Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:48 pm BST

PDB ID	:	4NRU
Title	:	Murine Norovirus RNA-dependent-RNA-polymerase in complex with Compound 6, a suramin derivative
Authors	:	Milani, M.; Croci, R.; Pezzullo, M.; Tarantino, D.; Mastrangelo, E.; Bolognesi, M.
Deposited on	:	2013-11-27
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 ⓘ symbol.

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

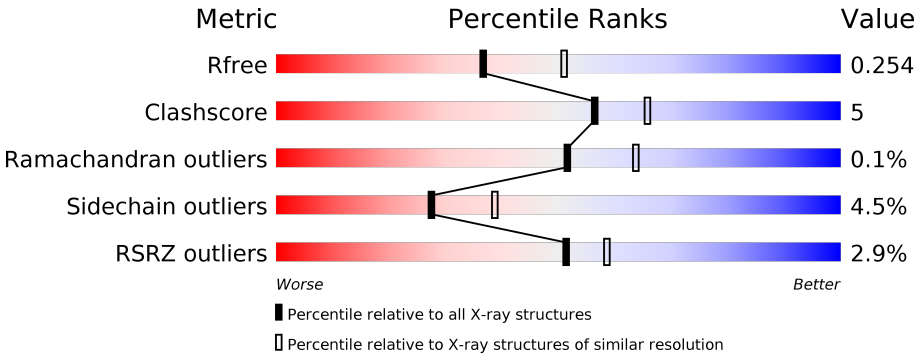
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.30 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 on 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	515	3% 83% 10% 7%
1	B	515	% 83% 10% • 6%
1	C	515	2% 82% 10% • 7%
1	D	515	2% 81% 11% • 7%
1	E	515	3% 80% 11% • 7%
1	F	515	6% 77% 14% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24851 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 RNA dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	4	0
			3821	2421	674	701	25			
1	B	482	Total	C	N	O	S	0	1	0
			3835	2424	678	709	24			
1	C	478	Total	C	N	O	S	0	0	0
			3803	2406	670	703	24			
1	D	479	Total	C	N	O	S	0	2	0
			3820	2415	674	707	24			
1	E	477	Total	C	N	O	S	0	2	0
			3807	2408	672	702	25			
1	F	473	Total	C	N	O	S	0	0	0
			3761	2381	659	697	24			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7
A	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
A	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
A	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
A	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
A	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
A	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
A	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7
B	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
B	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
B	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7

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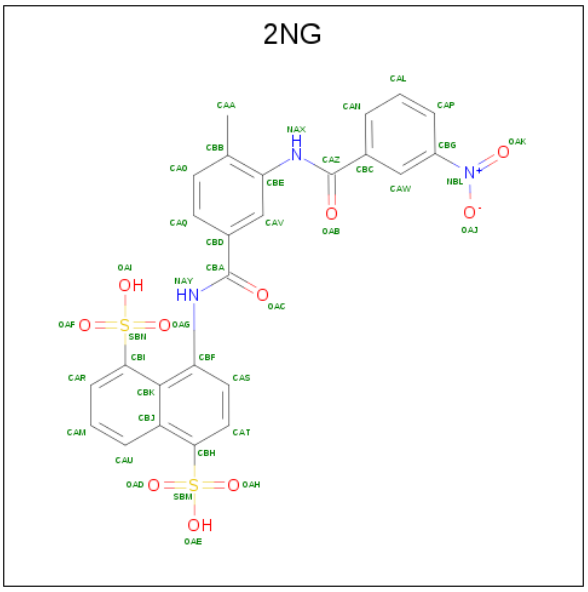
Chain	Residue	Modelled	Actual	Comment	Reference
C	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
C	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
C	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7
D	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
D	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
D	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7
E	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
E	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
E	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	508	LEU	-	EXPRESSION TAG	UNP S4V9Y7
F	509	GLU	-	EXPRESSION TAG	UNP S4V9Y7
F	510	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	511	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	512	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	513	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	514	HIS	-	EXPRESSION TAG	UNP S4V9Y7
F	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7

