Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 10:27 PM EDT

PDB ID	:	5K3N
Title	:	Crystal structure of Retinoic acid receptor-related orphan receptor (ROR) gamma ligand binding domain complex with ML209
Authors	:	Huang, P.; Rastinejad, F.; Lu, J.
Deposited on	:	2016-05-19
Resolution	:	2.67 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 (i)) were used in the production of this report:

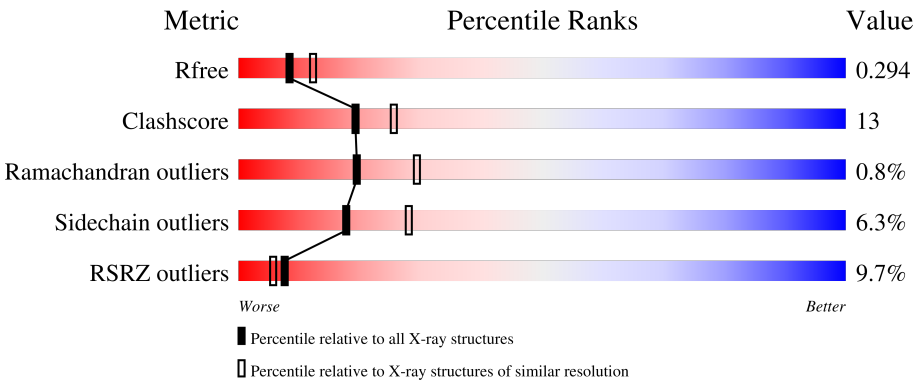
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.67 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	247	9% 65% 26% • 8%
1	B	247	7% 63% 25% • 9%
1	C	247	10% 61% 29% • 8%
1	D	247	9% 60% 29% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7604 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.

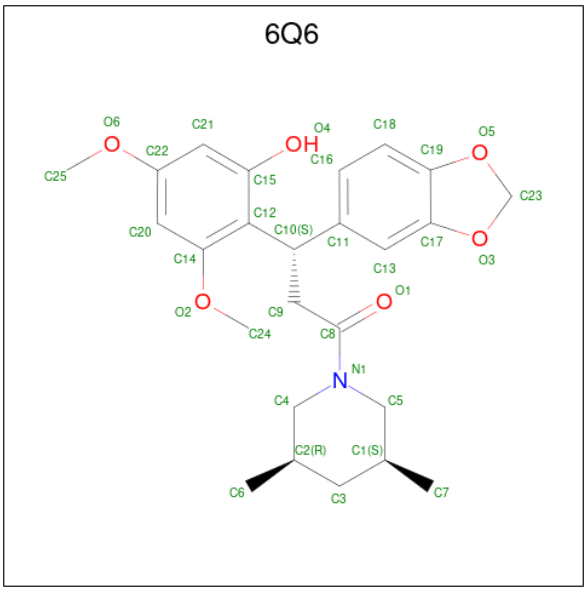
- Molecule 1 is a protein called Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	228	1865	1182	338	331	14	0	0	0
1	B	226	1850	1171	336	329	14	0	0	0
1	C	228	1865	1182	338	331	14	0	0	0
1	D	228	1865	1182	338	331	14	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLY	-	expression tag	UNP P51449
A	262	SER	-	expression tag	UNP P51449
A	263	HIS	-	expression tag	UNP P51449
A	264	MET	-	expression tag	UNP P51449
B	261	GLY	-	expression tag	UNP P51449
B	262	SER	-	expression tag	UNP P51449
B	263	HIS	-	expression tag	UNP P51449
B	264	MET	-	expression tag	UNP P51449
C	261	GLY	-	expression tag	UNP P51449
C	262	SER	-	expression tag	UNP P51449
C	263	HIS	-	expression tag	UNP P51449
C	264	MET	-	expression tag	UNP P51449
D	261	GLY	-	expression tag	UNP P51449
D	262	SER	-	expression tag	UNP P51449
D	263	HIS	-	expression tag	UNP P51449
D	264	MET	-	expression tag	UNP P51449

- Molecule 2 is (3S)-3-(2H-1,3-benzodioxol-5-yl)-1-[(3R,5S)-3,5-dimethylpiperidin-1-yl]-3-(2-hydroxy-4,6-dimethoxyphenyl)propan-1-one (three-letter code: 6Q6) (formula: $C_{25}H_{31}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	32	25	1	6	0	0
2	B	1	32	25	1	6	0	0
2	C	1	32	25	1	6	0	0
2	D	1	32	25	1	6	0	0

- Molecule 3 is water.

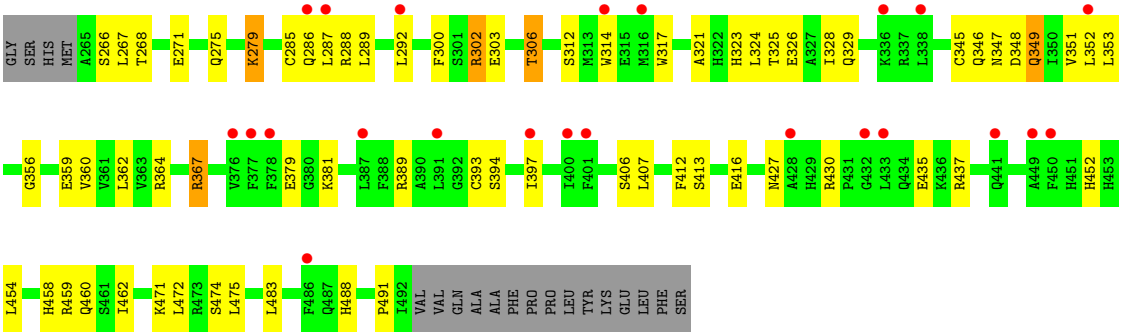
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	6	6	6	0	0
3	B	9	9	9	0	0
3	C	12	12	12	0	0
3	D	4	4	4	0	0

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.

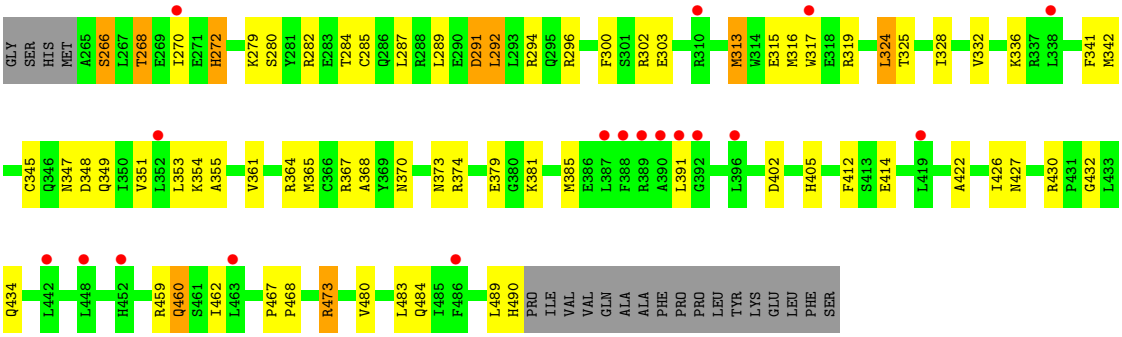
• Molecule 1: Nuclear receptor ROR-gamma

Chain A:



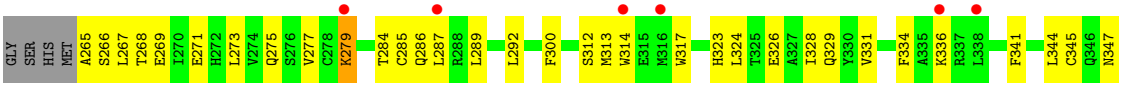
• Molecule 1: Nuclear receptor ROR-gamma

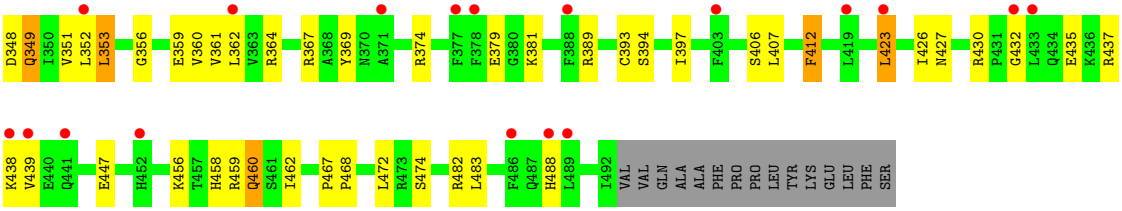
Chain B:



