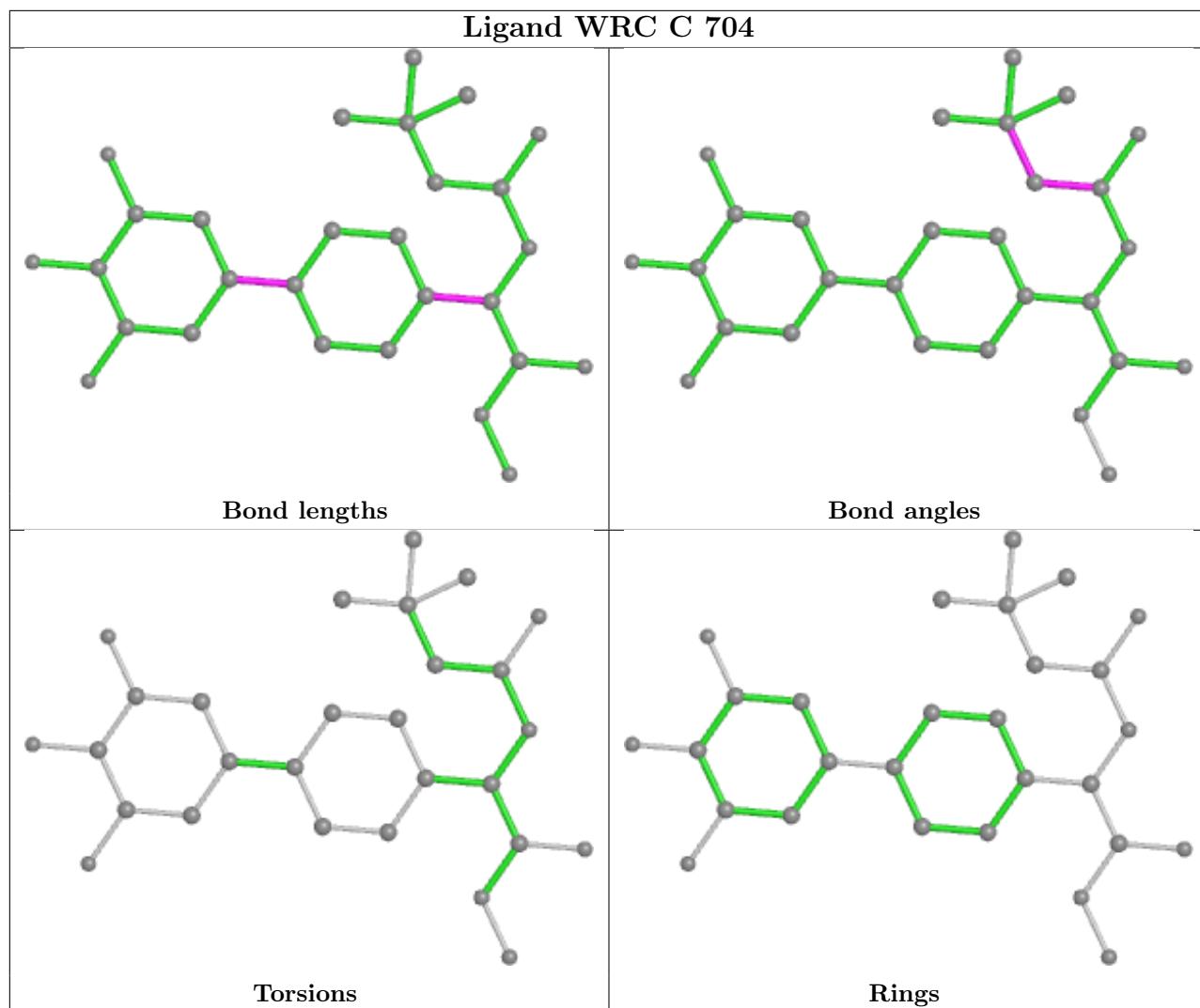
24 monomers are involved in 28 short contacts:

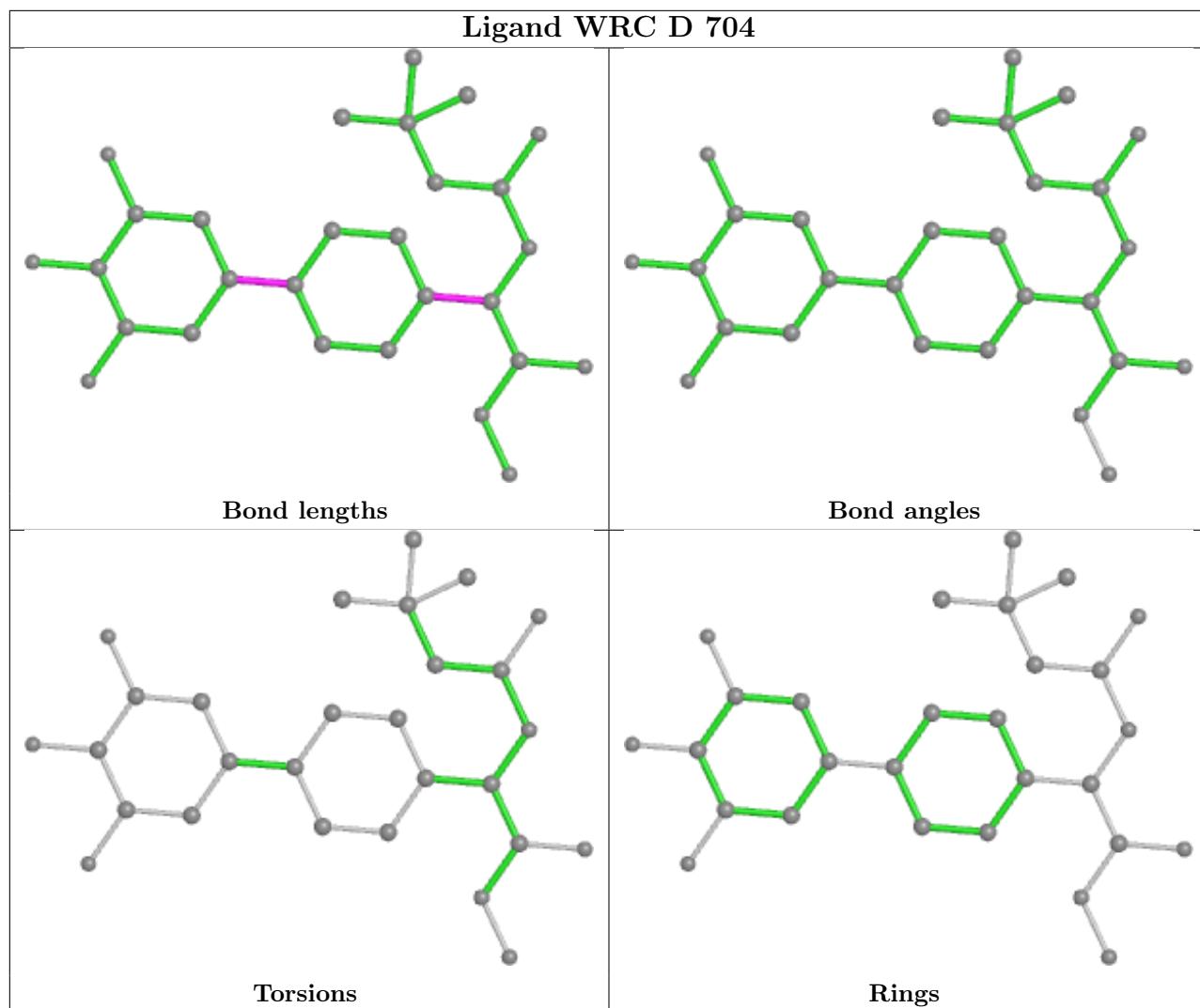
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	705	1PE	1	0
5	K	705	1PE	1	0
5	I	706	1PE	1	0
5	H	706	1PE	2	0
5	G	705	1PE	1	0
5	F	706	1PE	2	0
5	F	705	1PE	1	0
5	L	705	1PE	1	0
5	L	707	1PE	1	0
6	A	708	SO4	1	0
5	I	707	1PE	2	0
4	G	704	WRC	1	0
5	G	706	1PE	2	0
5	E	705	1PE	1	0
4	F	704	WRC	1	0
5	I	705	1PE	1	0
5	E	707	1PE	1	0
5	D	706	1PE	1	0
5	J	705	1PE	1	0
2	K	701	CO3	1	0
6	C	708	SO4	1	0
5	C	705	1PE	1	0
6	G	707	SO4	1	0
5	A	707	1PE	2	0