- Molecule 2 is 4-({4-methyl-3-[(3-nitrobenzoyl)amino]benzoyl}amino)naphthalene-1,5-disulfonic acid (three-letter code: 2NG) (formula: $C_{25}H_{19}N_3O_{10}S_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 40 25 3 10 2	0	0
2	B	1	Total C N O S 40 25 3 10 2	0	0
2	C	1	Total C N O S 40 25 3 10 2	0	0
2	D	1	Total C N O S 40 25 3 10 2	0	0
2	E	1	Total C N O S 40 25 3 10 2	0	0
2	E	1	Total C N O S 40 25 3 10 2	0	0
2	F	1	Total C N O S 40 25 3 10 2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is water.

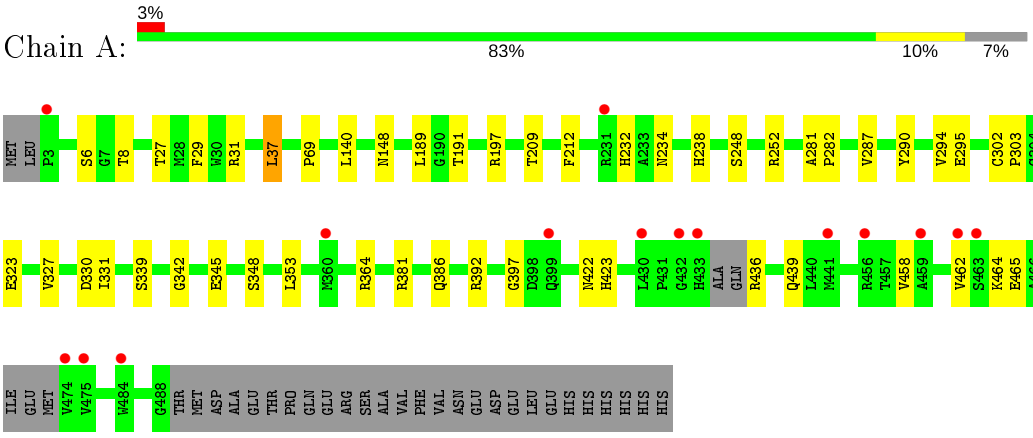
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	384	Total O 385 385	0	1
4	B	331	Total O 332 332	0	1
4	C	304	Total O 305 305	0	1
4	D	302	Total O 303 303	0	1
4	E	248	Total O 248 248	0	1
4	F	145	Total O 145 145	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

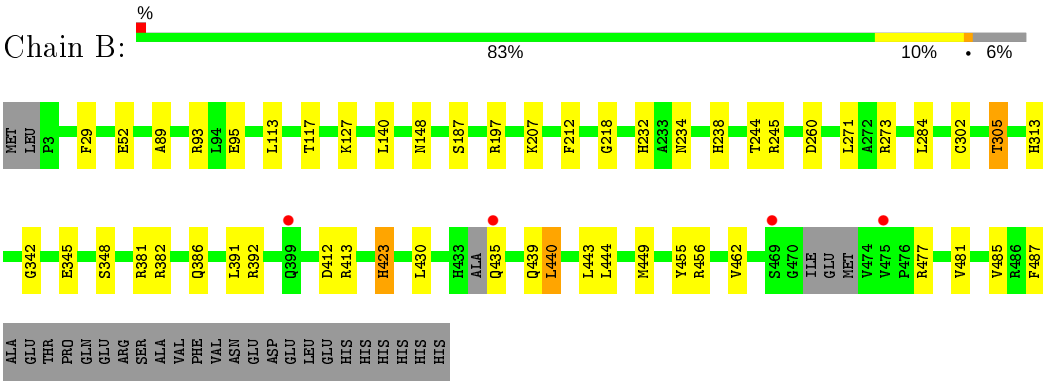
- Molecule 1: RNA dependent RNA polymerase

Chain A:



