



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:37 AM UTC

PDB ID : 3BGL / pdb_00003bgl
Title : Hepatoselectivity of Statins: Design and synthesis of 4-sulfamoyl pyrroles as HMG-CoA reductase inhibitors
Authors : Finzel, B.C.; Pavlovsky, A.; Park, W.K.C.
Deposited on : 2007-11-26
Resolution : 2.23 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

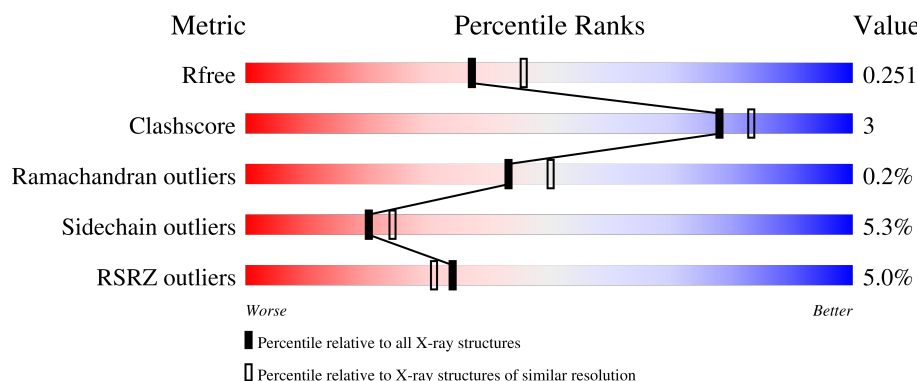
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	441	5% 83% 12% 5%
1	B	441	4% 86% 8% 5%
1	C	441	9% 85% 8% 6%
1	D	441	2% 87% 6% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13232 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 3-hydroxy-3-methylglutaryl-coenzyme A reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	B	421	Total	C	N	O	S	0	0	0
			3133	1951	551	601	30			
1	C	414	Total	C	N	O	S	0	0	0
			3073	1915	538	590	30			
1	D	410	Total	C	N	O	S	0	0	0
			3050	1901	535	584	30			

There are 28 discrepancies between the modelled and reference sequences:

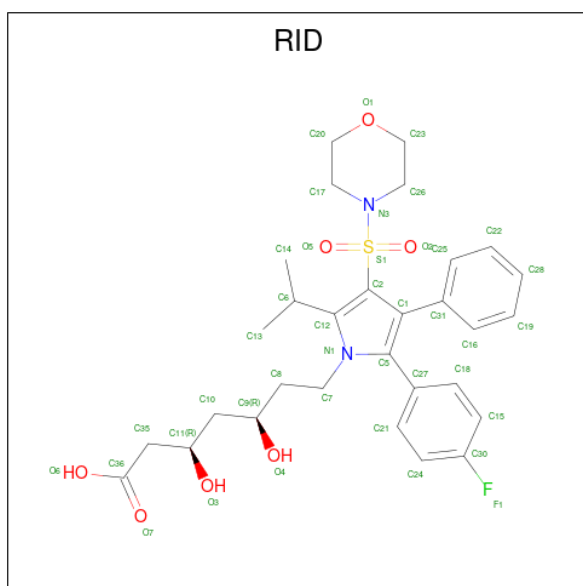
Chain	Residue	Modelled	Actual	Comment	Reference
A	435	HIS	-	expression tag	UNP P04035
A	436	HIS	-	expression tag	UNP P04035
A	437	HIS	-	expression tag	UNP P04035
A	438	HIS	-	expression tag	UNP P04035
A	439	HIS	-	expression tag	UNP P04035
A	440	HIS	-	expression tag	UNP P04035
A	485	ILE	MET	engineered mutation	UNP P04035
B	435	HIS	-	expression tag	UNP P04035
B	436	HIS	-	expression tag	UNP P04035
B	437	HIS	-	expression tag	UNP P04035
B	438	HIS	-	expression tag	UNP P04035
B	439	HIS	-	expression tag	UNP P04035
B	440	HIS	-	expression tag	UNP P04035
B	485	ILE	MET	engineered mutation	UNP P04035
C	435	HIS	-	expression tag	UNP P04035
C	436	HIS	-	expression tag	UNP P04035
C	437	HIS	-	expression tag	UNP P04035
C	438	HIS	-	expression tag	UNP P04035
C	439	HIS	-	expression tag	UNP P04035
C	440	HIS	-	expression tag	UNP P04035
C	485	ILE	MET	engineered mutation	UNP P04035

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	435	HIS	-	expression tag	UNP P04035
D	436	HIS	-	expression tag	UNP P04035
D	437	HIS	-	expression tag	UNP P04035
D	438	HIS	-	expression tag	UNP P04035
D	439	HIS	-	expression tag	UNP P04035
D	440	HIS	-	expression tag	UNP P04035
D	485	ILE	MET	engineered mutation	UNP P04035

- Molecule 2 is (3R,5R)-7-[2-(4-fluorophenyl)-5-(1-methylethyl)-4-(morpholin-4-ylsulfonyl)-3-phenyl-1H-pyrrol-1-yl]-3,5-dihydroxyheptanoic acid (CCD ID: RID) (formula: C₃₀H₃₇FN₂O₇S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			41	30	1	2	7	1		
2	B	1	Total	C	F	N	O	S	0	0
			41	30	1	2	7	1		
2	C	1	Total	C	F	N	O	S	0	0
			41	30	1	2	7	1		
2	D	1	Total	C	F	N	O	S	0	0
			41	30	1	2	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	191	Total	O	0	0
			191	191		

Continued on next page...

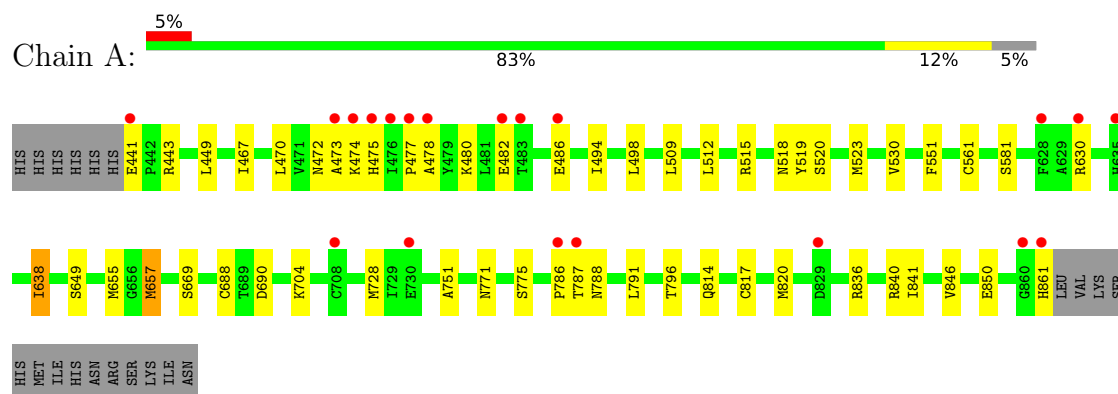
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	169	Total 169	O 169	0	0
3	C	134	Total 134	O 134	0	0
3	D	185	Total 185	O 185	0	0