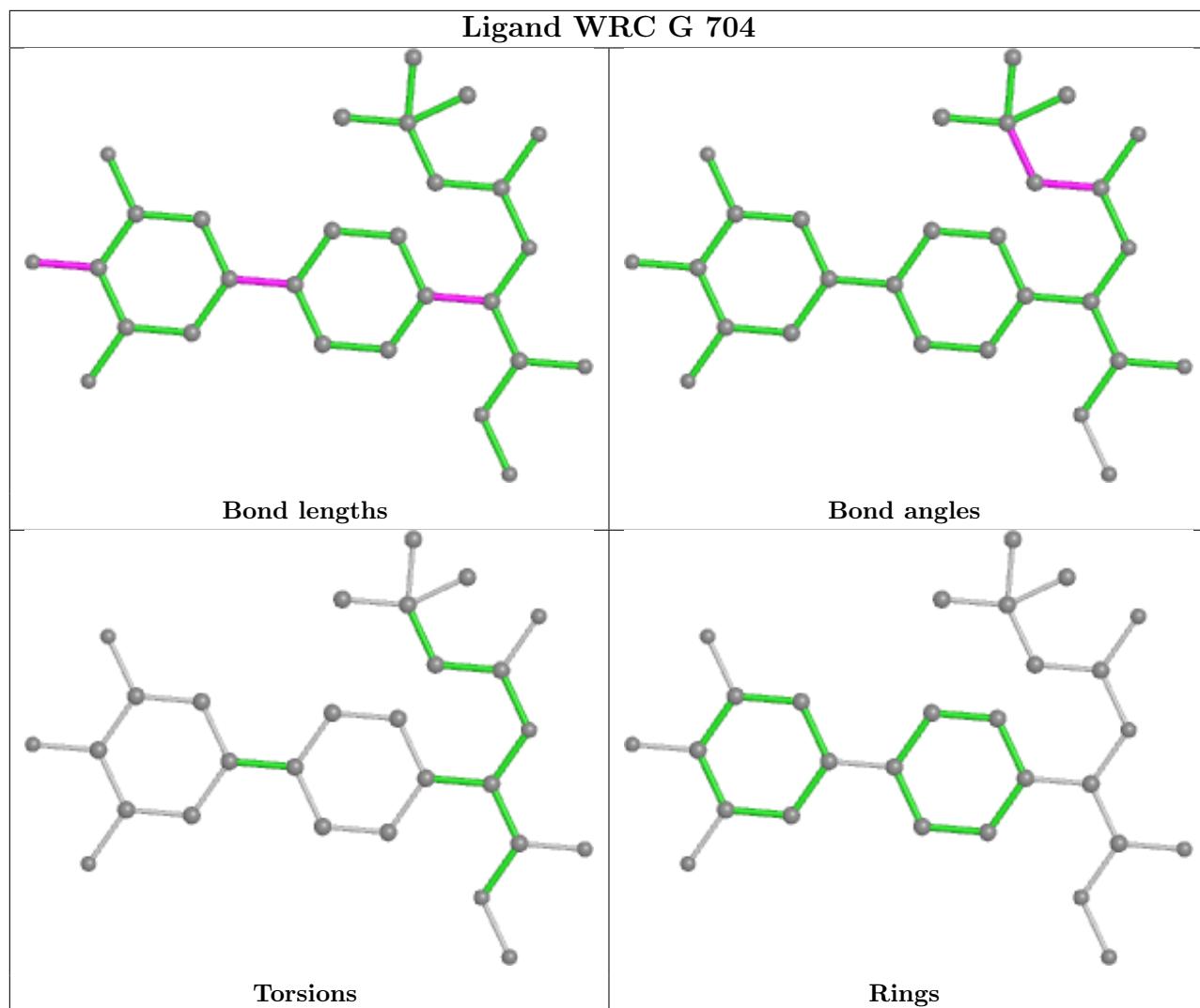
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