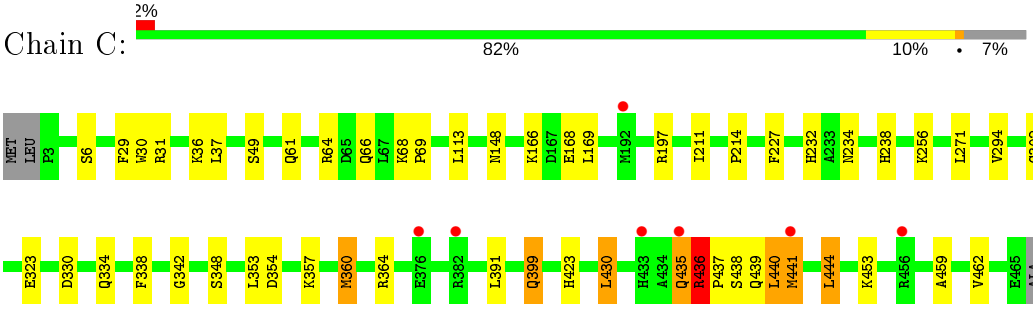
- Molecule 1: RNA dependent RNA polymerase

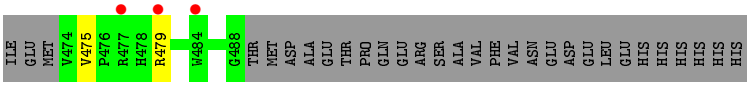
Chain B:



- Molecule 1: RNA dependent RNA polymerase

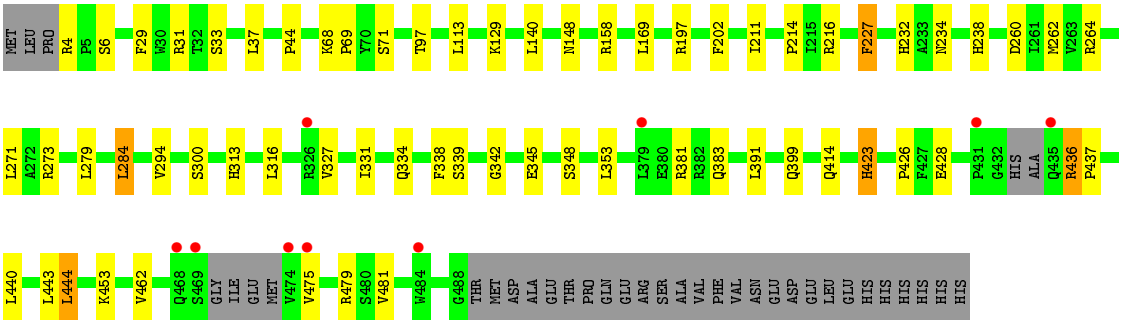
Chain C:





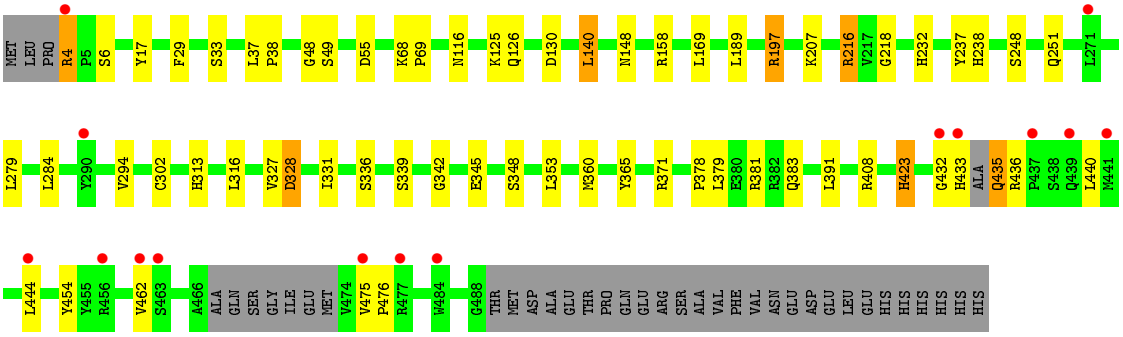
• Molecule 1: RNA dependent RNA polymerase

Chain D:



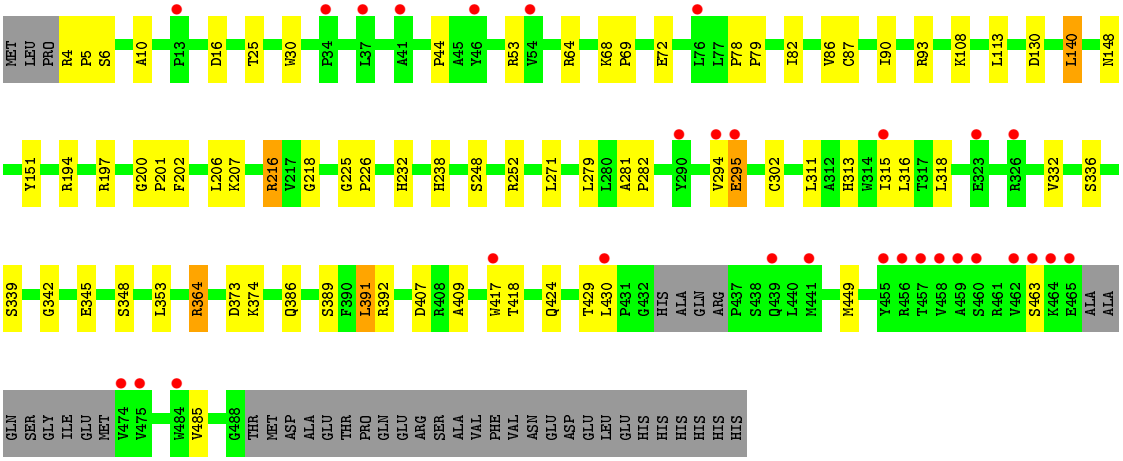
• Molecule 1: RNA dependent RNA polymerase

Chain E:



• Molecule 1: RNA dependent RNA polymerase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.22Å 162.42Å 122.96Å 90.00° 97.04° 90.00°	Depositor
Resolution (Å)	61.09 – 2.30 61.02 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (61.09-2.30) 99.8 (61.02-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.78 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.191 , 0.254 0.194 , 0.254	Depositor DCC
R_{free} test set	9445 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.1	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	24851	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 2NG

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	0.52	0/3928	0.71	0/5319
1	B	0.49	0/3932	0.70	2/5324 (0.0%)
1	C	0.49	0/3898	0.69	0/5281
1	D	0.49	0/3918	0.70	0/5305
1	E	0.47	0/3906	0.69	0/5290
1	F	0.45	0/3853	0.65	0/5218
All	All	0.49	0/23435	0.69	2/31737 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	412	ASP	CB-CG-OD1	5.85	123.56	118.30
1	B	413	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3821	0	3792	36	0
1	B	3835	0	3794	25	0
1	C	3803	0	3761	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3820	0	3784	33	0
1	E	3807	0	3770	34	0
1	F	3761	0	3720	41	0
2	A	40	0	19	5	0
2	B	40	0	19	2	0
2	C	40	0	19	2	0
2	D	40	0	19	1	0
2	E	80	0	38	5	0
2	F	40	0	19	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	385	0	0	2	0
4	B	332	0	0	1	0
4	C	305	0	0	3	0
4	D	303	0	0	3	0
4	E	248	0	0	3	0
4	F	145	0	0	1	0
All	All	24851	0	22754	229	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 5.