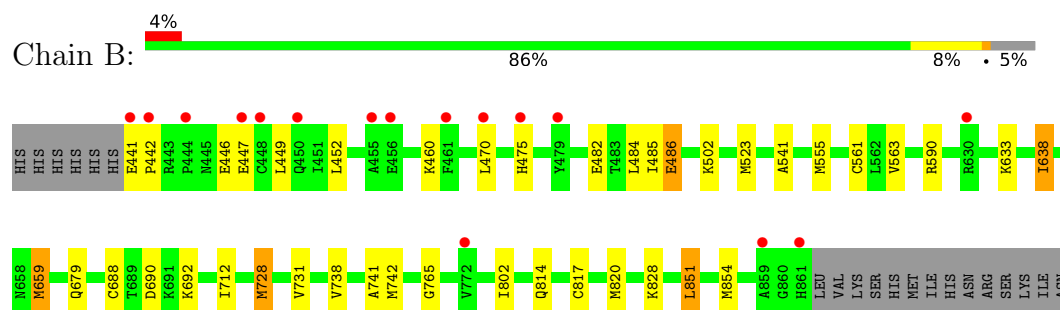
3 Residue-property plots

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

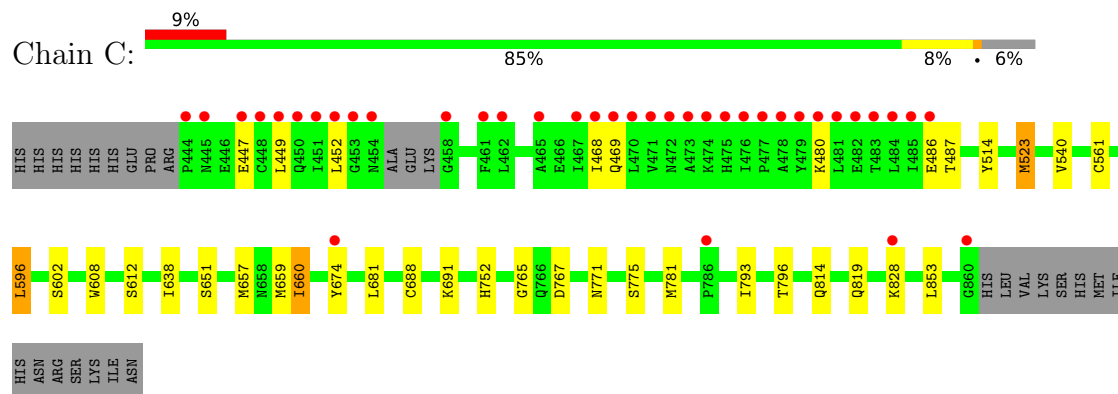
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



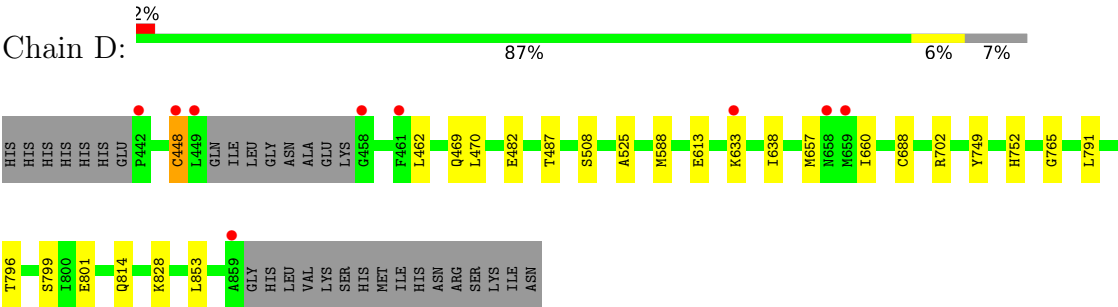
- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



- Molecule 1: 3-hydroxy-3-methylglutaryl-coenzyme A reductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.59Å 172.16Å 75.15Å 90.00° 117.24° 90.00°	Depositor
Resolution (Å)	30.00 – 2.23 30.00 – 2.23	Depositor EDS
% Data completeness (in resolution range)	82.2 (30.00-2.23) 82.2 (30.00-2.23)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.78 (at 2.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.208 , 0.251 0.208 , 0.251	Depositor DCC
R_{free} test set	3345 reflections (2.53%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.843	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 25.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13232	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% of the height of the origin peak. No significant pseudotranslation is detected.*

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: RID

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	0.50	0/3179	0.79	0/4298
1	B	0.49	0/3179	0.79	0/4298
1	C	0.51	0/3116	0.79	1/4211 (0.0%)
1	D	0.50	0/3094	0.80	0/4182
All	All	0.50	0/12568	0.79	1/16989 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	469	GLN	N-CA-C	-5.05	107.11	113.28