• Molecule 1: Nuclear receptor ROR-gamma

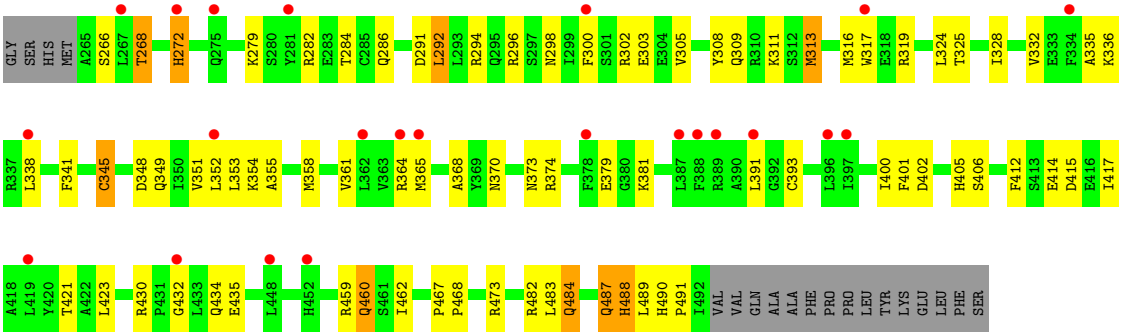
Chain C:





- Molecule 1: Nuclear receptor ROR-gamma

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	89.47Å 89.47Å 153.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.73 – 2.67 44.73 – 2.67	Depositor EDS
% Data completeness (in resolution range)	97.9 (44.73-2.67) 97.9 (44.73-2.67)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.51 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.257 , 0.285 0.251 , 0.294	Depositor DCC
R_{free} test set	1930 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 95.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.467 for -h,-k,l 0.477 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.490 for -h,-k,l	Depositor
Outliers	0 of 38437 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7604	wwPDB-VP
Average B, all atoms (Å^2)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 6Q6

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	0.31	0/1903	0.45	0/2560
1	B	0.32	0/1887	0.46	0/2537
1	C	0.31	0/1903	0.45	0/2560
1	D	0.33	0/1903	0.49	0/2560
All	All	0.32	0/7596	0.46	0/10217

There are no bond length outliers.

There are no bond angle outliers.

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	1865	0	1867	45	0
1	B	1850	0	1849	49	0
1	C	1865	0	1867	54	0
1	D	1865	0	1867	54	0
2	A	32	0	0	0	0
2	B	32	0	0	0	0
2	C	32	0	0	0	0
2	D	32	0	0	0	0
3	A	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	9	0	0	1	0
3	C	12	0	0	3	0
3	D	4	0	0	0	0
All	All	7604	0	7450	193	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 13.