All (229) 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:F:364:ARG:HB2	1:F:364:ARG:NH1	1.24	1.47
2:F:1101:2NG:NBL	2:F:1101:2NG:OAJ	1.73	1.19
1:F:364:ARG:CB	1:F:364:ARG:NH1	2.11	1.13
1:F:364:ARG:CB	1:F:364:ARG:HH11	1.68	1.04
1:C:435:GLN:CB	1:C:437:PRO:HD3	1.90	1.00
1:D:148:ASN:HD21	1:D:197:ARG:HH11	1.13	0.95
1:C:435:GLN:HB3	1:C:437:PRO:HD3	1.58	0.85
1:C:435:GLN:C	1:C:437:PRO:HD3	2.02	0.80
1:A:8:THR:HG22	4:A:1492:HOH:O	1.83	0.78
1:C:436:ARG:N	1:C:437:PRO:CD	2.46	0.78
1:F:364:ARG:CZ	1:F:364:ARG:HB2	2.14	0.77
1:A:148:ASN:HD21	1:A:197:ARG:HH11	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.33	0.76
1:C:435:GLN:HB3	1:C:437:PRO:CD	2.16	0.76
1:C:435:GLN:HB3	1:C:436:ARG:C	2.07	0.75
1:E:238:HIS:HD2	1:E:348:SER:OG	1.69	0.75
1:B:302:CYS:O	1:B:305:THR:HG23	1.88	0.74
1:C:435:GLN:HB3	1:C:436:ARG:CA	2.19	0.72
1:C:435:GLN:CG	1:C:436:ARG:HB3	2.19	0.72
1:D:148:ASN:ND2	1:D:197:ARG:HH11	1.86	0.71
1:F:364:ARG:HH11	1:F:364:ARG:HB2	0.76	0.70
1:A:232:HIS:HD2	1:A:348:SER:OG	1.75	0.69
1:D:479:ARG:HD3	4:D:1502[A]:HOH:O	1.92	0.69
1:F:364:ARG:CB	1:F:364:ARG:CZ	2.66	0.68
1:B:238:HIS:HD2	1:B:348:SER:OG	1.76	0.67
1:F:238:HIS:HD2	1:F:348:SER:OG	1.77	0.67
1:D:148:ASN:HD21	1:D:197:ARG:NH1	1.89	0.67
1:B:302:CYS:SG	1:B:305:THR:HG22	2.35	0.66
1:D:313:HIS:HD2	1:D:342:GLY:O	1.78	0.66
1:E:433:HIS:O	1:E:435:GLN:N	2.29	0.66
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.44	0.66
1:B:232:HIS:HE1	1:B:339:SER:OG	1.80	0.65
1:C:435:GLN:HA	1:C:436:ARG:HB2	1.78	0.65
1:E:68:LYS:HB2	1:E:69:PRO:HD3	1.79	0.64
1:C:438:SER:O	1:C:441:MET:HB3	1.98	0.64
1:F:90:ILE:HD12	1:F:315:ILE:HD13	1.79	0.62
1:C:435:GLN:HB3	1:C:437:PRO:N	2.15	0.62
1:F:79:PRO:HG2	1:F:82:ILE:HD12	1.82	0.62
1:A:212[B]:PHE:CZ	1:B:487:PHE:HB3	2.34	0.61
1:F:30:TRP:CD2	1:F:430:LEU:HD13	2.35	0.61
1:A:302[A]:CYS:SG	1:A:305:THR:HG23	2.41	0.61
1:F:44:PRO:HD3	1:F:417:TRP:CH2	2.36	0.61
1:B:313:HIS:HD2	1:B:342:GLY:O	1.84	0.61
1:C:435:GLN:CA	1:C:437:PRO:HD3	2.30	0.61
2:E:1101:2NG:OAG	2:E:1101:2NG:H8	2.01	0.61
1:E:29:PHE:O	1:E:423:HIS:HE1	1.83	0.61
1:A:353:LEU:O	1:A:381:ARG:NH1	2.34	0.60
1:C:435:GLN:C	1:C:437:PRO:CD	2.70	0.60
1:E:216:ARG:HD3	1:E:339:SER:OG	2.00	0.60