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	3133	0	3167	23	0
1	B	3133	0	3167	24	0
1	C	3073	0	3110	16	0
1	D	3050	0	3088	10	0
2	A	41	0	36	2	0
2	B	41	0	36	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	41	0	36	2	0
2	D	41	0	36	3	0
3	A	191	0	0	0	0
3	B	169	0	0	2	0
3	C	134	0	0	1	0
3	D	185	0	0	0	0
All	All	13232	0	12676	70	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 (70) 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:A:657:MET:HE1	1:A:690:ASP:OD2	1.94	0.66
1:B:817:CYS:HA	1:B:820:MET:HE3	1.81	0.62
1:B:657:MET:HE1	1:B:690:ASP:OD2	2.01	0.60
1:B:655:MET:SD	1:B:657:MET:HG3	2.42	0.59
1:A:655:MET:SD	1:A:657:MET:HG3	2.44	0.58
1:B:441:GLU:N	1:B:442:PRO:CD	2.68	0.56
1:A:472:ASN:O	1:A:473:ALA:HB3	2.07	0.54
1:A:817:CYS:HA	1:A:820:MET:HE3	1.90	0.54
2:A:2:RID:H13B	2:A:2:RID:O2	2.09	0.53
1:A:477:PRO:O	1:A:478:ALA:HB2	2.09	0.53
1:D:448:CYS:HB3	1:D:462:LEU:HD22	1.91	0.53
1:B:728:MET:HE1	1:B:851:LEU:HD23	1.91	0.52
1:B:590:ARG:HD2	3:B:989:HOH:O	2.09	0.52
1:C:596:LEU:HD13	1:C:602:SER:HA	1.93	0.51
1:A:523:MET:HE1	1:A:530:VAL:HG21	1.92	0.51
1:A:509:LEU:HD11	1:B:820:MET:HE2	1.91	0.51
1:A:581:SER:OG	1:A:840:ARG:HD2	2.12	0.50
1:A:771:ASN:OD1	1:A:775:SER:OG	2.30	0.50
1:B:449:LEU:HD11	1:B:475:HIS:ND1	2.27	0.49
1:C:561:CYS:HB2	2:D:3:RID:C14	2.43	0.49
1:A:518:ASN:ND2	1:A:520:SER:OG	2.44	0.48
1:B:441:GLU:N	1:B:442:PRO:HD3	2.28	0.48
1:D:752:HIS:CD2	1:D:853:LEU:HD23	2.50	0.47
1:C:468:ILE:HG22	1:C:468:ILE:O	2.13	0.47
1:C:771:ASN:OD1	1:C:775:SER:OG	2.33	0.46
1:B:712:ILE:HG13	1:B:851:LEU:HD11	1.98	0.46
2:B:1:RID:O2	2:B:1:RID:H14B	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:691:LYS:HZ3	1:C:767:ASP:CG	2.24	0.45
1:A:474:LYS:O	1:A:475:HIS:CB	2.64	0.45
1:A:551:PHE:CE2	1:A:841:ILE:HD11	2.52	0.45
1:C:561:CYS:HB2	2:D:3:RID:H14B	1.98	0.44
1:D:765:GLY:CA	1:D:814:GLN:HG2	2.48	0.44
1:A:561:CYS:HB2	2:B:1:RID:C14	2.48	0.44
1:C:819:GLN:HB3	1:D:508:SER:HB3	1.99	0.44
2:A:2:RID:C14	1:B:561:CYS:HB2	2.48	0.44
2:D:3:RID:O2	2:D:3:RID:H13B	2.16	0.44
1:A:519:TYR:HB3	1:A:523:MET:HE3	2.00	0.44
1:B:638:ILE:O	1:C:796:THR:HG21	2.16	0.44
1:C:752:HIS:CD2	1:C:853:LEU:HD23	2.52	0.44
1:A:474:LYS:O	1:A:475:HIS:HB2	2.17	0.44
1:A:751:ALA:O	1:B:692:LYS:NZ	2.48	0.44
1:B:541:ALA:HB2	1:B:555:MET:HE2	2.00	0.44
1:A:796:THR:HG21	1:D:638:ILE:O	2.18	0.44
1:B:765:GLY:HA2	1:B:814:GLN:HG2	2.00	0.44
1:A:638:ILE:O	1:D:796:THR:HG21	2.18	0.43
1:B:555:MET:HE3	1:B:563:VAL:HG22	2.00	0.43
1:A:509:LEU:CD1	1:B:820:MET:HE2	2.48	0.43
1:B:541:ALA:HB2	1:B:555:MET:CE	2.49	0.42
2:C:4:RID:O2	2:C:4:RID:H14B	2.18	0.42
1:A:728:MET:HE3	1:A:791:LEU:CD2	2.50	0.42
1:B:738:VAL:O	1:B:742:MET:HG2	2.19	0.42
1:B:460:LYS:HB2	1:B:486:GLU:HG2	2.00	0.42
1:B:731:VAL:HG12	1:B:854:MET:HE1	2.01	0.42
1:C:781:MET:HE2	1:C:793:ILE:HD12	2.01	0.41
1:B:659:MET:HE3	1:B:659:MET:HB3	1.94	0.41
1:C:608:TRP:CZ2	1:C:674:TYR:CD2	3.08	0.41
1:C:651:SER:HA	1:C:659:MET:HE3	2.02	0.41
1:C:659:MET:SD	1:C:660:ILE:HD12	2.60	0.41
1:C:752:HIS:CD2	1:C:853:LEU:CD2	3.02	0.41
2:C:4:RID:O2	2:C:4:RID:H13B	2.20	0.41
1:A:861:HIS:HA	2:B:1:RID:H28	2.02	0.41
1:C:765:GLY:HA2	1:C:814:GLN:HG2	2.03	0.41
1:B:741:ALA:HB1	1:D:749:TYR:CE1	2.56	0.41
1:C:523:MET:CE	3:C:919:HOH:O	2.67	0.41
1:D:765:GLY:HA2	1:D:814:GLN:HG2	2.03	0.41
1:A:472:ASN:O	1:A:473:ALA:CB	2.69	0.40
1:A:846:VAL:O	1:A:850:GLU:HG2	2.21	0.40
1:B:502:LYS:NZ	3:B:939:HOH:O	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:702:ARG:O	1:D:799:SER:HA	2.22	0.40
1:D:588:MET:HE1	1:D:801:GLU:HG2	2.04	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	311/441 (70%)	297 (96%)	13 (4%)	1 (0%)	36	41
1	B	419/441 (95%)	402 (96%)	17 (4%)	0	100	100
1	C	410/441 (93%)	390 (95%)	19 (5%)	1 (0%)	43	50
1	D	406/441 (92%)	392 (97%)	13 (3%)	1 (0%)	43	50
All	All	1546/1764 (88%)	1481 (96%)	62 (4%)	3 (0%)	43	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	786	PRO
1	C	514	TYR
1	D	525	ALA

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	335/355 (94%)	312 (93%)	23 (7%)	14	15
1	B	335/355 (94%)	316 (94%)	19 (6%)	18	21
1	C	329/355 (93%)	313 (95%)	16 (5%)	22	27
1	D	327/355 (92%)	315 (96%)	12 (4%)	30	39
All	All	1326/1420 (93%)	1256 (95%)	70 (5%)	20	24

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	441	GLU
1	A	443	ARG
1	A	449	LEU
1	A	467	ILE
1	A	470	LEU
1	A	480	LYS
1	A	482	GLU
1	A	486	GLU
1	A	494	ILE
1	A	498	LEU
1	A	512	LEU
1	A	515	ARG
1	A	630	ARG
1	A	638	ILE
1	A	649	SER
1	A	657	MET
1	A	669	SER
1	A	688	CYS
1	A	704	LYS
1	A	787	THR
1	A	788	ASN
1	A	814	GLN
1	A	836	ARG
1	B	446	GLU
1	B	447	GLU
1	B	452	LEU
1	B	470	LEU
1	B	482	GLU
1	B	484	LEU
1	B	485	ILE
1	B	486	GLU
1	B	523	MET
1	B	633	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	638	ILE
1	B	657	MET
1	B	659	MET
1	B	679	GLN
1	B	688	CYS
1	B	728	MET
1	B	802	ILE
1	B	828	LYS
1	B	851	LEU
1	C	447	GLU
1	C	449	LEU
1	C	452	LEU
1	C	480	LYS
1	C	486	GLU
1	C	487	THR
1	C	523	MET
1	C	540	VAL
1	C	596	LEU
1	C	612	SER
1	C	638	ILE
1	C	657	MET
1	C	660	ILE
1	C	681	LEU
1	C	688	CYS
1	C	828	LYS
1	D	448	CYS
1	D	469	GLN
1	D	470	LEU
1	D	482	GLU
1	D	487	THR
1	D	613	GLU
1	D	633	LYS
1	D	657	MET
1	D	660	ILE
1	D	688	CYS
1	D	791	LEU
1	D	828	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	488	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	ASN
1	A	567	ASN
1	A	632	GLN
1	A	679	GLN
1	A	788	ASN
1	A	819	GLN
1	B	454	ASN
1	B	472	ASN
1	B	510	GLN
1	B	529	ASN
1	B	632	GLN
1	B	658	ASN
1	B	679	GLN
1	B	819	GLN
1	C	497	GLN
1	C	632	GLN
1	C	635	HIS
1	C	672	HIS
1	D	472	ASN
1	D	518	ASN
1	D	642	ASN
1	D	770	GLN

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](#)

4 ligands are modelled in this entry.