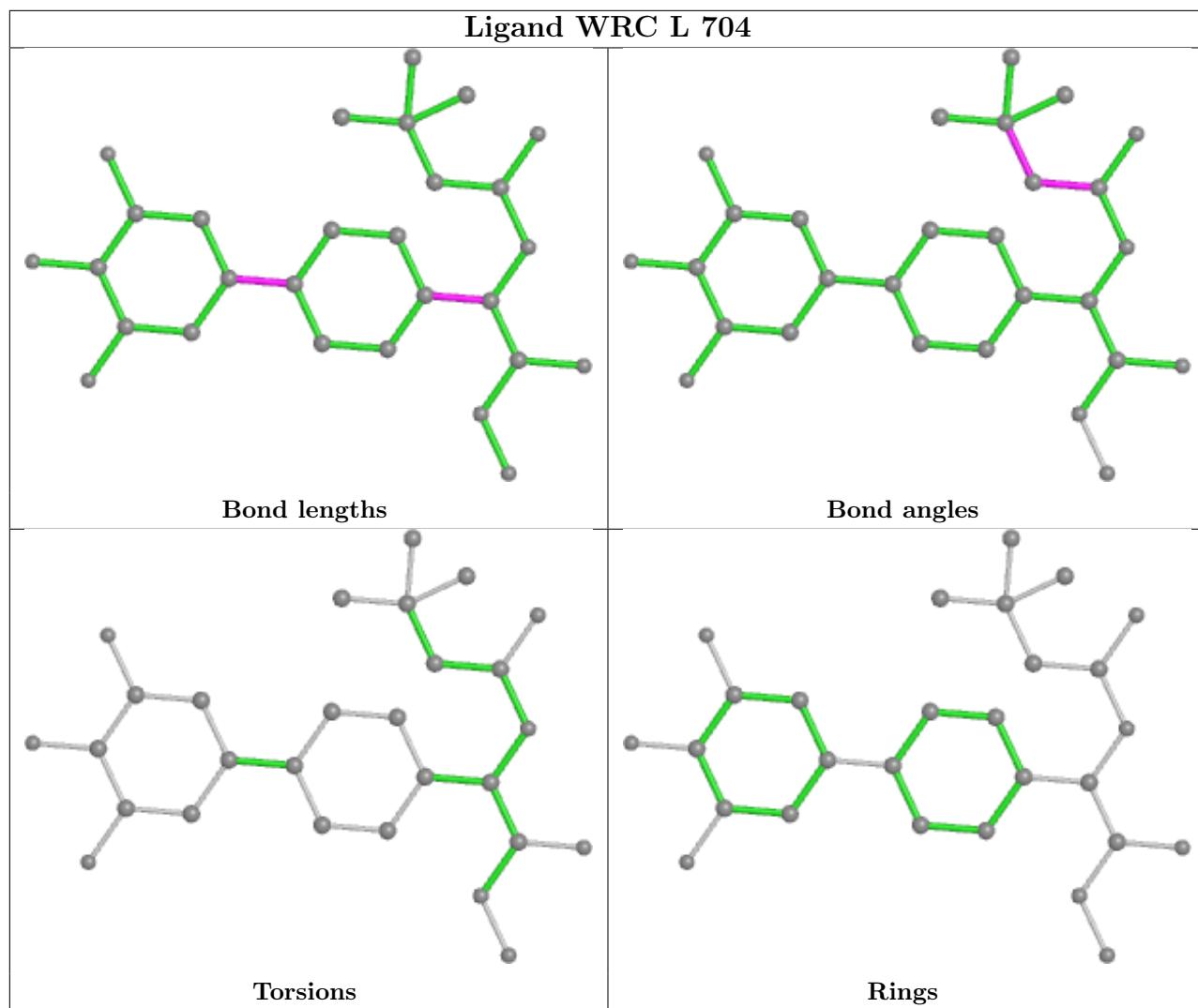


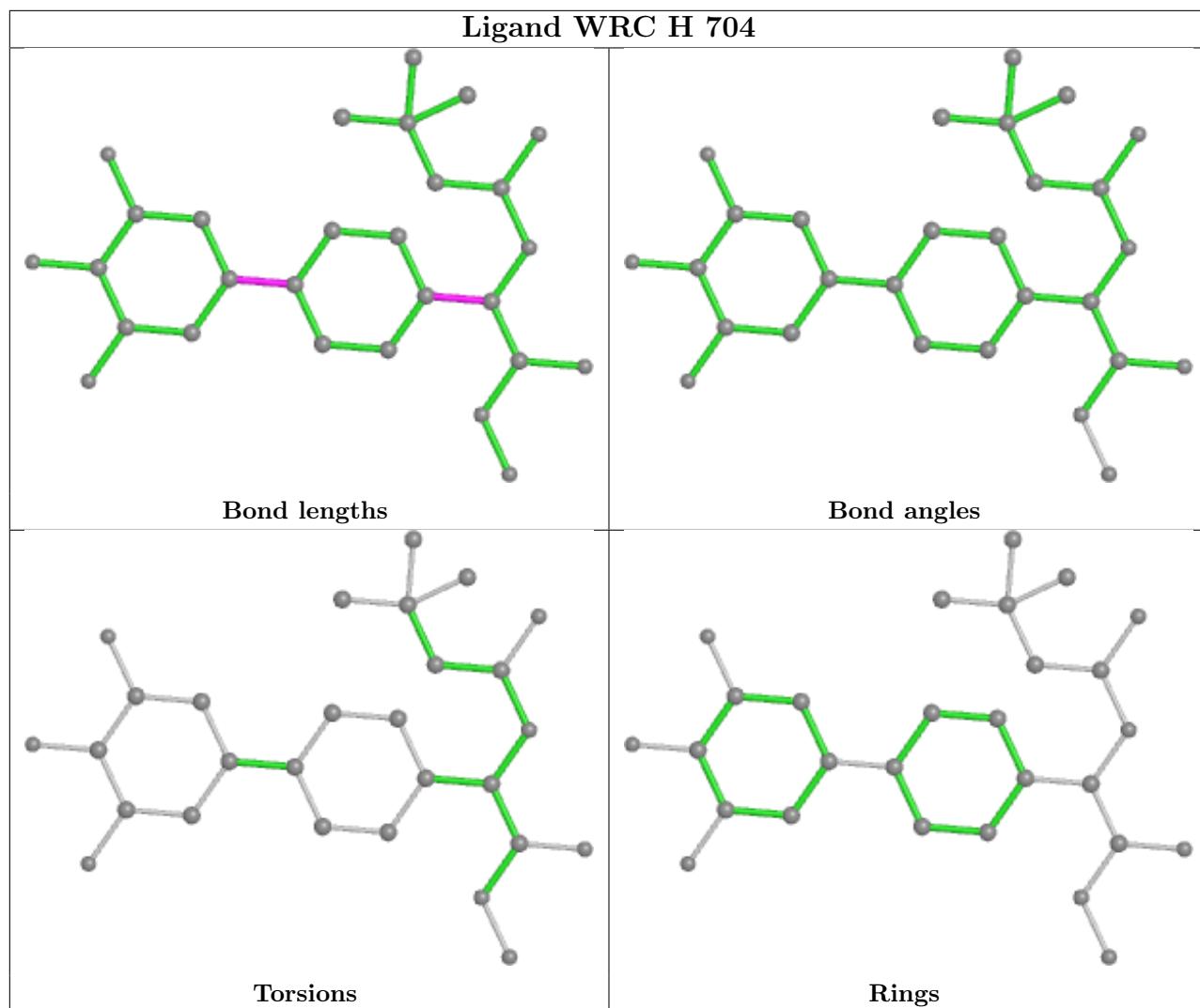


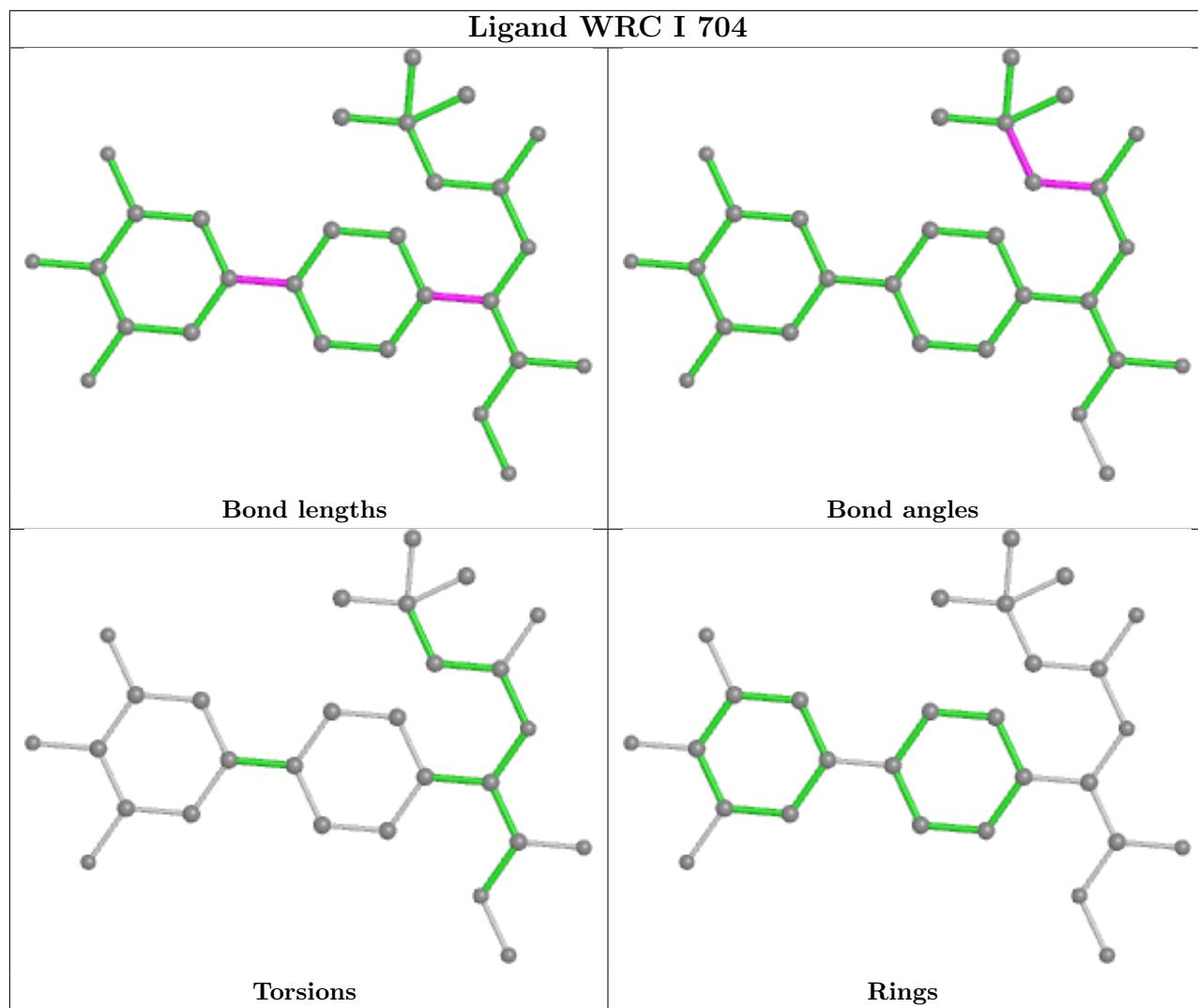


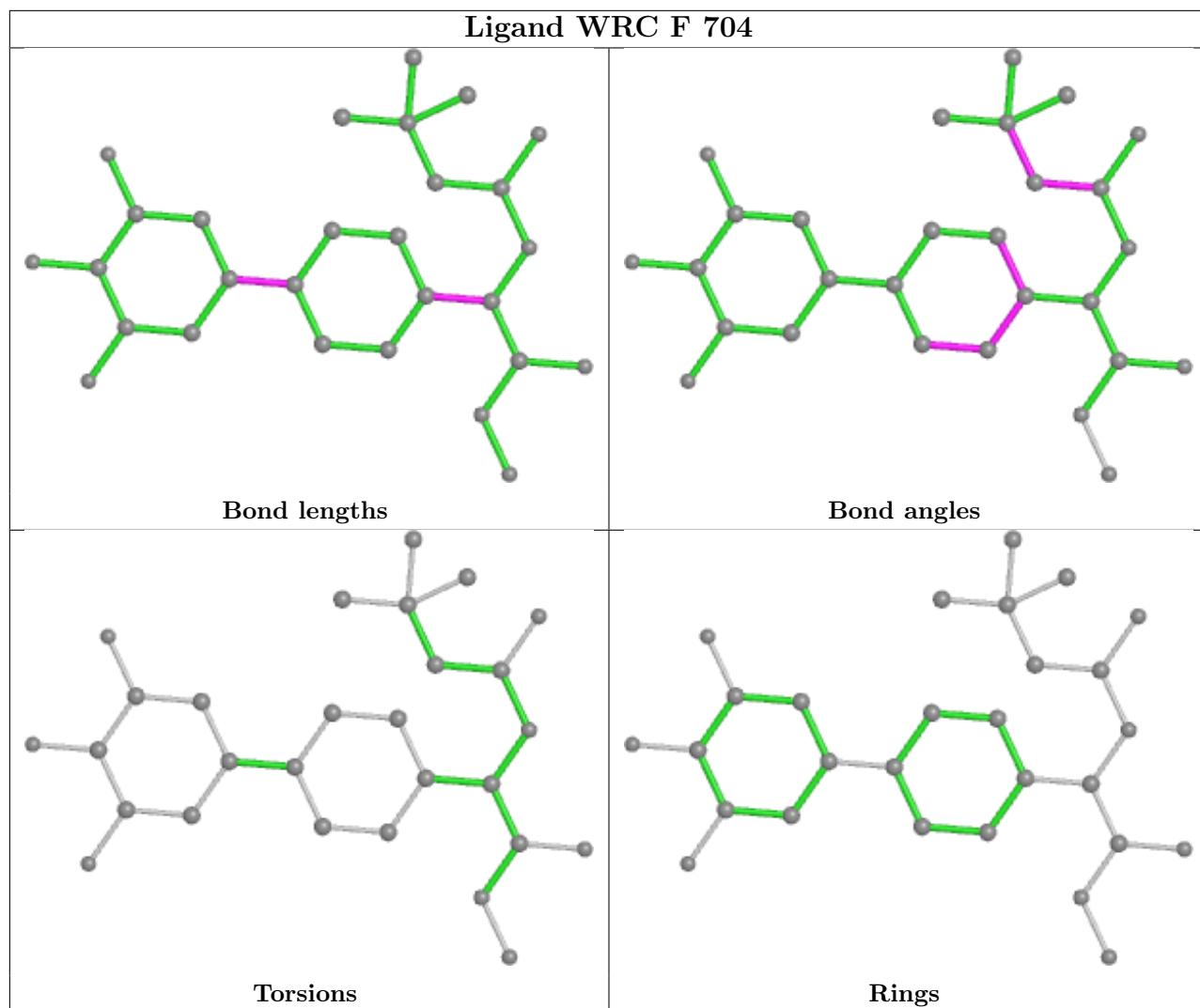


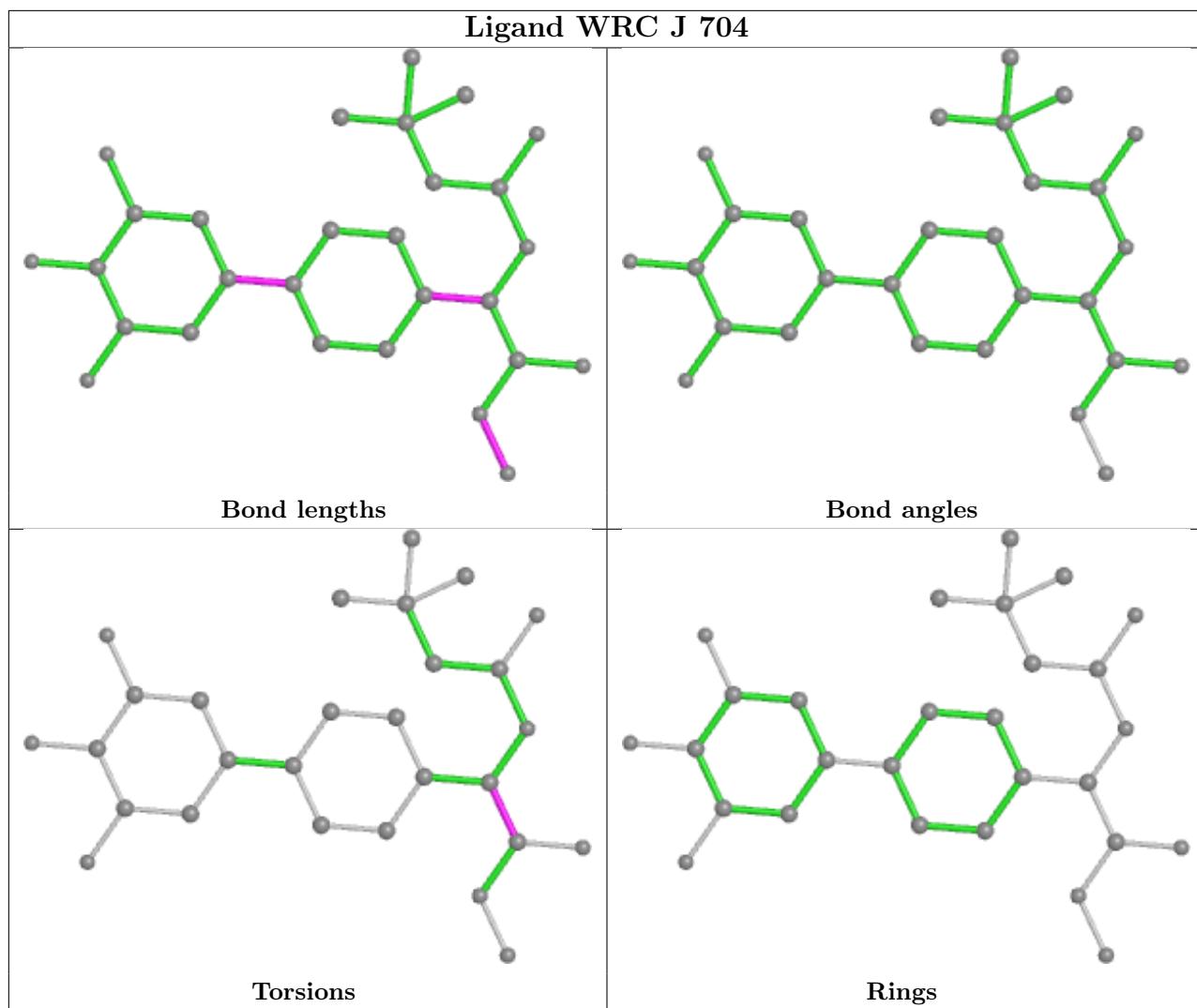


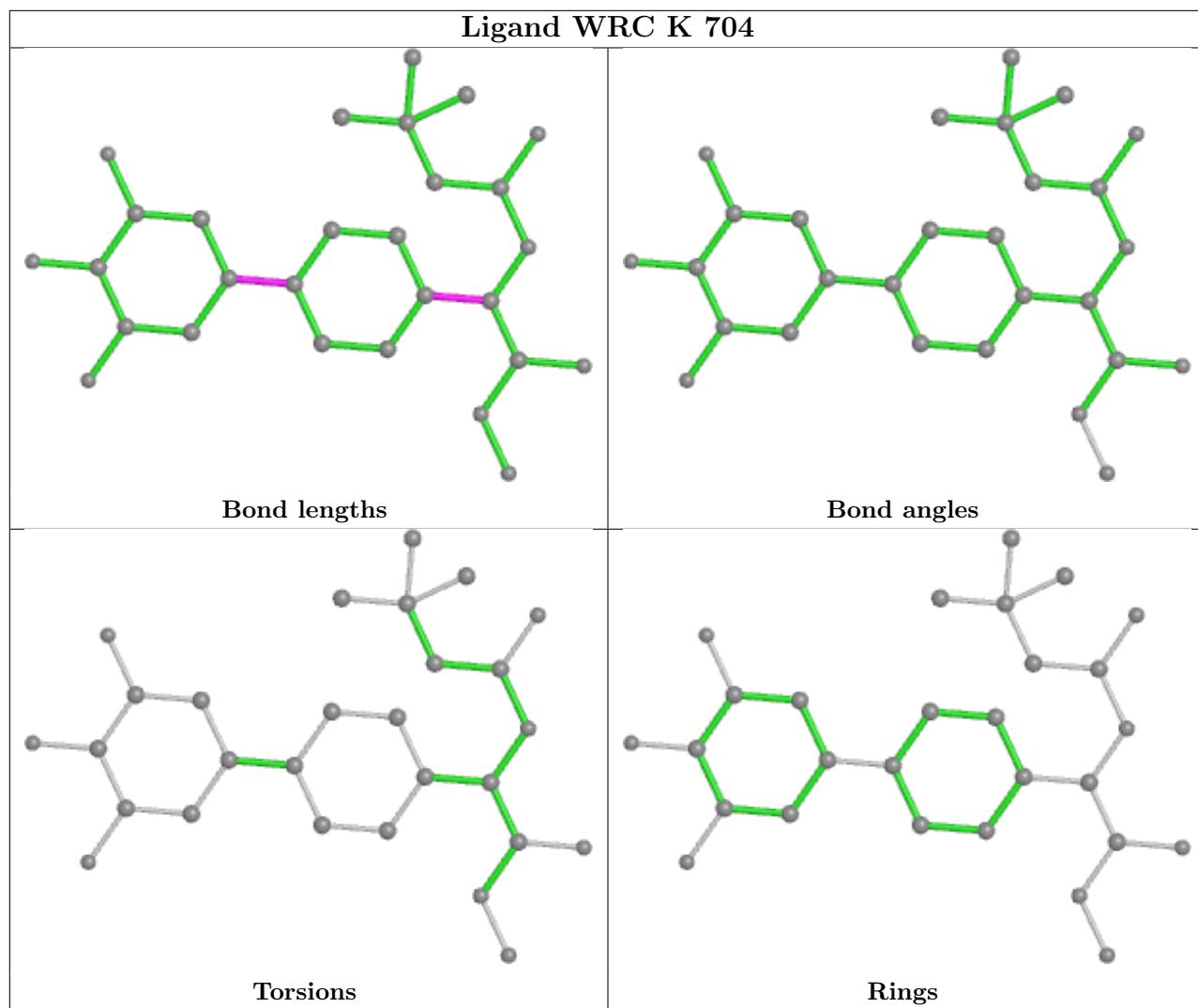


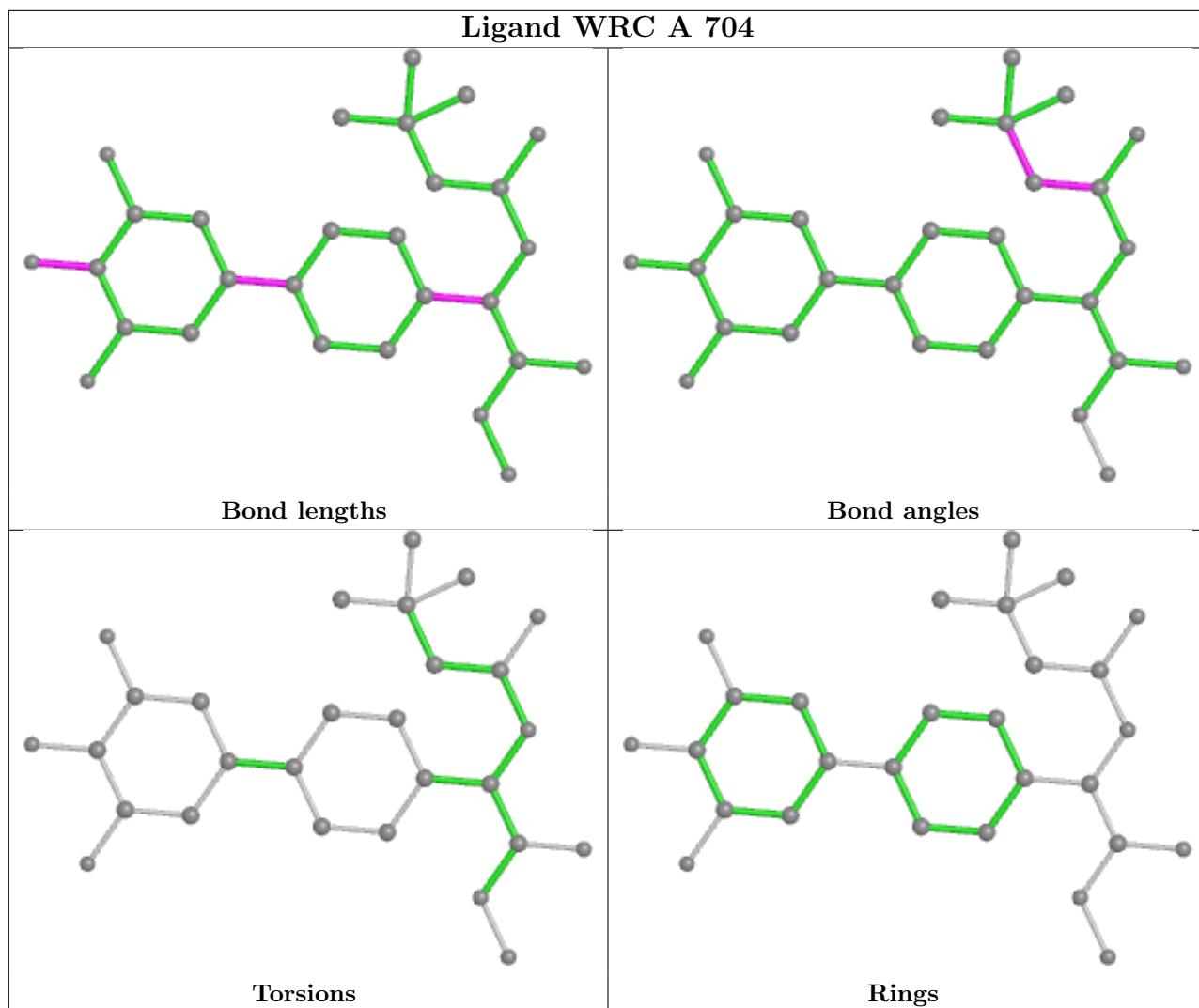












5.7 Other polymers [\(i\)](#)

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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	519/528 (98%)	-0.29	2 (0%)	92	95	12, 23, 42, 68
1	B	517/528 (97%)	-0.10	9 (1%)	70	76	13, 26, 56, 84
1	C	516/528 (97%)	-0.24	1 (0%)	95	96	10, 23, 48, 76
1	D	514/528 (97%)	-0.36	6 (1%)	79	83	9, 23, 43, 87
1	E	509/528 (96%)	-0.41	1 (0%)	95	96	11, 22, 38, 76
1	F	512/528 (96%)	-0.23	4 (0%)	86	89	11, 26, 50, 72
1	G	519/528 (98%)	-0.28	2 (0%)	92	95	11, 23, 42, 74
1	H	517/528 (97%)	-0.13	10 (1%)	66	73	12, 26, 58, 85
1	I	518/528 (98%)	-0.25	3 (0%)	89	92	11, 24, 46, 93
1	J	514/528 (97%)	-0.34	8 (1%)	72	77	10, 22, 44, 79
1	K	509/528 (96%)	-0.39	3 (0%)	89	92	12, 22, 38, 65
1	L	512/528 (96%)	-0.27	3 (0%)	89	92	12, 25, 49, 75