1:A:313:HIS:HD2	1:A:342:GLY:O	1.84	0.60
2:E:1102:2NG:NAY	2:E:1102:2NG:SBN	2.74	0.60
1:A:140:LEU:HG	1:A:189:LEU:HD22	1.84	0.59
1:C:211:ILE:HG21	1:C:227:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:475:VAL:O	1:C:475:VAL:HG13	2.04	0.58
1:C:435:GLN:CB	1:C:436:ARG:HB3	2.33	0.58
1:C:435:GLN:HB2	1:C:437:PRO:HD3	1.81	0.58
1:D:44:PRO:HG2	1:D:426:PRO:HB3	1.86	0.58
1:B:477:ARG:O	1:B:481:VAL:HG12	2.04	0.58
1:D:232:HIS:HE1	1:D:339:SER:OG	1.86	0.58
1:C:435:GLN:HG2	1:C:440:LEU:HD22	1.86	0.57
1:F:151:TYR:HB2	1:F:194:ARG:HG2	1.86	0.57
1:D:238:HIS:HD2	1:D:348:SER:OG	1.88	0.57
2:E:1101:2NG:OAG	2:E:1101:2NG:NAY	2.36	0.56
1:A:148:ASN:ND2	1:A:197:ARG:HH11	2.01	0.56
1:F:87:CYS:SG	1:F:315:ILE:HD12	2.46	0.56
1:A:148:ASN:HD21	1:A:197:ARG:NH1	2.04	0.55
1:F:148:ASN:HD21	1:F:197:ARG:HH11	1.52	0.55
1:B:244:THR:HG22	1:B:245:ARG:HG3	1.88	0.55
1:B:260:ASP:OD1	1:B:273:ARG:NH2	2.39	0.55
1:E:327:VAL:HG12	1:E:331:ILE:HB	1.89	0.55
1:F:216:ARG:HD3	1:F:339:SER:OG	2.07	0.55
1:A:302[A]:CYS:HB2	1:A:303:PRO:HD2	1.88	0.54
1:C:435:GLN:CA	1:C:436:ARG:CB	2.85	0.54
1:C:436:ARG:N	1:C:437:PRO:HD3	2.18	0.54
1:A:232:HIS:HE1	1:A:339:SER:OG	1.90	0.54
1:C:435:GLN:CB	1:C:436:ARG:CB	2.84	0.54
2:A:1101:2NG:SBN	2:A:1101:2NG:NAY	2.81	0.54
1:C:440:LEU:HG	1:C:462:VAL:HG13	1.88	0.54
1:D:353:LEU:O	1:D:381:ARG:NH1	2.41	0.54
1:A:323:GLU:OE2	1:A:364[A]:ARG:NH2	2.41	0.53
1:B:449:MET:HE2	1:B:485:VAL:HG13	1.90	0.53
1:C:238:HIS:HD2	1:C:348:SER:OG	1.90	0.53
2:C:1101:2NG:OAG	2:C:1101:2NG:H8	2.09	0.53
1:C:214:PRO:HB3	1:C:338:PHE:HB2	1.91	0.53
1:E:125:LYS:HE3	1:E:140:LEU:HD13	1.91	0.53
1:F:86:VAL:HG13	1:F:318:LEU:HD23	1.91	0.53
1:A:386:GLN:NE2	1:A:397:GLY:H	2.06	0.53
2:B:1101:2NG:NAY	2:B:1101:2NG:SBN	2.83	0.52
1:B:29:PHE:O	1:B:423:HIS:HE1	1.93	0.52
1:D:227:PHE:HB2	4:D:1267:HOH:O	2.09	0.52
2:C:1101:2NG:SBN	2:C:1101:2NG:NAY	2.83	0.52
1:F:130:ASP:HB2	1:F:140:LEU:HD22	1.92	0.52
1:B:440:LEU:HG	1:B:462:VAL:HG13	1.93	0.51
1:A:209:THR:HG22	1:A:212[B]:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:444:LEU:HD21	1:D:462:VAL:HG11	1.93	0.51
1:A:313:HIS:HE1	1:A:345:GLU:OE2	1.93	0.51
1:C:439:GLN:NE2	4:C:1472:HOH:O	2.44	0.51