All (193) 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:285:CYS:HB2	1:A:367:ARG:HH12	1.46	0.81
1:B:325:THR:HA	1:B:328:ILE:HD12	1.67	0.74
1:D:351:VAL:HA	1:D:354:LYS:HE3	1.69	0.74
1:D:355:ALA:HB3	1:D:430:ARG:HD2	1.69	0.74
1:B:351:VAL:HA	1:B:354:LYS:HE3	1.71	0.73
1:C:279:LYS:NZ	3:C:701:HOH:O	2.21	0.73
1:C:265:ALA:N	3:C:702:HOH:O	2.23	0.71
1:B:355:ALA:HB3	1:B:430:ARG:HD2	1.73	0.69
1:B:345:CYS:SG	3:B:702:HOH:O	2.52	0.67
1:B:348:ASP:OD1	1:B:434:GLN:N	2.26	0.67
1:D:488:HIS:CD2	1:D:491:PRO:HG3	2.29	0.67
1:C:289:LEU:HA	1:C:292:LEU:HB2	1.79	0.64
1:B:284:THR:O	1:B:364:ARG:NH2	2.29	0.64
1:D:374:ARG:HH11	1:D:401:PHE:HB3	1.65	0.62
1:D:319:ARG:NH1	1:D:379:GLU:OE2	2.33	0.61
1:C:427:ASN:HB3	1:C:430:ARG:HG2	1.82	0.61
1:B:480:VAL:HG22	1:B:484:GLN:HG3	1.83	0.61
1:C:394:SER:HA	1:C:397:ILE:HD12	1.83	0.60
1:D:284:THR:O	1:D:364:ARG:NH2	2.28	0.60
1:C:285:CYS:HB2	1:C:367:ARG:HH12	1.66	0.59
1:D:348:ASP:OD1	1:D:434:GLN:N	2.29	0.59
1:A:289:LEU:HB2	1:A:367:ARG:HH21	1.69	0.58
1:C:289:LEU:HB2	1:C:367:ARG:HH21	1.68	0.58
1:C:323:HIS:NE2	1:C:379:GLU:OE2	2.35	0.58
1:B:303:GLU:OE1	1:B:303:GLU:N	2.37	0.57
1:D:484:GLN:HA	1:D:490:HIS:HE1	1.70	0.57
1:A:394:SER:HA	1:A:397:ILE:HD12	1.87	0.57
1:B:291:ASP:OD1	1:B:294:ARG:NH2	2.36	0.57
1:A:362:LEU:HD23	1:A:472:LEU:HD12	1.87	0.57
1:A:279:LYS:NZ	3:A:702:HOH:O	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:355:ALA:O	1:D:430:ARG:NH1	2.39	0.56
1:B:459:ARG:HH21	1:B:462:ILE:HG21	1.70	0.56
1:D:303:GLU:N	1:D:303:GLU:OE1	2.39	0.56
1:D:325:THR:HA	1:D:328:ILE:HD12	1.87	0.56
1:B:292:LEU:HD21	1:B:368:ALA:HA	1.87	0.56
1:D:488:HIS:NE2	1:D:491:PRO:HG3	2.20	0.55
1:D:393:CYS:SG	1:D:482:ARG:NH2	2.79	0.55
1:A:324:LEU:O	1:A:328:ILE:HG13	2.07	0.55
1:A:300:PHE:CE2	1:A:381:LYS:HB2	2.42	0.55
1:B:473:ARG:HH11	1:B:473:ARG:HB3	1.71	0.55
1:B:268:THR:O	1:B:272:HIS:N	2.37	0.54
1:D:351:VAL:HG21	1:D:432:GLY:O	2.07	0.54
1:D:473:ARG:HH11	1:D:473:ARG:HB3	1.71	0.54
1:A:427:ASN:HB3	1:A:430:ARG:HG2	1.89	0.54
1:C:459:ARG:HH21	1:C:462:ILE:HG21	1.72	0.54
1:D:296:ARG:NH2	1:D:370:ASN:OD1	2.39	0.54
1:D:370:ASN:ND2	1:D:373:ASN:OD1	2.40	0.54
1:D:332:VAL:HG22	1:D:353:LEU:HD22	1.89	0.54
1:A:407:LEU:HD22	1:A:412:PHE:HE2	1.73	0.53
1:A:347:ASN:O	1:A:351:VAL:HG23	2.09	0.53
1:A:359:GLU:OE2	1:A:430:ARG:NH2	2.42	0.53
1:D:374:ARG:NH1	1:D:402:ASP:OD1	2.31	0.52
1:B:370:ASN:ND2	1:B:373:ASN:OD1	2.43	0.52
1:D:292:LEU:HD21	1:D:368:ALA:HA	1.91	0.52
1:A:459:ARG:HH21	1:A:462:ILE:HG21	1.74	0.52
1:B:355:ALA:O	1:B:430:ARG:NH1	2.42	0.52
1:A:289:LEU:HA	1:A:292:LEU:HB2	1.92	0.52
1:D:291:ASP:OD1	1:D:294:ARG:NH2	2.41	0.52
1:B:374:ARG:NH1	1:B:402:ASP:OD1	2.27	0.51
1:C:344:LEU:HB2	1:C:349:GLN:HG3	1.92	0.51
1:D:459:ARG:HH21	1:D:462:ILE:HG21	1.76	0.51
1:A:323:HIS:NE2	1:A:379:GLU:OE2	2.37	0.51
1:B:319:ARG:NH1	1:B:379:GLU:OE2	2.43	0.51
1:C:345:CYS:O	1:C:349:GLN:N	2.43	0.50
1:A:348:ASP:OD2	1:A:435:GLU:N	2.38	0.50
1:C:285:CYS:O	1:C:287:LEU:N	2.45	0.50
1:D:268:THR:O	1:D:272:HIS:N	2.37	0.50
1:D:324:LEU:O	1:D:328:ILE:HG13	2.11	0.50
1:A:326:GLU:O	1:A:329:GLN:HB3	2.12	0.50
1:C:331:VAL:HG21	1:C:361:VAL:HG22	1.93	0.50
1:A:285:CYS:O	1:A:287:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:TRP:CE3	1:B:483:LEU:HD13	2.48	0.49
1:C:317:TRP:CE3	1:C:483:LEU:HD13	2.47	0.49
1:C:352:LEU:O	1:C:356:GLY:N	2.46	0.49
1:A:325:THR:HG23	1:A:491:PRO:HG3	1.94	0.49
1:C:347:ASN:O	1:C:351:VAL:HG23	2.13	0.49
1:C:359:GLU:CD	1:C:430:ARG:HH22	2.16	0.49
1:D:300:PHE:CE2	1:D:381:LYS:HD2	2.48	0.49
1:B:347:ASN:O	1:B:351:VAL:HG23	2.13	0.49
1:C:353:LEU:HB2	3:C:703:HOH:O	2.12	0.49
1:D:365:MET:HE3	1:D:368:ALA:HB3	1.94	0.48
1:D:487:GLN:O	1:D:489:LEU:N	2.45	0.48
1:C:317:TRP:HE3	1:C:483:LEU:HD13	1.78	0.48
1:C:324:LEU:O	1:C:328:ILE:HG13	2.12	0.48
1:A:346:GLN:HA	1:A:349:GLN:HB2	1.95	0.48
1:C:393:CYS:HB3	1:C:482:ARG:HH11	1.78	0.48
1:B:316:MET:HB2	1:B:391:LEU:HD21	1.95	0.48
1:B:285:CYS:O	1:B:287:LEU:N	2.47	0.48
1:D:345:CYS:O	1:D:349:GLN:HG3	2.12	0.48
1:C:326:GLU:O	1:C:329:GLN:HB3	2.14	0.48
1:D:317:TRP:CE3	1:D:483:LEU:HD13	2.49	0.47
1:B:332:VAL:HG22	1:B:353:LEU:HD22	1.97	0.47
1:B:422:ALA:O	1:B:426:ILE:HG12	2.14	0.47
1:C:266:SER:OG	1:C:267:LEU:N	2.47	0.47
1:C:407:LEU:HD21	1:C:467:PRO:HD3	1.95	0.47
1:A:454:LEU:O	1:A:458:HIS:N	2.47	0.47
1:A:303:GLU:OE1	1:A:303:GLU:N	2.43	0.47
1:A:317:TRP:HE3	1:A:483:LEU:HD13	1.80	0.47
1:A:317:TRP:CE3	1:A:483:LEU:HD13	2.50	0.47
1:C:348:ASP:OD2	1:C:435:GLU:N	2.48	0.47
1:C:389:ARG:NH2	1:D:459:ARG:HD3	2.30	0.47