All	All	6176/6336 (97%)	-0.27	52 (0%)	86	89	9, 24, 49, 93
							91 (1%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	398	PHE	4.4
1	H	144	ILE	3.9
1	G	551	VAL	3.4
1	I	549	SER	3.3
1	D	85	ALA	3.3
1	L	398	PHE	3.1
1	J	260	ASN	3.1
1	D	136	GLY	3.0
1	J	261	MET	2.9
1	J	219	LEU	2.9
1	B	228	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	H	180	ASP	2.8
1	I	398	PHE	2.8
1	J	398	PHE	2.7
1	C	398	PHE	2.7
1	J	255	THR	2.7
1	F	123	VAL	2.7
1	L	146	SER	2.6
1	B	194	SER	2.6
1	E	551	VAL	2.6
1	H	152	GLN	2.5
1	J	229	ASN	2.5
1	H	159	ASP	2.5
1	D	260	ASN	2.4
1	H	198	LEU	2.4
1	B	261	MET	2.4
1	D	603	ASP	2.3
1	K	272	ASN	2.3
1	B	136	GLY	2.3
1	K	273	ASN	2.3
1	B	195	VAL	2.3
1	H	602	ASN	2.3
1	B	145	SER	2.3
1	H	195	VAL	2.2
1	F	196	ALA	2.2
1	J	136	GLY	2.2
1	I	135	PRO	2.2
1	F	138	GLU	2.2
1	A	137	LYS	2.2
1	D	261	MET	2.2
1	B	119	GLY	2.2
1	B	120	GLY	2.2
1	H	603	ASP	2.2
1	D	195	VAL	2.2
1	A	136	GLY	2.1
1	B	603	ASP	2.1
1	F	273	ASN	2.1
1	J	123	VAL	2.1
1	H	273	ASN	2.1
1	H	276	THR	2.1
1	L	137	LYS	2.1
1	K	362	LYS	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 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
5	1PE	L	706	10/16	0.32	0.63	82,95,103,104	0