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
2	RID	D	3	-	42,44,44	1.17	4 (9%)	54,63,63	2.09	12 (22%)
2	RID	C	4	-	42,44,44	1.18	3 (7%)	54,63,63	2.61	11 (20%)
2	RID	B	1	-	42,44,44	1.13	4 (9%)	54,63,63	2.07	12 (22%)
2	RID	A	2	-	42,44,44	1.21	4 (9%)	54,63,63	1.83	7 (12%)

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
2	RID	D	3	-	-	6/35/45/45	0/4/4/4
2	RID	C	4	-	-	6/35/45/45	0/4/4/4
2	RID	B	1	-	-	8/35/45/45	0/4/4/4
2	RID	A	2	-	-	4/35/45/45	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	RID	C1-C5	4.52	1.46	1.39
2	C	4	RID	C1-C5	4.39	1.46	1.39
2	A	2	RID	C1-C5	4.25	1.46	1.39
2	A	2	RID	C5-N1	-3.96	1.33	1.39
2	B	1	RID	C1-C5	3.86	1.45	1.39
2	C	4	RID	C5-N1	-3.75	1.33	1.39
2	B	1	RID	C5-N1	-3.62	1.33	1.39
2	D	3	RID	C5-N1	-3.55	1.33	1.39
2	A	2	RID	C1-C2	-2.98	1.37	1.43
2	C	4	RID	C1-C2	-2.79	1.38	1.43
2	D	3	RID	C1-C2	-2.76	1.38	1.43
2	B	1	RID	C1-C2	-2.62	1.38	1.43
2	A	2	RID	C12-C2	2.46	1.42	1.39
2	B	1	RID	C12-C2	2.36	1.42	1.39
2	D	3	RID	C12-C2	2.14	1.42	1.39

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	RID	C26-N3-C17	10.53	124.22	112.12
2	D	3	RID	O2-S1-O5	-8.48	107.53	119.69
2	C	4	RID	O2-S1-O5	-8.16	107.99	119.69
2	C	4	RID	C20-C17-N3	7.50	113.61	108.27
2	B	1	RID	O2-S1-O5	-7.45	108.99	119.69
2	A	2	RID	O2-S1-O5	-6.92	109.76	119.69
2	B	1	RID	C26-N3-C17	6.17	119.20	112.12
2	D	3	RID	C26-N3-C17	5.97	118.98	112.12
2	A	2	RID	C27-C5-N1	4.95	132.27	122.89
2	D	3	RID	C27-C5-N1	4.75	131.89	122.89
2	A	2	RID	C26-N3-C17	4.74	117.56	112.12
2	C	4	RID	C27-C5-N1	4.59	131.59	122.89
2	B	1	RID	C27-C5-N1	4.33	131.09	122.89
2	A	2	RID	C27-C5-C1	-4.29	119.21	128.66
2	C	4	RID	C27-C5-C1	-3.99	119.88	128.66
2	B	1	RID	C21-C27-C5	-3.94	114.62	120.56
2	C	4	RID	C21-C27-C5	-3.76	114.88	120.56
2	D	3	RID	C27-C5-C1	-3.73	120.44	128.66
2	C	4	RID	C7-C8-C9	-3.44	106.22	113.31
2	B	1	RID	C27-C5-C1	-3.39	121.19	128.66
2	D	3	RID	C23-C26-N3	3.35	110.66	108.27
2	B	1	RID	C7-N1-C5	-3.16	120.85	126.72
2	D	3	RID	C21-C27-C5	-2.98	116.06	120.56
2	B	1	RID	C7-C8-C9	-2.96	107.20	113.31
2	A	2	RID	C21-C27-C5	-2.94	116.12	120.56
2	D	3	RID	C7-C8-C9	-2.94	107.24	113.31
2	B	1	RID	C18-C27-C5	2.81	124.80	120.56
2	B	1	RID	C11-C10-C9	-2.69	110.03	114.28
2	A	2	RID	C7-N1-C5	-2.65	121.78	126.72
2	D	3	RID	C7-N1-C5	-2.57	121.94	126.72
2	B	1	RID	C31-C1-C5	-2.53	122.10	127.01
2	C	4	RID	C18-C27-C5	2.46	124.29	120.56
2	B	1	RID	O2-S1-C2	2.46	112.71	107.67
2	C	4	RID	C7-N1-C5	-2.36	122.33	126.72
2	C	4	RID	C10-C11-C35	-2.24	108.39	112.96
2	D	3	RID	C10-C11-C35	-2.19	108.49	112.96
2	A	2	RID	C11-C10-C9	-2.13	110.91	114.28
2	B	1	RID	C13-C6-C12	-2.10	108.81	112.92
2	D	3	RID	O2-S1-C2	2.09	111.96	107.67
2	C	4	RID	O2-S1-C2	2.09	111.96	107.67
2	D	3	RID	C10-C9-C8	-2.04	108.10	112.42
2	D	3	RID	C18-C27-C5	2.03	123.64	120.56

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	RID	C17-N3-S1-O5
2	B	1	RID	C17-N3-S1-O2
2	C	4	RID	C26-N3-S1-O5
2	C	4	RID	C26-N3-S1-O2
2	D	3	RID	C26-N3-S1-O2
2	D	3	RID	C26-N3-S1-C2
2	B	1	RID	C17-N3-S1-C2
2	C	4	RID	C26-N3-S1-C2
2	A	2	RID	C26-N3-S1-C2
2	A	2	RID	C1-C2-S1-O5
2	B	1	RID	C1-C2-S1-O5
2	D	3	RID	C1-C2-S1-O5
2	D	3	RID	C26-N3-S1-O5
2	B	1	RID	C7-C8-C9-O4
2	A	2	RID	C2-C1-C31-C25
2	B	1	RID	C7-C8-C9-C10
2	A	2	RID	C2-C1-C31-C16
2	C	4	RID	C2-C1-C31-C25
2	C	4	RID	C1-C2-S1-O5
2	C	4	RID	C2-C1-C31-C16
2	D	3	RID	C2-C1-C31-C25
2	B	1	RID	C2-C1-C31-C25
2	B	1	RID	C2-C1-C31-C16
2	D	3	RID	C2-C1-C31-C16