1:B:317:TRP:HE3	1:B:483:LEU:HD13	1.79	0.47
1:C:300:PHE:CZ	1:C:381:LYS:HB2	2.50	0.47
1:B:289:LEU:HB2	1:B:367:ARG:HH21	1.80	0.47
1:C:393:CYS:O	1:C:397:ILE:HG13	2.15	0.47
1:C:271:GLU:OE2	1:C:456:LYS:NZ	2.48	0.46
1:C:407:LEU:HD22	1:C:412:PHE:HE2	1.81	0.46
1:B:351:VAL:O	1:B:354:LYS:HB3	2.16	0.46
1:C:458:HIS:HA	1:C:460:GLN:NE2	2.31	0.46
1:A:271:GLU:O	1:A:275:GLN:HG3	2.16	0.46
1:C:359:GLU:OE2	1:C:430:ARG:NH2	2.49	0.46
1:C:271:GLU:O	1:C:275:GLN:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:CYS:O	1:A:397:ILE:HG13	2.17	0.45
1:B:313:MET:H	1:B:313:MET:HG2	1.58	0.45
1:B:467:PRO:HA	1:B:468:PRO:HD3	1.74	0.45
1:C:435:GLU:HB3	1:C:438:LYS:HB2	1.98	0.45
1:D:351:VAL:O	1:D:354:LYS:HB3	2.16	0.45
1:D:335:ALA:HA	1:D:338:LEU:HG	1.99	0.45
1:B:427:ASN:HB3	1:B:430:ARG:HG2	1.97	0.45
1:C:266:SER:N	1:C:269:GLU:OE1	2.30	0.45
1:A:314:TRP:HB3	1:B:282:ARG:NH2	2.32	0.45
1:D:317:TRP:HE3	1:D:483:LEU:HD13	1.82	0.45
1:A:302:ARG:O	1:A:306:THR:OG1	2.32	0.45
1:A:452:HIS:O	1:A:452:HIS:ND1	2.50	0.45
1:A:285:CYS:HB2	1:A:367:ARG:NH1	2.23	0.45
1:C:273:LEU:O	1:C:277:VAL:HG23	2.17	0.45
1:C:312:SER:HB3	1:D:414:GLU:HB2	2.00	0.44
1:C:313:MET:O	1:C:317:TRP:HD1	1.99	0.44
1:B:484:GLN:HG2	1:B:490:HIS:NE2	2.31	0.44
1:C:300:PHE:CD2	1:C:381:LYS:HD2	2.51	0.44
1:A:300:PHE:CZ	1:A:381:LYS:HB2	2.53	0.44
1:D:341:PHE:HE1	1:D:352:LEU:HD12	1.82	0.44
1:D:300:PHE:CE2	1:D:381:LYS:HB2	2.53	0.43
1:D:467:PRO:HA	1:D:468:PRO:HD3	1.75	0.43
1:C:423:LEU:HD21	1:C:447:GLU:HG3	2.00	0.43
1:C:435:GLU:O	1:C:439:VAL:HG23	2.18	0.43
1:A:314:TRP:HB3	1:B:282:ARG:HH21	1.83	0.43
1:C:336:LYS:HA	1:C:341:PHE:CE2	2.53	0.43
1:C:393:CYS:HB3	1:C:482:ARG:NH1	2.33	0.43
1:C:467:PRO:HA	1:C:468:PRO:HD3	1.86	0.43
1:B:361:VAL:O	1:B:365:MET:HG2	2.19	0.43
1:D:423:LEU:HD23	1:D:423:LEU:HA	1.83	0.43
1:A:314:TRP:HB2	1:B:282:ARG:HD3	2.01	0.43
1:B:345:CYS:O	1:B:349:GLN:HG3	2.18	0.43
1:C:300:PHE:CE2	1:C:381:LYS:HB2	2.54	0.43
1:A:359:GLU:CD	1:A:430:ARG:HH22	2.23	0.43
1:C:345:CYS:O	1:C:349:GLN:HB2	2.19	0.43
1:D:305:VAL:O	1:D:309:GLN:HG3	2.19	0.43
1:B:300:PHE:CE2	1:B:381:LYS:HD2	2.54	0.42
1:B:336:LYS:HA	1:B:341:PHE:CD2	2.54	0.42
1:D:460:GLN:N	1:D:460:GLN:OE1	2.53	0.42
1:A:321:ALA:HA	1:A:324:LEU:HB3	2.01	0.42
1:B:300:PHE:CE2	1:B:381:LYS:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:358:MET:HE3	1:D:358:MET:HB3	1.92	0.42
1:A:458:HIS:HA	1:A:460:GLN:NE2	2.35	0.42
1:C:313:MET:HG2	1:D:415:ASP:OD2	2.19	0.42
1:D:308:TYR:HA	1:D:311:LYS:HE2	2.01	0.42
1:D:417:ILE:O	1:D:421:THR:HG23	2.19	0.42
1:D:488:HIS:CE1	1:D:491:PRO:HG3	2.54	0.42
1:D:316:MET:HB2	1:D:391:LEU:HD21	2.00	0.42
1:B:324:LEU:O	1:B:328:ILE:HG13	2.19	0.42
1:D:490:HIS:N	1:D:491:PRO:CD	2.83	0.42
1:A:312:SER:HB3	1:B:414:GLU:HB2	2.01	0.42
1:D:313:MET:H	1:D:313:MET:HG2	1.40	0.41
1:A:406:SER:O	1:A:407:LEU:HD23	2.20	0.41
1:D:300:PHE:CZ	1:D:381:LYS:HB2	2.55	0.41
1:A:367:ARG:H	1:A:367:ARG:HG3	1.52	0.41
1:C:406:SER:O	1:C:407:LEU:HD23	2.20	0.41
1:A:266:SER:OG	1:A:267:LEU:N	2.53	0.41
1:B:342:MET:HA	1:B:349:GLN:NE2	2.35	0.41
1:D:490:HIS:N	1:D:491:PRO:HD2	2.36	0.41
1:A:345:CYS:O	1:A:349:GLN:N	2.50	0.41
1:B:296:ARG:NH2	1:B:370:ASN:OD1	2.51	0.41
1:C:351:VAL:HG21	1:C:432:GLY:O	2.21	0.41
1:D:328:ILE:HG12	1:D:361:VAL:HG21	2.02	0.41
1:B:280:SER:O	1:B:284:THR:HG23	2.20	0.41
1:B:300:PHE:CZ	1:B:381:LYS:HB2	2.56	0.41
1:C:284:THR:OG1	1:C:334:PHE:HB2	2.21	0.41
1:C:314:TRP:HB3	1:D:282:ARG:HH21	1.85	0.41
1:C:360:VAL:HG12	1:C:364:ARG:HD2	2.03	0.41
1:C:362:LEU:HD23	1:C:472:LEU:HD12	2.03	0.41
1:D:336:LYS:HA	1:D:341:PHE:HD2	1.86	0.41
1:A:352:LEU:O	1:A:356:GLY:N	2.52	0.41
1:A:413:SER:H	1:A:416:GLU:HB2	1.85	0.41
1:B:460:GLN:N	1:B:460:GLN:OE1	2.54	0.41
1:A:471:LYS:HE2	1:A:475:LEU:HD13	2.02	0.40
1:B:266:SER:O	1:B:270:ILE:HG13	2.21	0.40
1:A:389:ARG:NH2	1:B:459:ARG:HD3	2.36	0.40
1:C:369:TYR:CE1	1:C:374:ARG:HA	2.57	0.40
1:D:345:CYS:N	1:D:435:GLU:OE1	2.50	0.40
1:A:360:VAL:HG12	1:A:364:ARG:HD2	2.04	0.40
1:B:351:VAL:HG21	1:B:432:GLY:O	2.21	0.40
1:B:473:ARG:HB3	1:B:473:ARG:NH1	2.36	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	226/247 (92%)	205 (91%)	20 (9%)	1 (0%)	34	48
1	B	224/247 (91%)	204 (91%)	19 (8%)	1 (0%)	34	48
1	C	226/247 (92%)	203 (90%)	21 (9%)	2 (1%)	17	26
1	D	226/247 (92%)	205 (91%)	18 (8%)	3 (1%)	12	18
All	All	902/988 (91%)	817 (91%)	78 (9%)	7 (1%)	19	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	C	286	GLN
1	D	488	HIS
1	B	324	LEU
1	D	286	GLN
1	D	406	SER
1	C	426	ILE