5	1PE	L	705	10/16	0.42	0.47	86,89,93,93	0
5	1PE	F	706	12/16	0.67	0.26	28,76,81,81	0
5	1PE	L	707	10/16	0.73	0.28	44,59,68,68	0
5	1PE	G	706	12/16	0.74	0.21	58,60,67,69	0
5	1PE	C	705	15/16	0.76	0.24	45,56,67,67	0
5	1PE	A	707	15/16	0.76	0.26	46,56,64,65	0
5	1PE	I	706	9/16	0.79	0.19	32,42,50,51	0
5	1PE	I	705	13/16	0.80	0.21	47,54,58,59	0
5	1PE	A	706	6/16	0.81	0.17	38,39,42,43	0
5	1PE	H	706	10/16	0.82	0.26	57,61,71,72	0
3	ZN	B	703	1/1	0.82	0.12	82,82,82,82	1
5	1PE	J	705	10/16	0.83	0.19	42,46,52,53	0
5	1PE	E	706	12/16	0.83	0.20	34,44,62,62	0
3	ZN	L	703	1/1	0.84	0.09	68,68,68,68	0
5	1PE	F	705	10/16	0.84	0.18	36,43,48,49	0
5	1PE	B	705	10/16	0.84	0.19	38,42,52,52	0
3	ZN	H	702	1/1	0.84	0.09	62,62,62,62	1
5	1PE	H	705	10/16	0.84	0.23	52,59,66,67	0
5	1PE	E	705	10/16	0.84	0.19	41,48,53,54	0
5	1PE	B	706	10/16	0.85	0.16	36,46,48,49	0
5	1PE	C	707	7/16	0.85	0.21	42,46,48,48	0
5	1PE	D	705	11/16	0.85	0.21	44,50,58,59	0
5	1PE	I	707	9/16	0.85	0.18	47,50,51,52	0
5	1PE	J	706	10/16	0.86	0.19	45,49,65,66	0
5	1PE	G	705	9/16	0.86	0.16	29,34,36,36	0
5	1PE	K	705	12/16	0.87	0.21	44,49,57,60	0