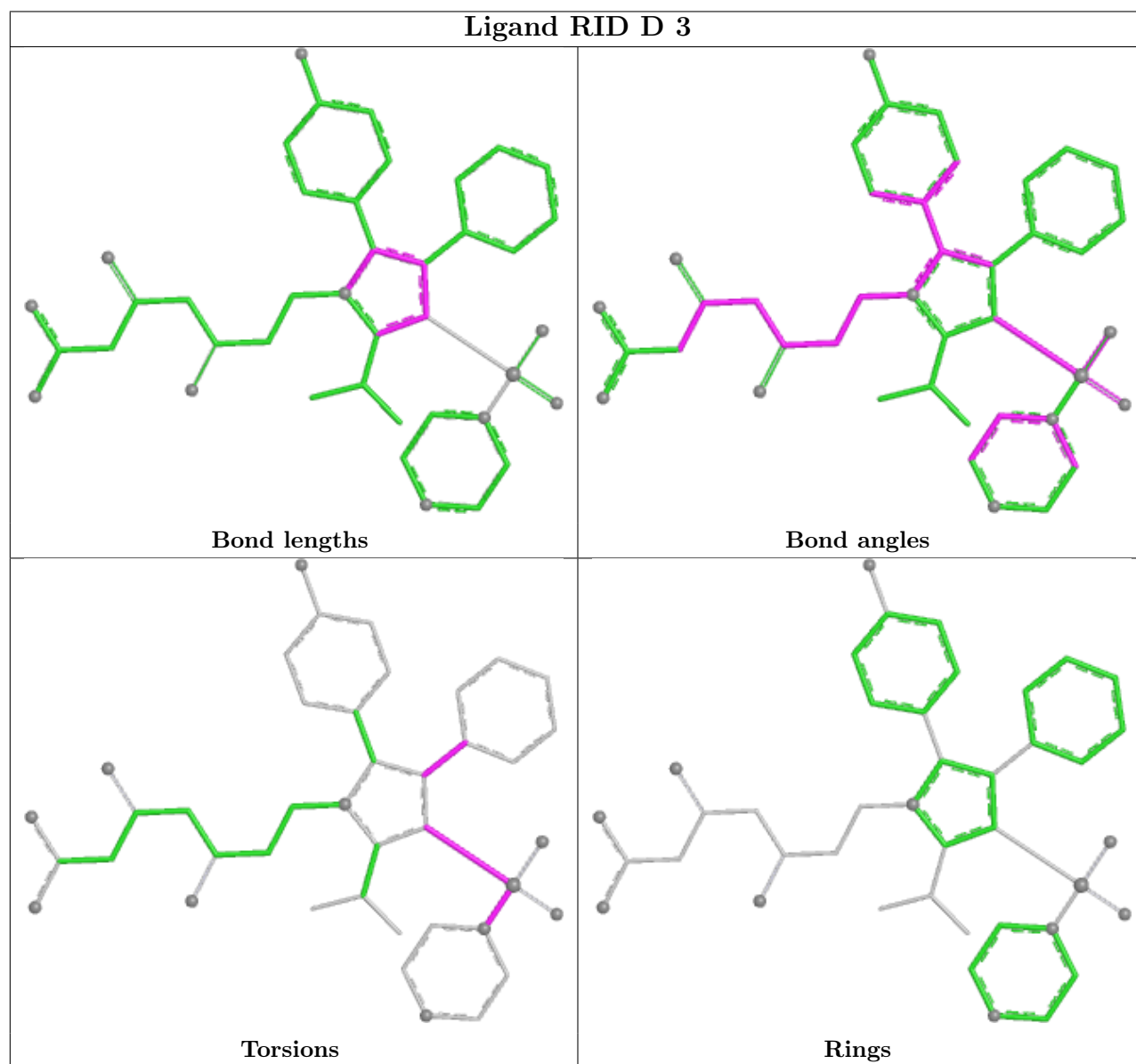
There are no ring outliers.

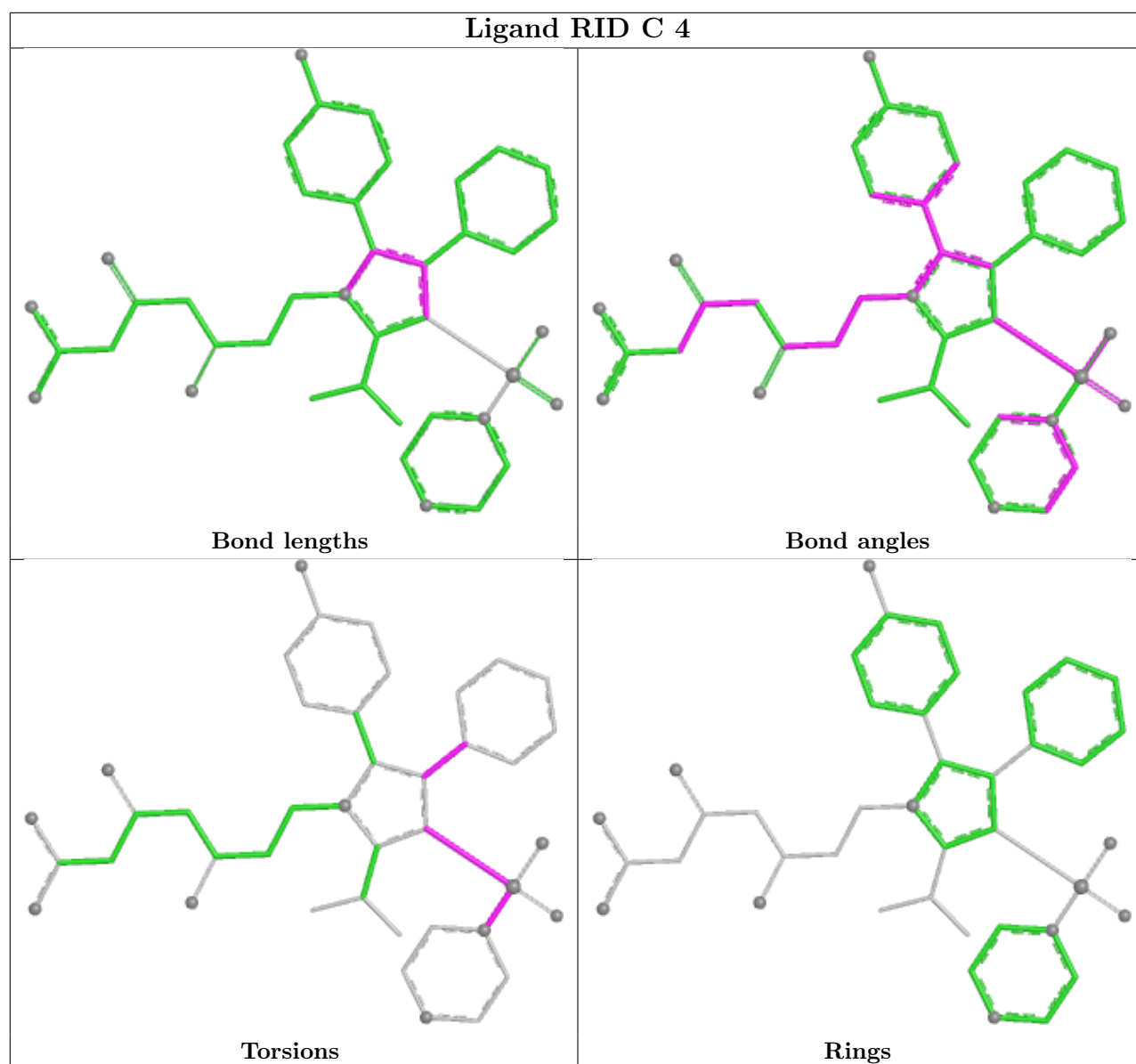
4 monomers are involved in 10 short contacts:

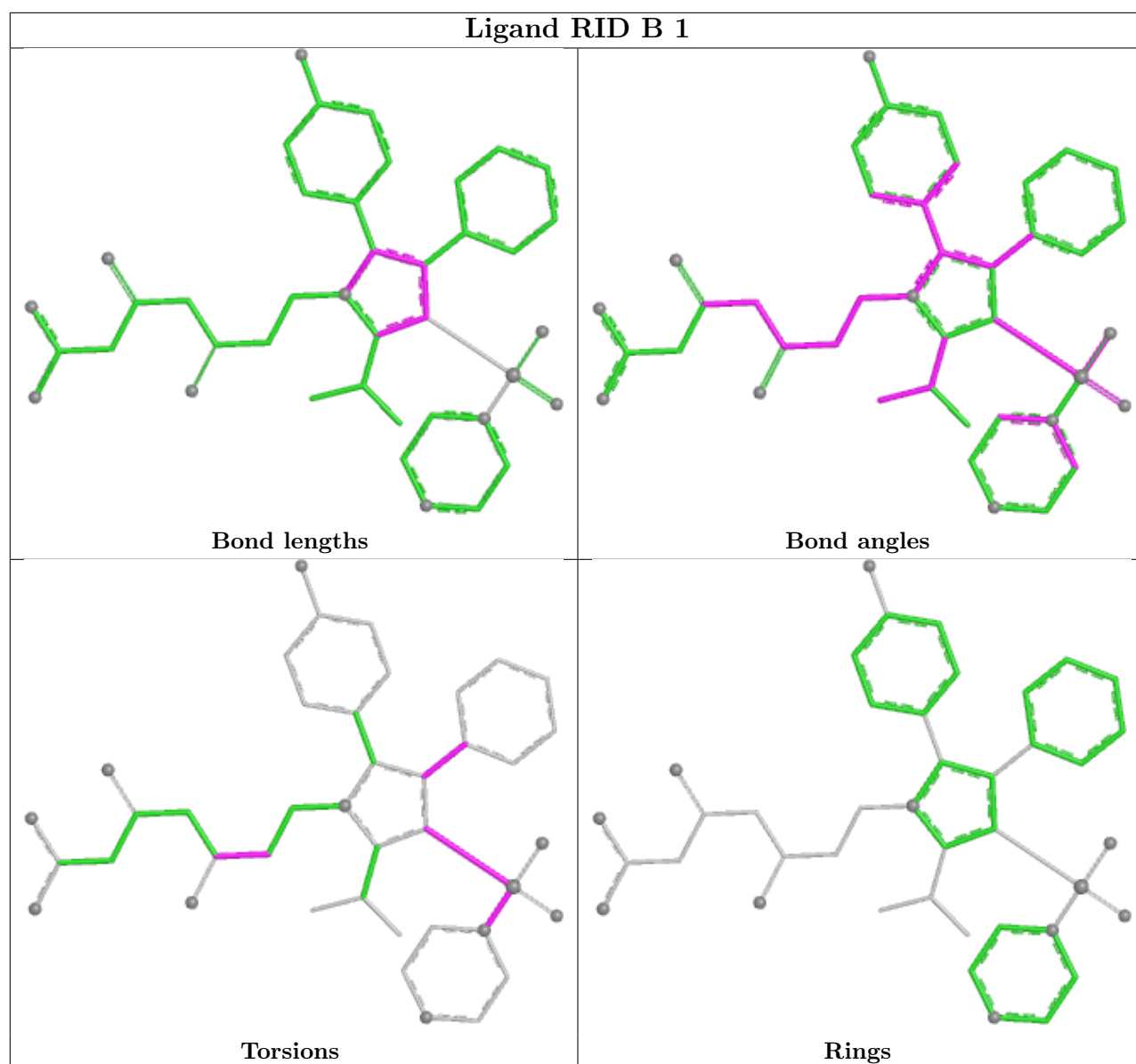
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	RID	3	0
2	C	4	RID	2	0
2	B	1	RID	3	0
2	A	2	RID	2	0

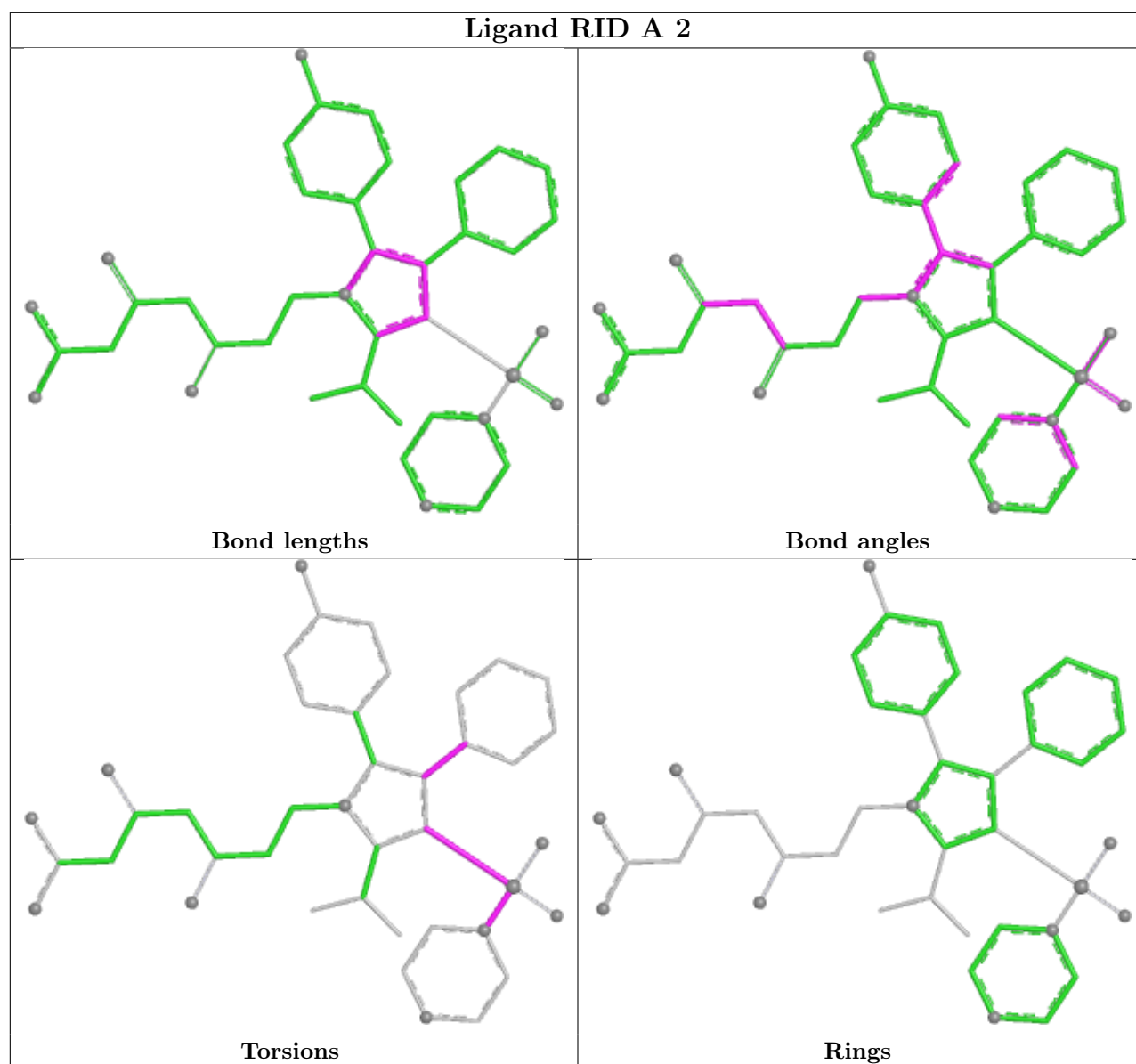
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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	421/441 (95%)	0.30	20 (4%) 35 32	22, 33, 46, 54	0
1	B	421/441 (95%)	0.35	17 (4%) 42 39	24, 34, 58, 64	0
1	C	414/441 (93%)	0.53	38 (9%) 14 12	24, 33, 65, 68	0
1	D	410/441 (92%)	0.28	9 (2%) 62 60	20, 33, 50, 64	0
All	All	1666/1764 (94%)	0.36	84 (5%) 34 31	20, 33, 54, 68	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	472	ASN	6.2
1	C	481	LEU	6.2
1	C	471	VAL	5.1
1	C	444	PRO	5.0
1	C	448	CYS	4.9
1	C	458	GLY	4.5
1	A	475	HIS	4.3
1	C	468	ILE	4.3
1	C	477	PRO	4.3
1	D	449	LEU	4.3
1	B	861	HIS	4.3
1	C	473	ALA	4.2
1	C	475	HIS	4.1
1	C	452	LEU	4.0
1	B	442	PRO	4.0
1	C	453	GLY	3.9
1	C	449	LEU	3.9
1	C	478	ALA	3.8
1	C	476	ILE	3.8
1	B	479	TYR	3.6
1	D	442	PRO	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	461	PHE	3.4
1	A	441	GLU	3.4
1	B	657	MET	3.3
1	C	445	ASN	3.3
1	A	474	LYS	3.3
1	C	474	LYS	3.3
1	C	484	LEU	3.2
1	A	473	ALA	3.1
1	A	786	PRO	3.1
1	D	633	LYS	3.1
1	C	486	GLU	3.0
1	C	451	ILE	3.0
1	C	828	LYS	3.0
1	C	469	GLN	2.9
1	A	476	ILE	2.9
1	C	483	THR	2.8
1	C	479	TYR	2.8
1	C	470	LEU	2.8
1	C	447	GLU	2.7
1	B	444	PRO	2.6
1	C	482	GLU	2.6
1	A	861	HIS	2.6
1	A	730	GLU	2.6
1	A	860	GLY	2.6
1	C	465	ALA	2.5
1	A	477	PRO	2.5
1	B	456	GLU	2.5
1	A	829	ASP	2.5
1	B	455	ALA	2.5
1	B	470	LEU	2.4
1	C	467	ILE	2.4
1	C	450	GLN	2.4
1	B	630	ARG	2.4
1	B	461	PHE	2.4
1	B	447	GLU	2.4
1	C	860	GLY	2.3
1	D	448	CYS	2.3
1	D	461	PHE	2.3
1	C	786	PRO	2.3
1	A	635	HIS	2.3
1	C	480	LYS	2.3
1	B	475	HIS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	482	GLU	2.3
1	A	630	ARG	2.3
1	D	859	ALA	2.2
1	A	628	PHE	2.2
1	B	441	GLU	2.2
1	A	708	CYS	2.2
1	A	486	GLU	2.2
1	C	454	ASN	2.2
1	D	458	GLY	2.2
1	C	674	TYR	2.1
1	C	462	LEU	2.1
1	B	448	CYS	2.1
1	A	478	ALA	2.1
1	A	483	THR	2.1
1	A	787	THR	2.1
1	D	659	MET	2.1
1	B	772	VAL	2.1
1	B	450	GLN	2.1
1	D	658	ASN	2.1
1	B	859	ALA	2.0
1	C	485	ILE	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.