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	204/220 (93%)	193 (95%)	11 (5%)	22	34
1	B	202/220 (92%)	187 (93%)	15 (7%)	13	21
1	C	204/220 (93%)	194 (95%)	10 (5%)	25	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	204/220 (93%)	189 (93%)	15 (7%)	13	21
All	All	814/880 (92%)	763 (94%)	51 (6%)	18	28

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	268	THR
1	A	279	LYS
1	A	288	ARG
1	A	302	ARG
1	A	306	THR
1	A	349	GLN
1	A	353	LEU
1	A	367	ARG
1	A	437	ARG
1	A	474	SER
1	A	488	HIS
1	B	266	SER
1	B	268	THR
1	B	272	HIS
1	B	279	LYS
1	B	291	ASP
1	B	292	LEU
1	B	302	ARG
1	B	313	MET
1	B	315	GLU
1	B	385	MET
1	B	405	HIS
1	B	412	PHE
1	B	460	GLN
1	B	473	ARG
1	B	489	LEU
1	C	268	THR
1	C	279	LYS
1	C	349	GLN
1	C	353	LEU
1	C	412	PHE
1	C	423	LEU
1	C	437	ARG
1	C	460	GLN
1	C	474	SER
1	C	488	HIS

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Mol	Chain	Res	Type
1	D	266	SER
1	D	268	THR
1	D	272	HIS
1	D	279	LYS
1	D	292	LEU
1	D	298	ASN
1	D	302	ARG
1	D	313	MET
1	D	345	CYS
1	D	400	ILE
1	D	405	HIS
1	D	412	PHE
1	D	460	GLN
1	D	484	GLN
1	D	487	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	309	GLN
1	A	349	GLN
1	A	434	GLN
1	B	346	GLN
1	C	309	GLN
1	C	434	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 monosaccharides 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	6Q6	B	600	-	35,35,35	1.04	2 (5%)	45,50,50	1.57	6 (13%)
2	6Q6	A	600	-	35,35,35	0.90	1 (2%)	45,50,50	1.71	7 (15%)
2	6Q6	C	600	-	35,35,35	0.80	1 (2%)	45,50,50	1.62	6 (13%)
2	6Q6	D	600	-	35,35,35	1.01	1 (2%)	45,50,50	1.70	11 (24%)

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	6Q6	B	600	-	-	2/20/38/38	0/4/4/4
2	6Q6	A	600	-	-	4/20/38/38	0/4/4/4
2	6Q6	C	600	-	-	2/20/38/38	0/4/4/4
2	6Q6	D	600	-	-	2/20/38/38	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	6Q6	C12-C10	-4.77	1.47	1.52
2	D	600	6Q6	C12-C10	-4.71	1.47	1.52
2	A	600	6Q6	C12-C10	-4.05	1.48	1.52
2	C	600	6Q6	C12-C10	-3.32	1.49	1.52
2	B	600	6Q6	C15-C12	-2.05	1.36	1.40

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	6Q6	O2-C14-C12	6.29	122.16	115.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	600	6Q6	O2-C14-C12	5.69	121.52	115.54
2	B	600	6Q6	O2-C14-C12	5.66	121.50	115.54
2	D	600	6Q6	O2-C14-C12	5.54	121.37	115.54
2	A	600	6Q6	C15-C12-C14	4.76	121.10	116.66
2	C	600	6Q6	C15-C12-C14	4.40	120.76	116.66
2	B	600	6Q6	O2-C14-C20	-4.31	116.71	124.12
2	D	600	6Q6	C15-C12-C14	3.78	120.19	116.66
2	D	600	6Q6	C24-O2-C14	3.64	123.03	117.53
2	A	600	6Q6	O2-C14-C20	-3.41	118.26	124.12
2	C	600	6Q6	O2-C14-C20	-3.25	118.52	124.12
2	B	600	6Q6	O3-C23-O5	-3.24	102.91	108.08
2	A	600	6Q6	C24-O2-C14	3.13	122.26	117.53
2	D	600	6Q6	O2-C14-C20	-3.06	118.85	124.12
2	D	600	6Q6	O3-C23-O5	-3.04	103.22	108.08
2	A	600	6Q6	C15-C12-C10	-3.00	115.96	122.00
2	A	600	6Q6	O3-C23-O5	-2.94	103.38	108.08
2	C	600	6Q6	O3-C23-O5	-2.70	103.77	108.08
2	C	600	6Q6	C24-O2-C14	2.68	121.57	117.53
2	B	600	6Q6	C15-C12-C14	2.63	119.11	116.66
2	D	600	6Q6	C7-C1-C3	-2.56	106.82	111.18
2	C	600	6Q6	C15-C12-C10	-2.56	116.86	122.00
2	D	600	6Q6	C6-C2-C3	-2.25	107.35	111.18
2	D	600	6Q6	C17-C13-C11	-2.25	116.24	119.83
2	D	600	6Q6	C16-C18-C19	-2.23	115.81	120.06
2	D	600	6Q6	C16-C11-C13	2.22	121.32	118.76
2	B	600	6Q6	C15-C12-C10	-2.14	117.69	122.00
2	D	600	6Q6	C15-C12-C10	-2.11	117.75	122.00
2	A	600	6Q6	C16-C18-C19	-2.07	116.12	120.06
2	B	600	6Q6	C1-C3-C2	-2.04	108.39	111.59