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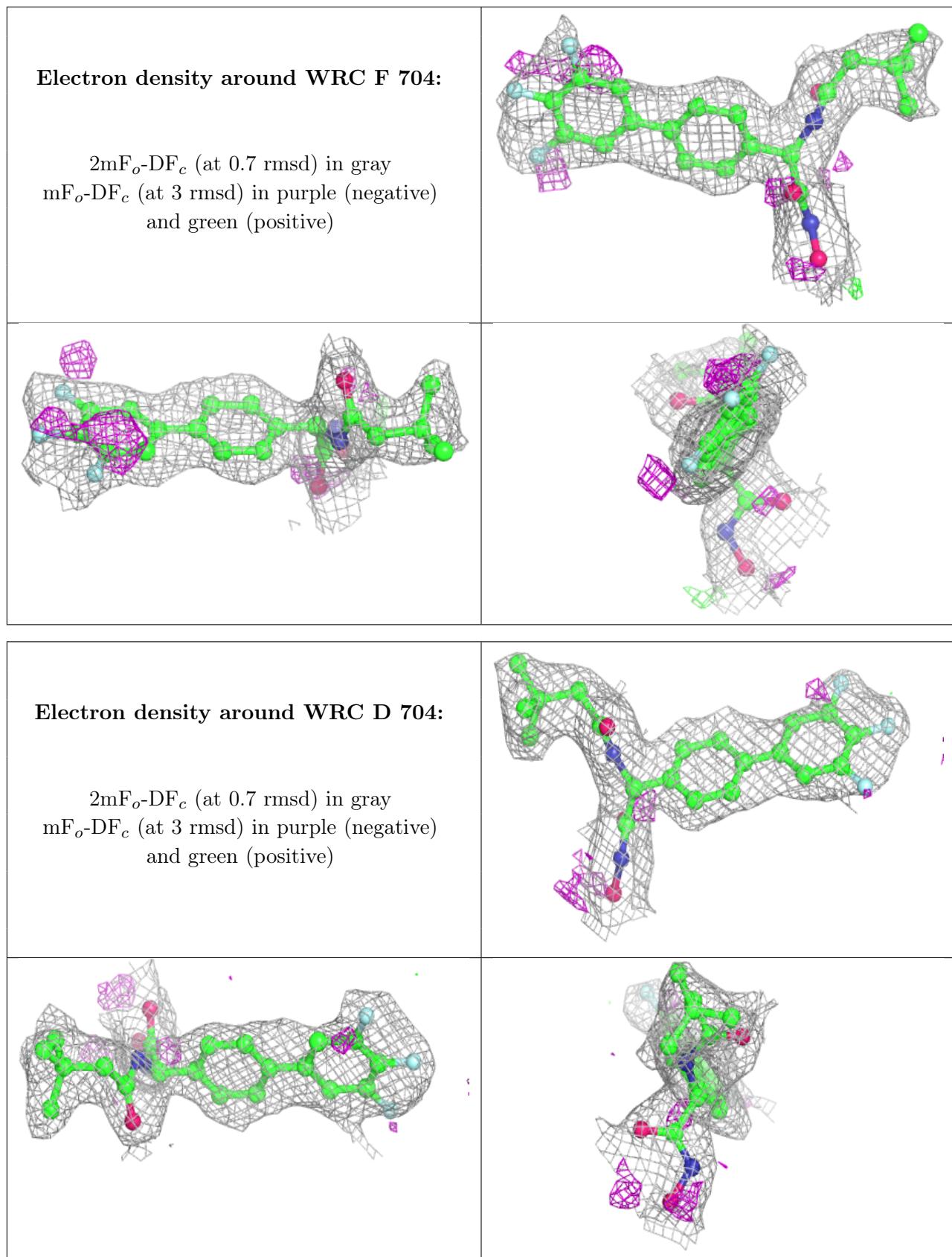
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	1PE	C	706	11/16	0.87	0.17	30,40,45,46	0
6	SO4	L	708	5/5	0.89	0.23	83,83,84,87	0
6	SO4	C	709	5/5	0.90	0.25	73,74,76,76	0
2	CO3	K	701	4/4	0.90	0.20	29,32,34,34	0
5	1PE	A	705	9/16	0.91	0.16	36,39,43,43	0
3	ZN	I	702	1/1	0.91	0.08	56,56,56,56	1
5	1PE	E	707	6/16	0.91	0.14	32,37,40,42	0
4	WRC	F	704	28/28	0.91	0.15	22,32,56,60	0
4	WRC	D	704	28/28	0.92	0.14	13,28,53,59	0
2	CO3	C	701	4/4	0.92	0.19	23,30,32,34	0
4	WRC	I	704	28/28	0.92	0.14	27,35,52,56	0
6	SO4	C	708	5/5	0.92	0.24	86,86,87,87	0
2	CO3	A	701	4/4	0.92	0.19	25,28,29,33	0
5	1PE	D	706	10/16	0.92	0.13	51,53,55,57	0
4	WRC	L	704	28/28	0.93	0.13	19,27,50,53	0
4	WRC	A	704	28/28	0.93	0.16	16,28,51,56	0
4	WRC	C	704	28/28	0.93	0.12	14,27,53,58	0
2	CO3	B	701	4/4	0.93	0.23	14,22,24,35	0
4	WRC	E	704	28/28	0.93	0.13	19,29,49,54	0
6	SO4	A	708	5/5	0.93	0.14	86,86,87,87	0
2	CO3	L	701	4/4	0.93	0.19	16,26,31,32	0
4	WRC	G	704	28/28	0.93	0.15	22,26,51,62	0
6	SO4	D	707	5/5	0.93	0.24	58,58,59,60	0
6	SO4	G	707	5/5	0.93	0.19	69,69,70,72	0
6	SO4	K	706	5/5	0.93	0.22	87,87,89,89	0
2	CO3	E	701	4/4	0.93	0.19	23,25,28,32	0
3	ZN	C	702	1/1	0.94	0.06	44,44,44,44	1
4	WRC	H	704	28/28	0.94	0.15	19,28,48,54	0
4	WRC	B	704	28/28	0.94	0.15	17,27,49,55	0
4	WRC	J	704	28/28	0.94	0.14	19,33,44,45	0
3	ZN	E	703	1/1	0.94	0.07	36,36,36,36	1
2	CO3	F	701	4/4	0.94	0.18	31,32,32,37	0
2	CO3	H	701	4/4	0.94	0.18	28,31,33,35	0
2	CO3	I	701	4/4	0.94	0.16	18,19,19,25	0
3	ZN	K	703	1/1	0.95	0.04	45,45,45,45	0
6	SO4	G	708	5/5	0.95	0.20	60,60,61,62	0
3	ZN	K	702	1/1	0.95	0.07	70,70,70,70	0
4	WRC	K	704	28/28	0.95	0.13	19,27,46,48	0
3	ZN	G	702	1/1	0.96	0.08	61,61,61,61	1
2	CO3	G	701	4/4	0.96	0.19	21,22,23,30	0
3	ZN	L	702	1/1	0.96	0.06	44,44,44,44	0
2	CO3	D	701	4/4	0.96	0.18	19,26,31,35	0