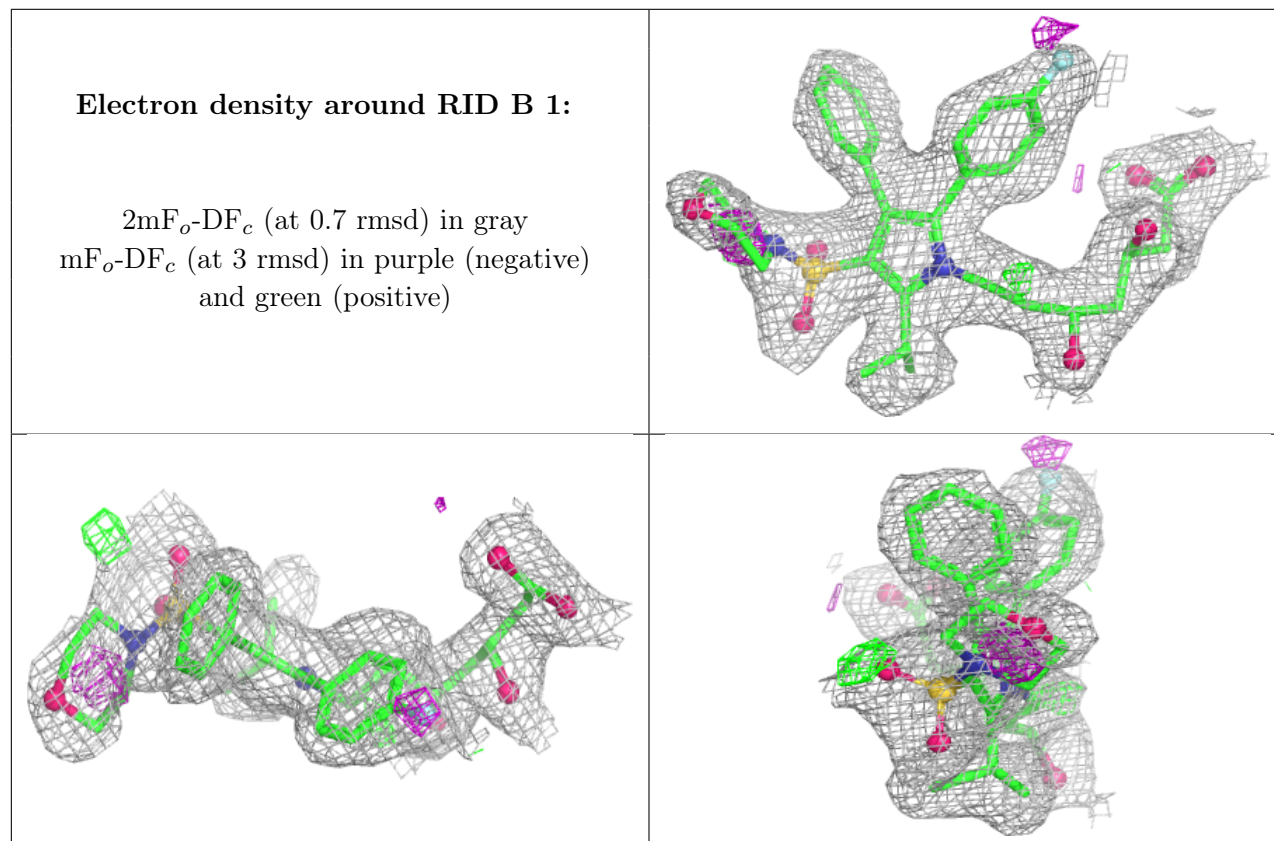
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RID	B	1	41/41	0.89	0.11	29,37,43,44	0
2	RID	C	4	41/41	0.90	0.10	24,32,38,38	0

Continued on next page...

Continued from previous page...