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	6Q6	C20-C14-O2-C24
2	C	600	6Q6	C20-C14-O2-C24
2	C	600	6Q6	C12-C14-O2-C24
2	A	600	6Q6	C12-C14-O2-C24
2	D	600	6Q6	C20-C14-O2-C24
2	D	600	6Q6	C12-C14-O2-C24
2	A	600	6Q6	O1-C8-C9-C10
2	B	600	6Q6	O1-C8-C9-C10

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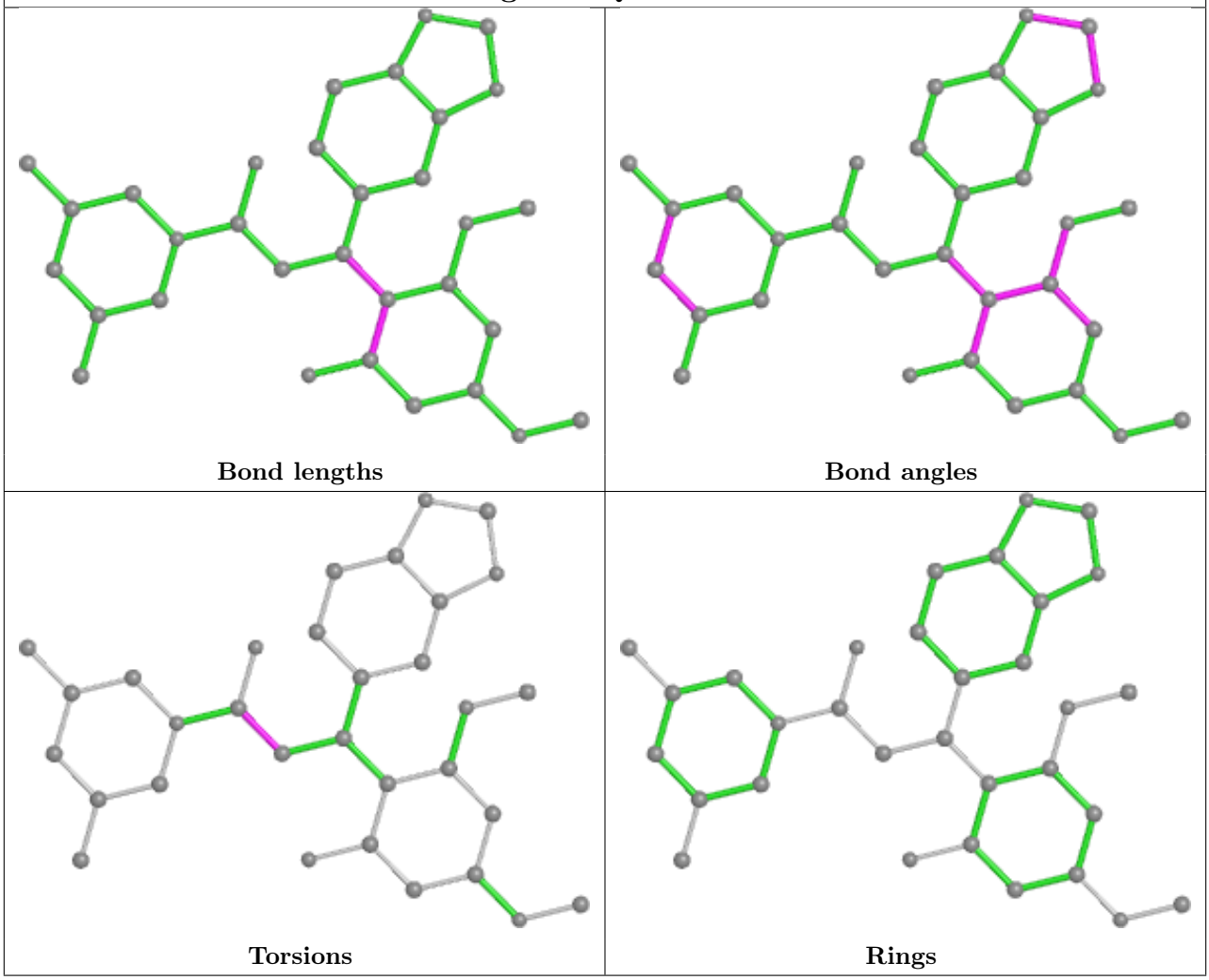
Mol	Chain	Res	Type	Atoms
2	A	600	6Q6	N1-C8-C9-C10
2	B	600	6Q6	N1-C8-C9-C10

There are no ring outliers.

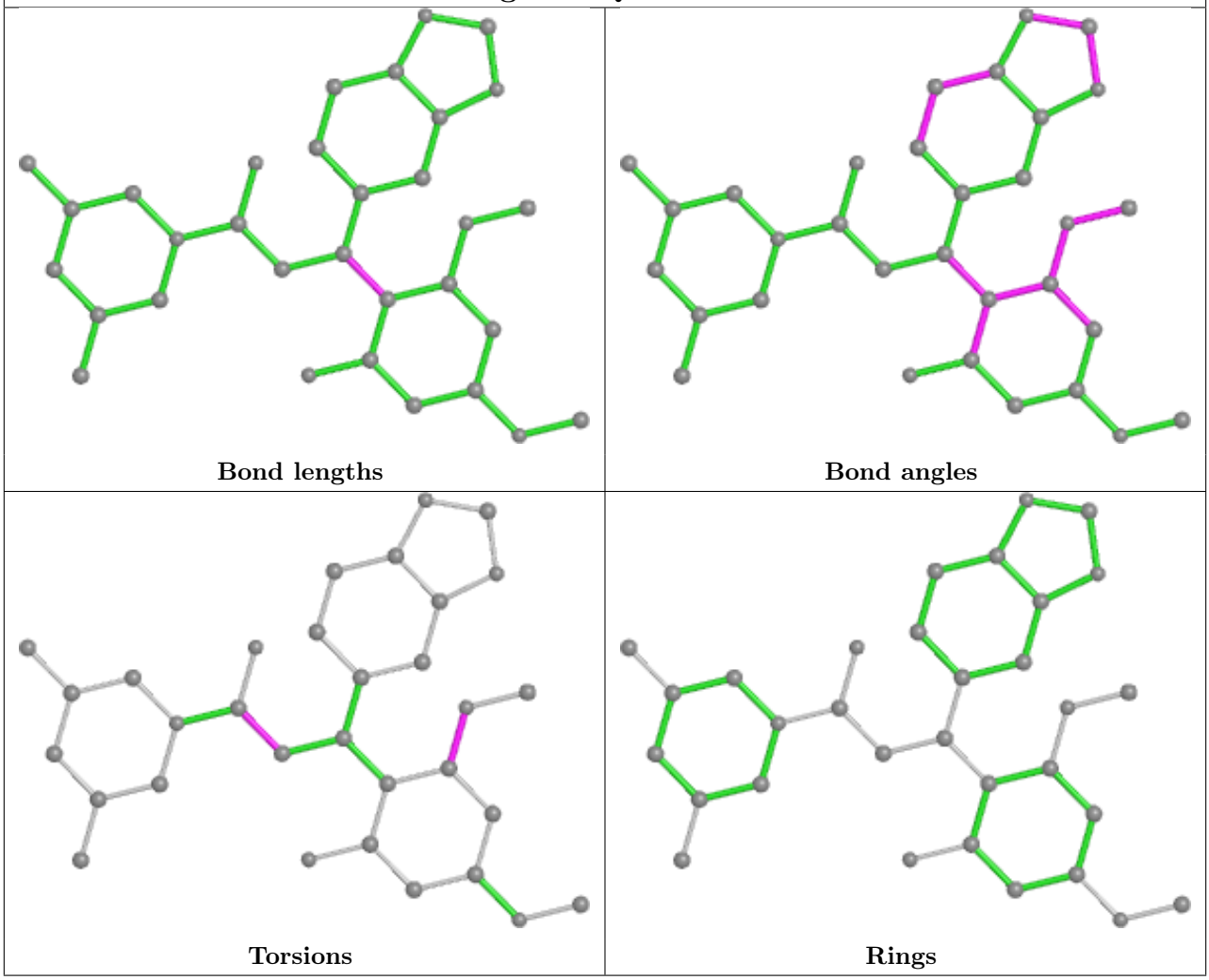
No monomer is involved in short contacts.