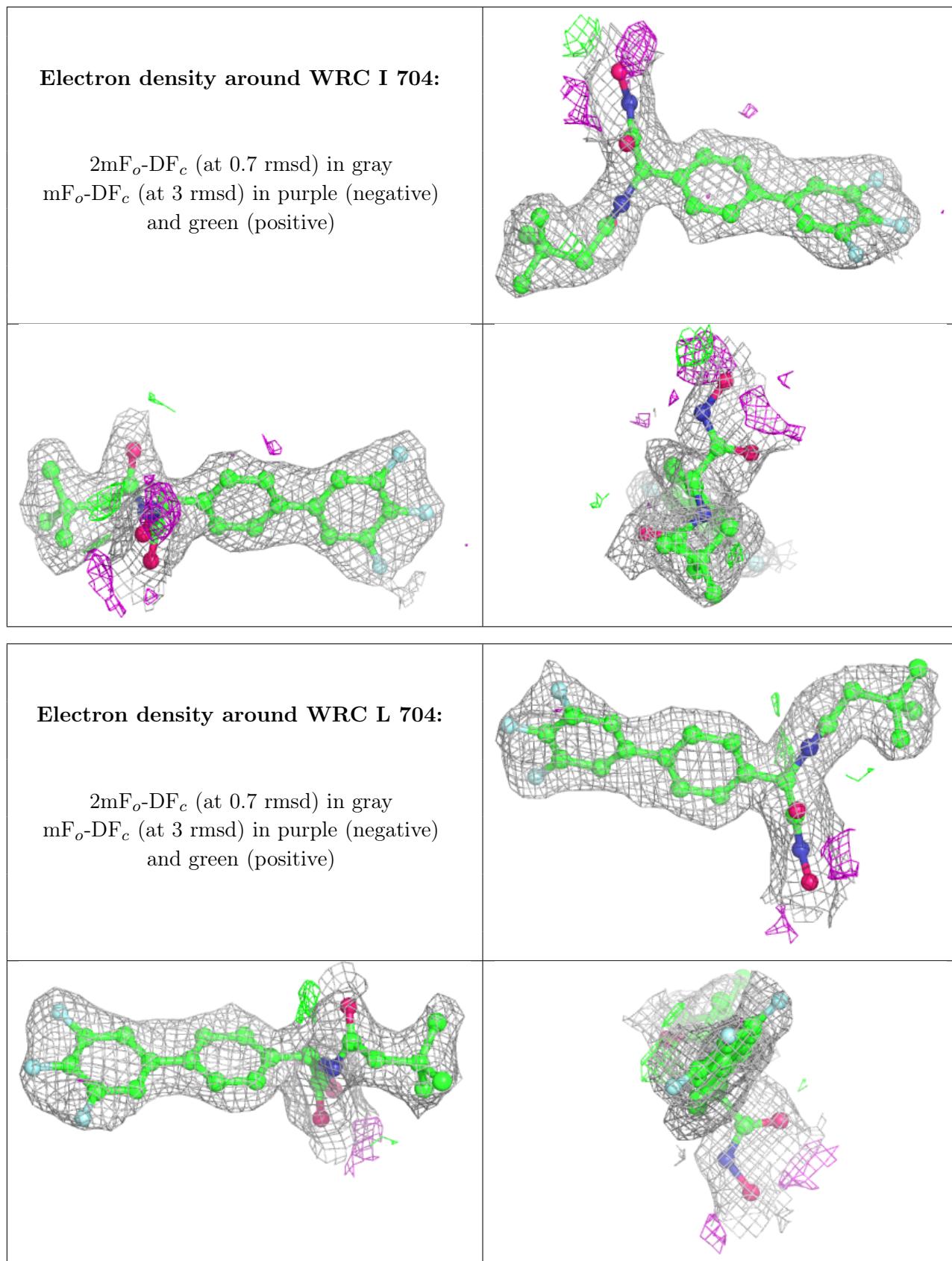
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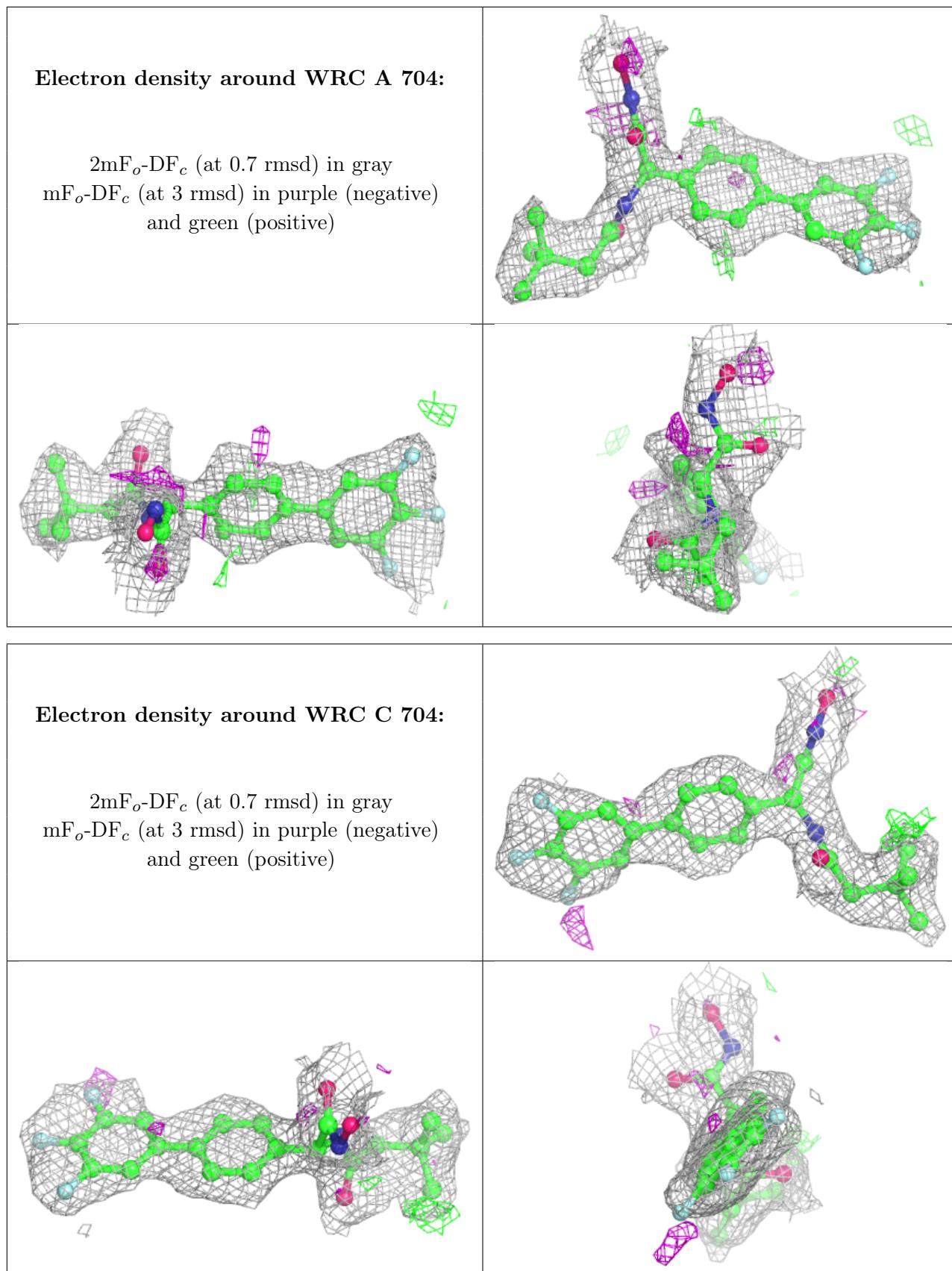
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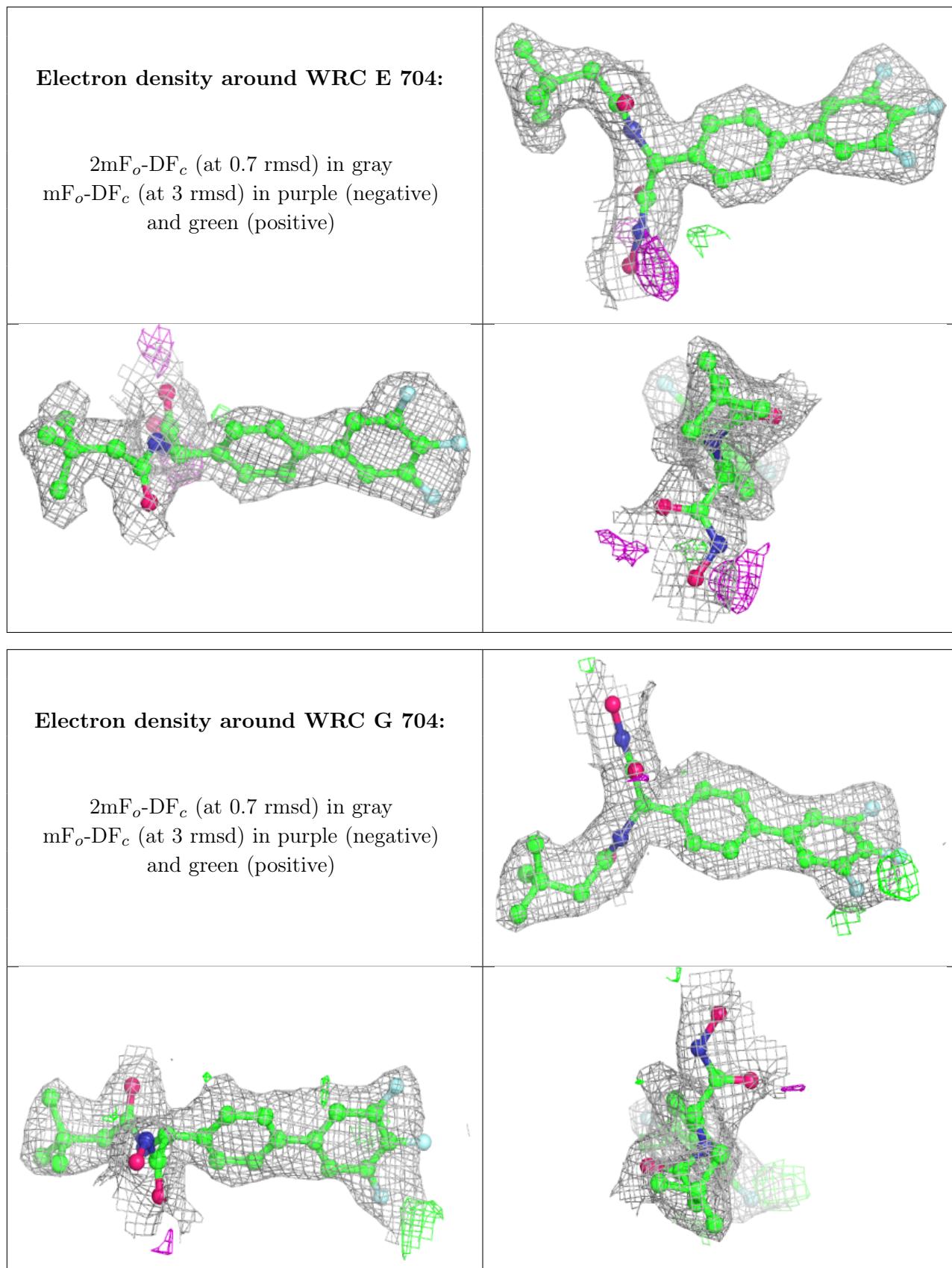
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	ZN	I	703	1/1	0.97	0.05	50,50,50,50	0
3	ZN	J	702	1/1	0.97	0.06	56,56,56,56	0
3	ZN	J	703	1/1	0.97	0.06	42,42,42,42	0
2	CO3	J	701	4/4	0.97	0.13	17,25,29,31	0
3	ZN	F	702	1/1	0.97	0.05	65,65,65,65	0
3	ZN	F	703	1/1	0.97	0.04	45,45,45,45	0
3	ZN	A	703	1/1	0.97	0.08	57,57,57,57	1
3	ZN	G	703	1/1	0.97	0.05	38,38,38,38	0
3	ZN	D	702	1/1	0.97	0.04	48,48,48,48	1
3	ZN	H	703	1/1	0.97	0.05	42,42,42,42	0
3	ZN	E	702	1/1	0.97	0.06	70,70,70,70	0
3	ZN	A	702	1/1	0.98	0.04	37,37,37,37	0
3	ZN	D	703	1/1	0.98	0.04	32,32,32,32	1
3	ZN	C	703	1/1	0.99	0.07	35,35,35,35	1
3	ZN	B	702	1/1	0.99	0.05	39,39,39,39	0
6	SO4	G	709	5/5	0.99	0.11	14,21,24,24	0
6	SO4	J	707	5/5	0.99	0.11	21,25,25,26	0
6	SO4	A	709	5/5	0.99	0.14	19,19,25,26	0
6	SO4	F	707	5/5	0.99	0.11	23,24,26,26	0