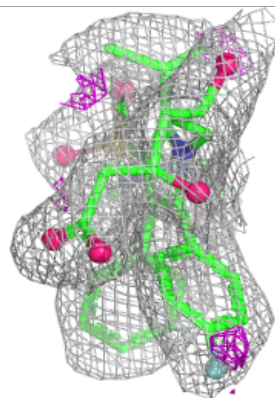
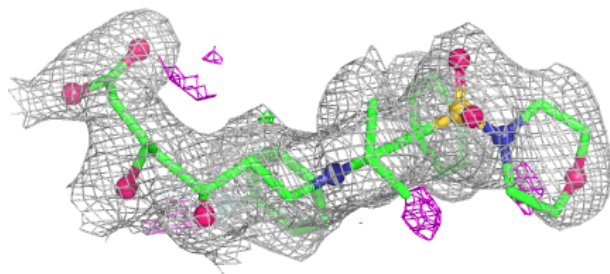
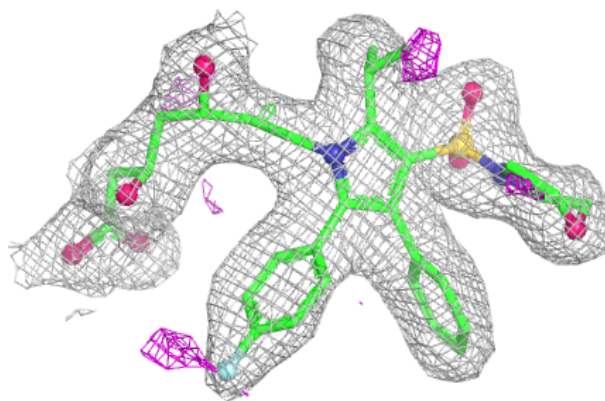
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	RID	D	3	41/41	0.92	0.10	29,37,41,42	0
2	RID	A	2	41/41	0.93	0.09	28,34,37,37	0

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.

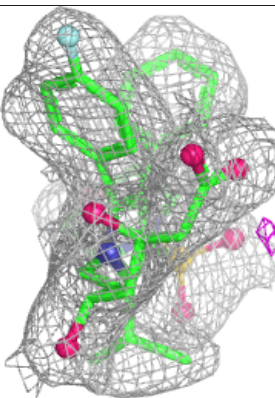
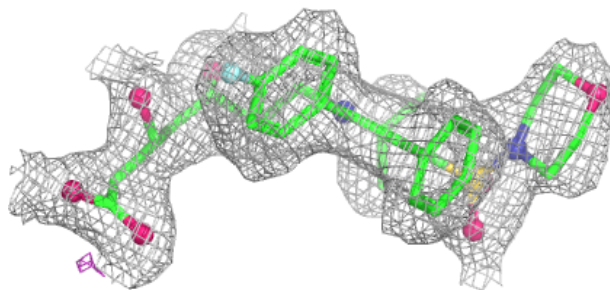
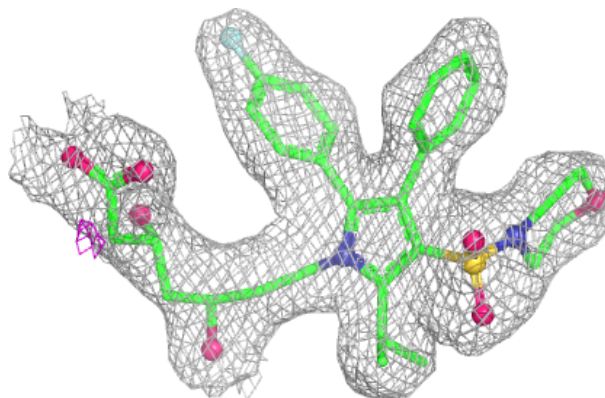


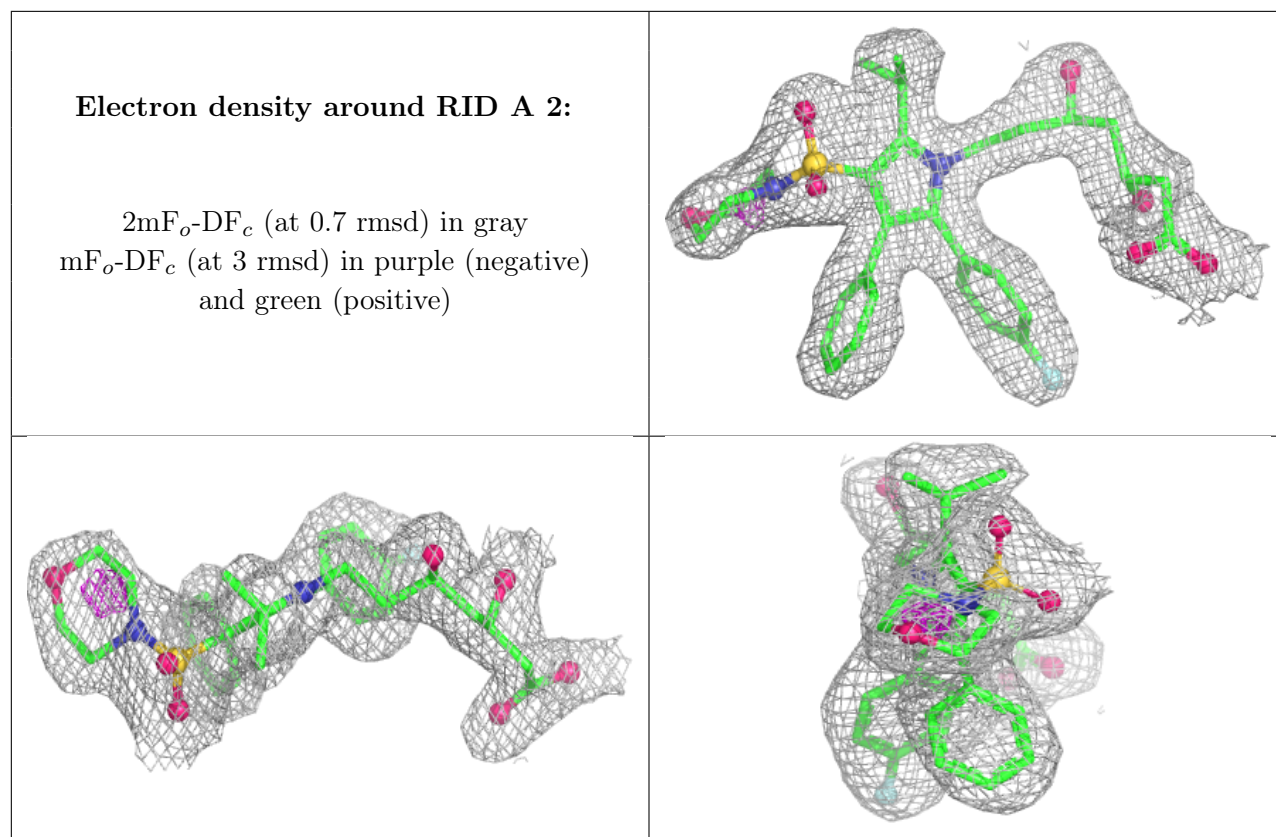
Electron density around RID C 4:

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

**Electron density around RID D 3:**

$2mF_o-DF_c$ (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.