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

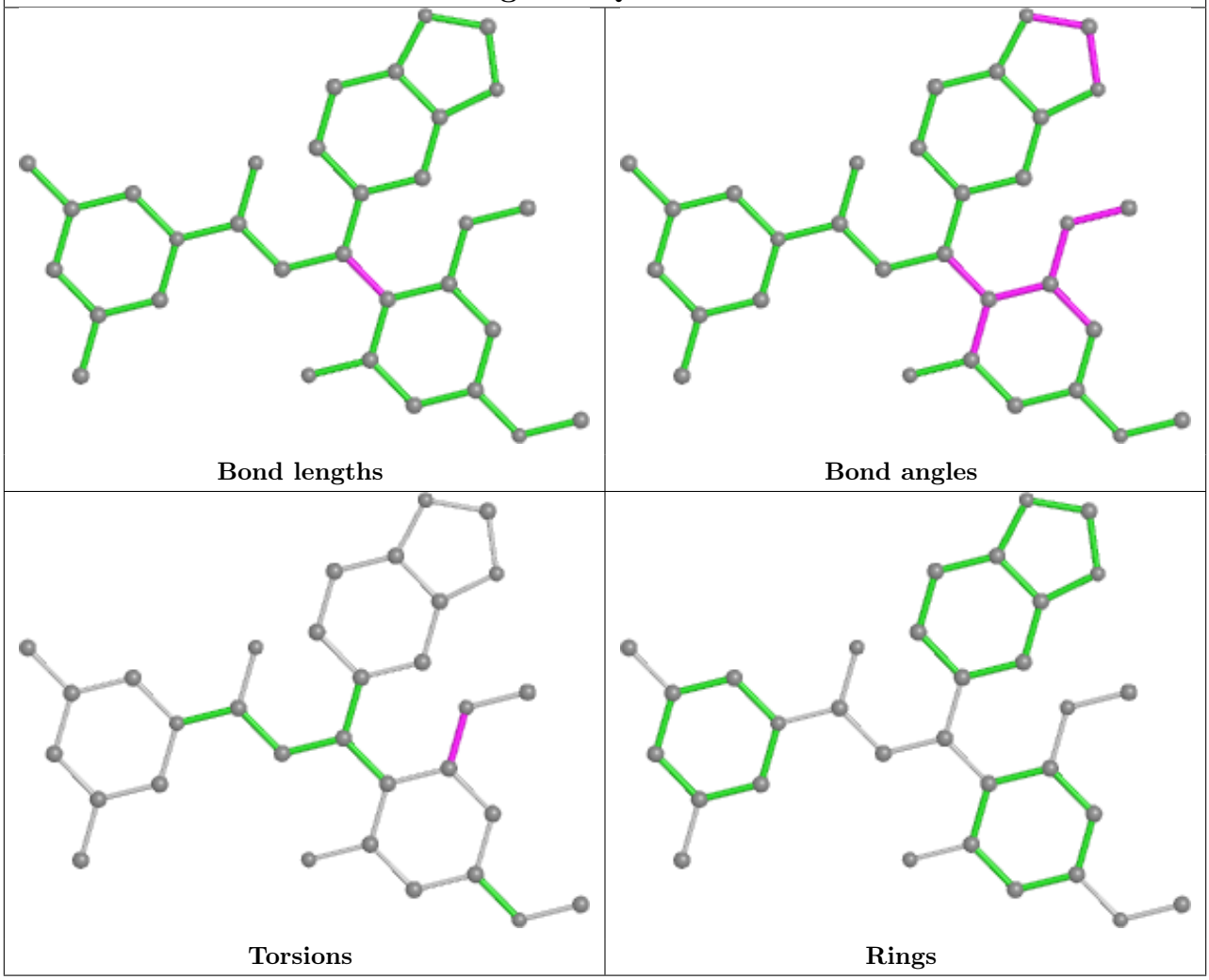
Ligand 6Q6 B 600



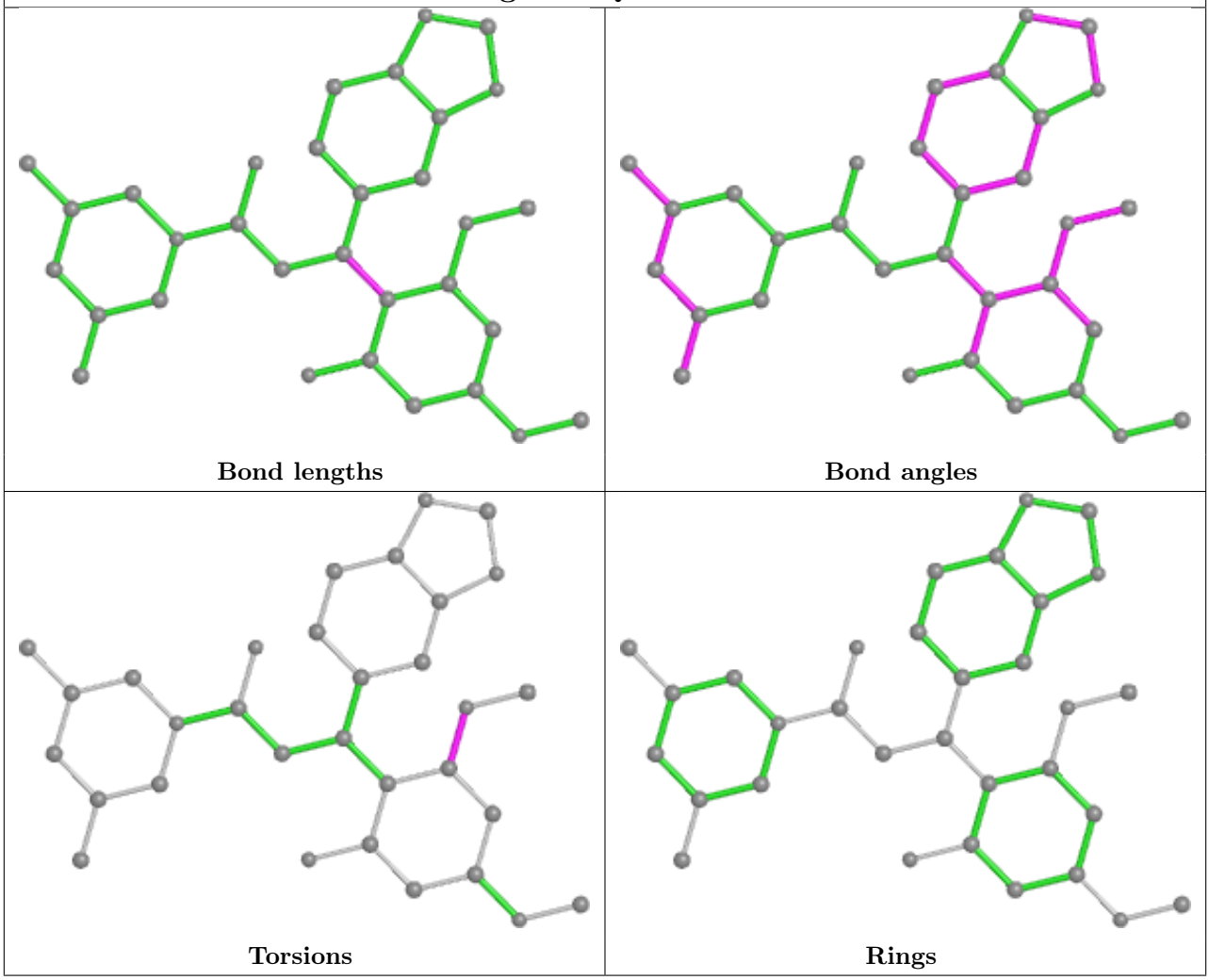
Ligand 6Q6 A 600



Ligand 6Q6 C 600



Ligand 6Q6 D 600



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	228/247 (92%)	0.65	23 (10%)	7	4	86, 125, 163, 192	0
1	B	226/247 (91%)	0.60	18 (7%)	12	9	78, 115, 149, 171	0
1	C	228/247 (92%)	0.62	24 (10%)	6	4	81, 115, 159, 209	0
1	D	228/247 (92%)	0.58	23 (10%)	7	4	76, 118, 159, 194	0
All	All	910/988 (92%)	0.61	88 (9%)	7	6	76, 119, 159, 209	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	377	PHE	5.6
1	D	389	ARG	5.3
1	A	377	PHE	4.9
1	C	378	PHE	4.9
1	A	352	LEU	4.8
1	A	336	LYS	4.7
1	C	336	LYS	4.6
1	B	389	ARG	4.6
1	B	388	PHE	4.5
1	A	286	GLN	4.3
1	D	352	LEU	4.2
1	B	390	ALA	4.2
1	D	387	LEU	4.1
1	C	419	LEU	3.9
1	D	378	PHE	3.6
1	C	352	LEU	3.5
1	A	391	LEU	3.5
1	C	287	LEU	3.5
1	D	338	LEU	3.4
1	B	391	LEU	3.4
1	D	388	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	270	ILE	3.2
1	D	272	HIS	3.1
1	C	441	GLN	3.1
1	A	378	PHE	3.1
1	B	317	TRP	3.1
1	A	316	MET	3.0
1	A	486	PHE	3.0
1	C	371	ALA	2.9
1	A	449	ALA	2.9
1	D	452	HIS	2.8
1	B	338	LEU	2.8
1	C	432	GLY	2.8
1	B	387	LEU	2.8
1	A	432	GLY	2.8
1	C	316	MET	2.7
1	A	428	ALA	2.7
1	A	338	LEU	2.7
1	A	433	LEU	2.7
1	C	388	PHE	2.7
1	D	419	LEU	2.7
1	D	397	ILE	2.7
1	C	439	VAL	2.6
1	C	438	LYS	2.6
1	D	281	TYR	2.6
1	B	419	LEU	2.5
1	C	362	LEU	2.5
1	A	397	ILE	2.5
1	A	441	GLN	2.4
1	C	338	LEU	2.4
1	D	267	LEU	2.4
1	D	334	PHE	2.4
1	B	442	LEU	2.4
1	D	396	LEU	2.4
1	B	452	HIS	2.3
1	A	387	LEU	2.3
1	B	448	LEU	2.3
1	C	433	LEU	2.3
1	D	391	LEU	2.3
1	B	310	ARG	2.3
1	C	489	LEU	2.3
1	B	352	LEU	2.3
1	B	392	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	300	PHE	2.3
1	C	452	HIS	2.2
1	C	488	HIS	2.2
1	D	275	GLN	2.2
1	C	314	TRP	2.2
1	C	279	LYS	2.2
1	A	450	PHE	2.2
1	B	486	PHE	2.2
1	C	486	PHE	2.2
1	B	463	LEU	2.2
1	A	376	VAL	2.2
1	C	423	LEU	2.2
1	D	448	LEU	2.2
1	A	400	ILE	2.1
1	A	287	LEU	2.1
1	D	364	ARG	2.1
1	A	401	PHE	2.1
1	D	362	LEU	2.1
1	A	292	LEU	2.1
1	A	314	TRP	2.1
1	D	317	TRP	2.1
1	D	365	MET	2.1
1	D	432	GLY	2.0
1	C	403	PHE	2.0
1	B	396	LEU	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)

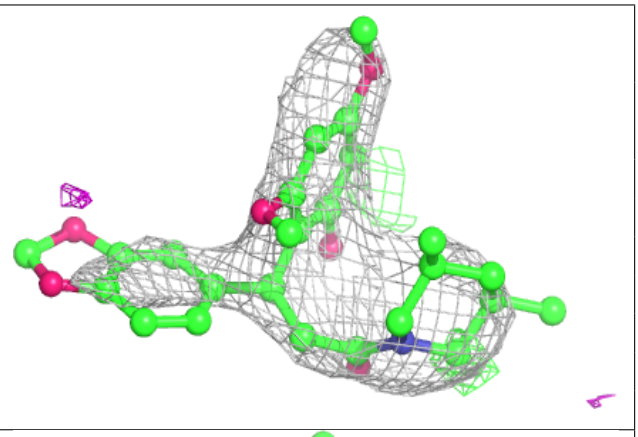
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

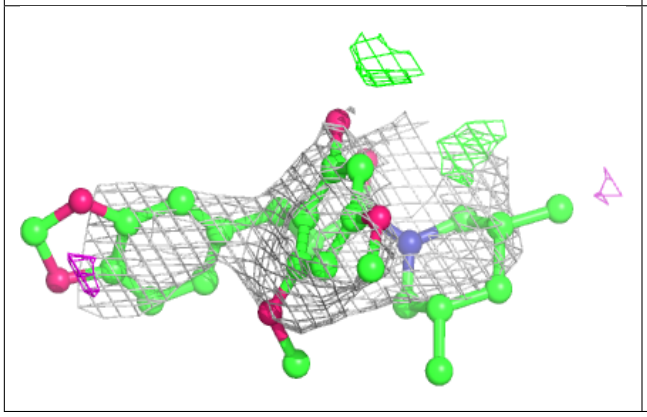
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	6Q6	C	600	32/32	0.86	0.59	132,169,188,188	0
2	6Q6	A	600	32/32	0.89	0.58	110,161,208,215	0
2	6Q6	B	600	32/32	0.94	0.33	86,110,132,139	0
2	6Q6	D	600	32/32	0.95	0.27	69,102,125,134	0

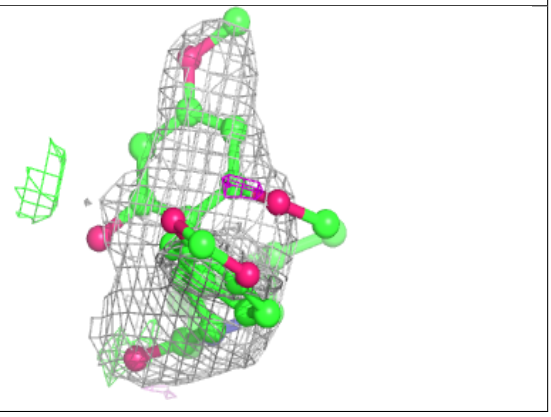
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 6Q6 C 600:

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

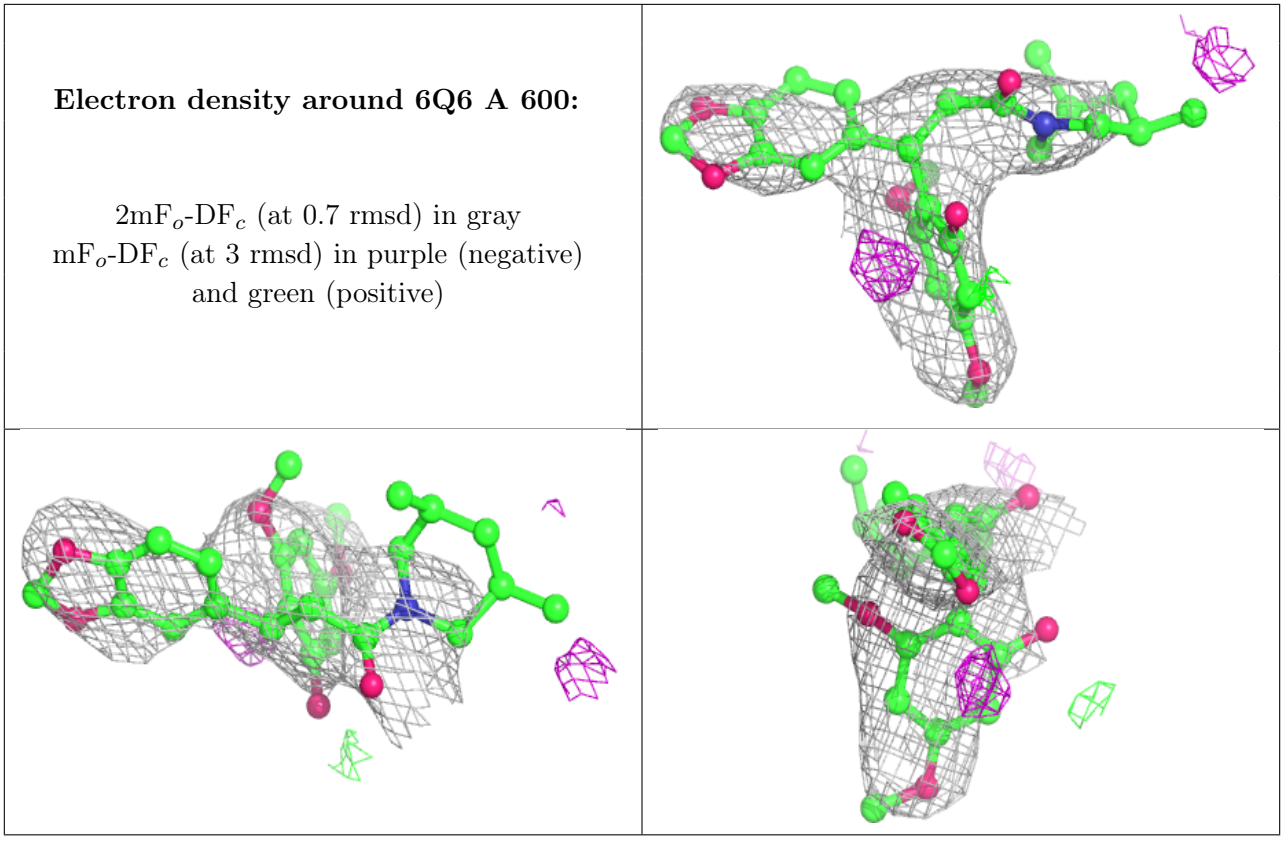






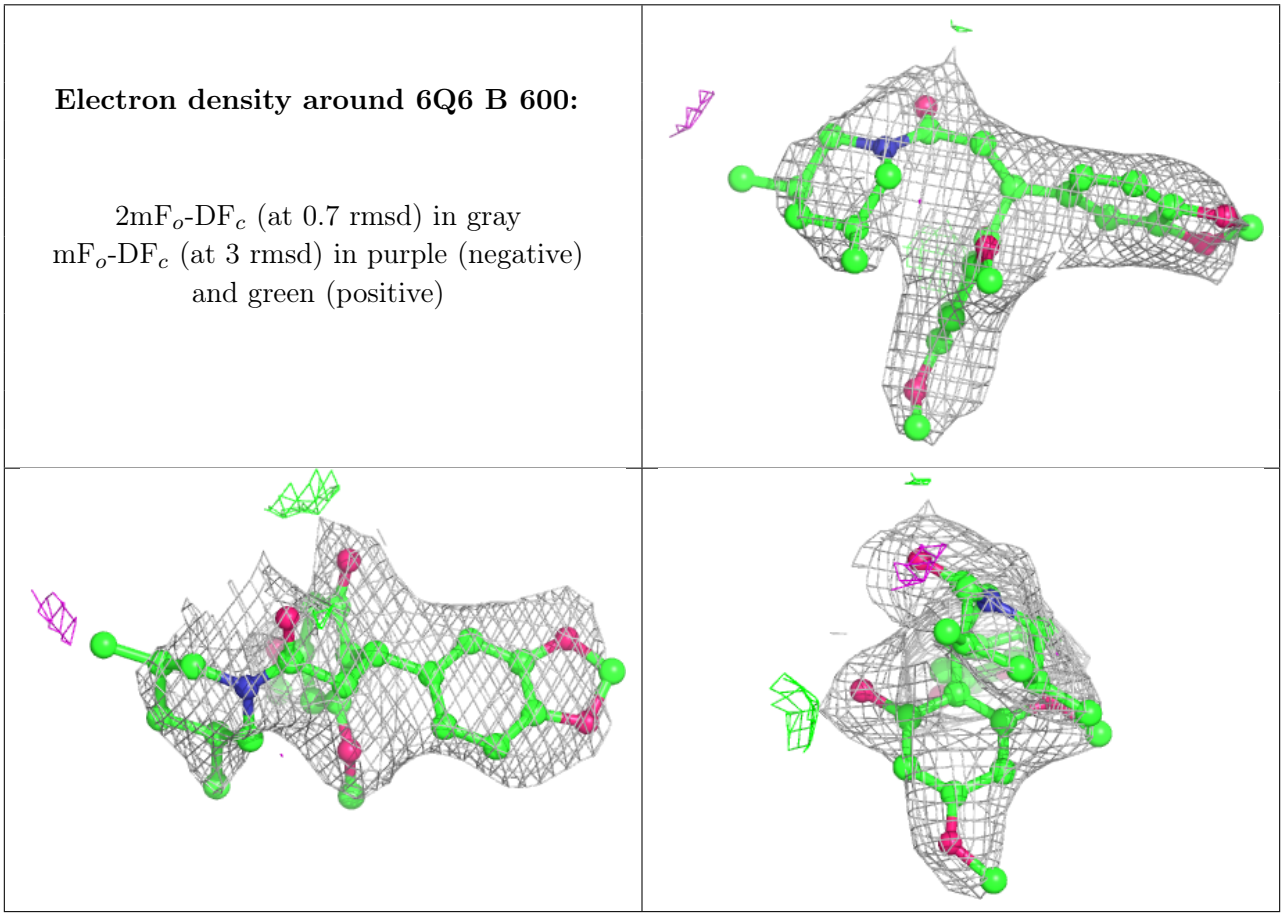
Electron density around 6Q6 A 600:

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



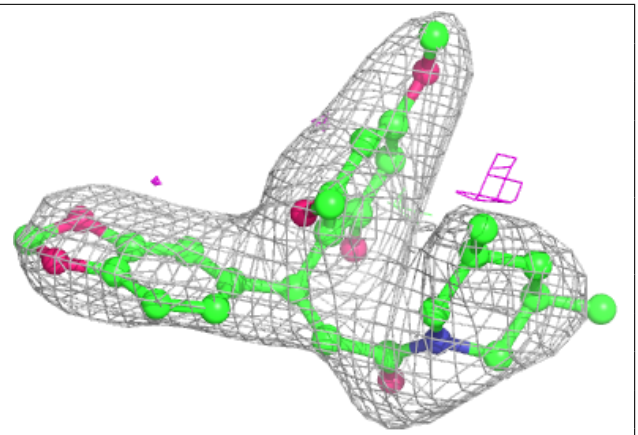
Electron density around 6Q6 B 600:

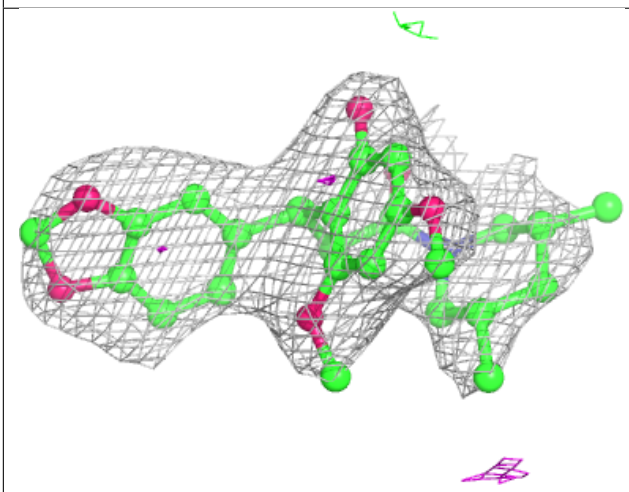
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

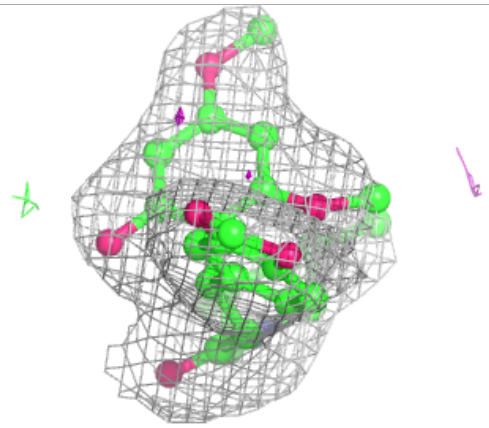


Electron density around 6Q6 D 600:

$2mF_o$-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.