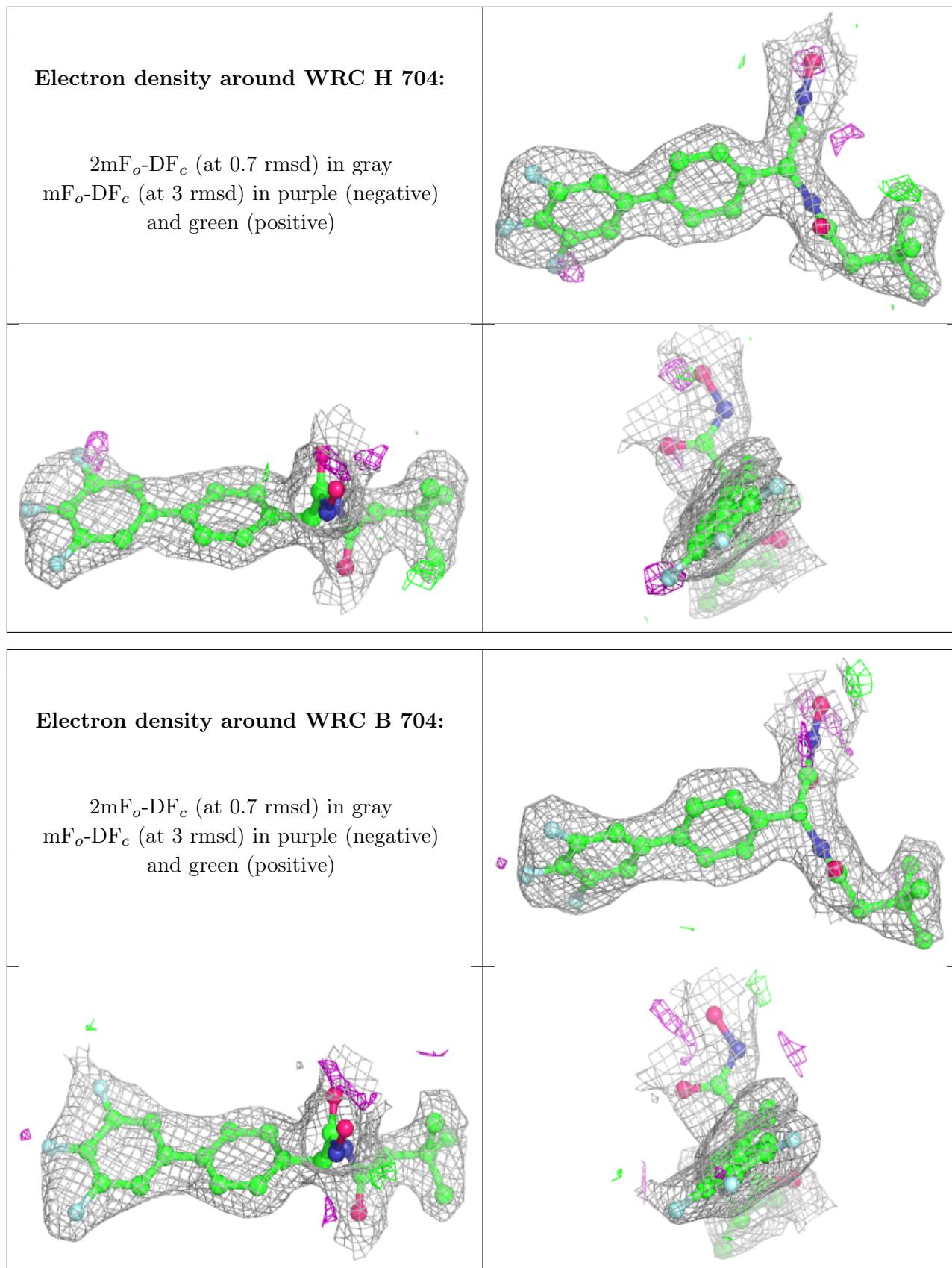
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

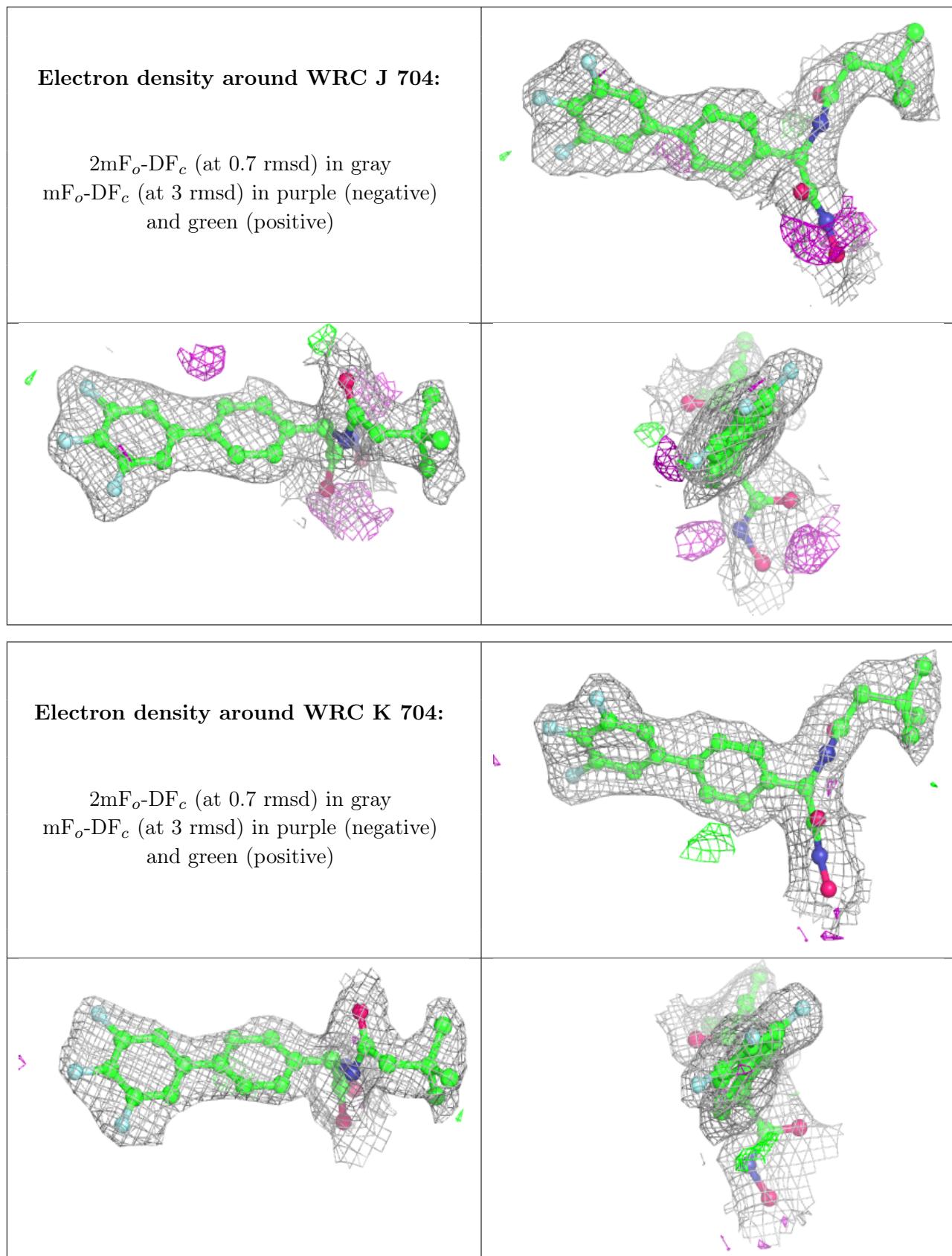












6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.