1:F:207:LYS:HG2	1:F:218:GLY:HA3	1.94	0.50
1:C:31:ARG:NE	1:C:37:LEU:HD13	2.27	0.50
1:E:158:ARG:NH2	1:E:284:LEU:HD13	2.26	0.50
1:A:191:THR:HG22	1:A:302[B]:CYS:SG	2.52	0.50
1:B:89:ALA:HB1	1:B:333:MET:CE	2.41	0.50
1:A:69:PRO:HB2	1:A:248:SER:HB2	1.95	0.49
1:F:25:THR:O	1:F:424:GLN:NE2	2.45	0.49
1:A:327:VAL:CG1	1:A:331:ILE:HB	2.43	0.49
2:D:1101:2NG:SBN	2:D:1101:2NG:NAY	2.86	0.49
1:A:232:HIS:CD2	1:A:348:SER:OG	2.62	0.49
1:E:371:ARG:NH1	1:E:378:PRO:O	2.42	0.49
1:A:464:LYS:HB3	4:A:1482:HOH:O	2.12	0.48
1:C:360:MET:HG2	4:C:1445:HOH:O	2.13	0.48
1:C:435:GLN:CA	1:C:436:ARG:HB2	2.40	0.48
1:C:436:ARG:N	1:C:437:PRO:HD2	2.26	0.48
1:B:117:THR:OG1	1:B:127:LYS:NZ	2.47	0.48
1:C:435:GLN:CB	1:C:437:PRO:CD	2.72	0.48
1:D:29:PHE:O	1:D:423:HIS:HE1	1.96	0.48
1:E:313:HIS:HD2	1:E:342:GLY:O	1.96	0.48
1:B:381:ARG:HD2	4:B:1484:HOH:O	2.13	0.48
1:A:323:GLU:OE1	1:A:364[B]:ARG:NH2	2.45	0.48
1:C:29:PHE:O	1:C:423:HIS:HE1	1.97	0.48
1:C:334:GLN:HG2	1:D:399[A]:GLN:HG3	1.95	0.48
1:E:251:GLN:NE2	1:E:365:TYR:O	2.47	0.48
1:D:232:HIS:HD2	1:D:348:SER:OG	1.97	0.48
1:D:414:GLN:O	1:D:436:ARG:NH2	2.38	0.48
1:C:435:GLN:HG2	1:C:440:LEU:CD2	2.44	0.47
2:E:1101:2NG:SBN	2:E:1101:2NG:NAY	2.87	0.47
1:E:237:TYR:HB3	1:E:381:ARG:HG2	1.96	0.47
1:C:444:LEU:HD13	1:C:462:VAL:HG21	1.96	0.47
1:C:459:ALA:HB1	1:C:475:VAL:HG21	1.95	0.47
1:D:158:ARG:NH2	1:D:284:LEU:HD13	2.30	0.47
1:C:435:GLN:HA	1:C:436:ARG:CB	2.44	0.47
1:D:260:ASP:OD1	1:D:273:ARG:NH2	2.47	0.47
1:E:327:VAL:HG11	1:E:331:ILE:HG21	1.97	0.47
1:C:166:LYS:HE3	1:C:168:GLU:OE1	2.14	0.47
1:C:313:HIS:HD2	1:C:342:GLY:O	1.97	0.46
1:F:313:HIS:HD2	1:F:342:GLY:O	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:O	1:A:423:HIS:HE1	1.98	0.46
1:E:207:LYS:HG3	1:E:218:GLY:HA3	1.97	0.46
1:C:435:GLN:HG3	1:C:436:ARG:HB3	1.95	0.46
1:D:264:ARG:HG3	4:D:1213:HOH:O	2.16	0.46
1:E:232:HIS:HD2	1:E:348:SER:OG	1.99	0.46
1:C:66:GLN:O	1:C:69:PRO:HD2	2.16	0.46
2:F:1101:2NG:H8	2:F:1101:2NG:OAI	2.16	0.45
1:F:311:LEU:O	1:F:315:ILE:HG12	2.16	0.45
1:C:256:LYS:NZ	4:C:1437:HOH:O	2.49	0.45
2:F:1101:2NG:SBN	2:F:1101:2NG:NAY	2.89	0.45
2:A:1101:2NG:H8	2:A:1101:2NG:OAG	2.17	0.45
1:F:5:PRO:HD2	1:F:16:ASP:HA	1.99	0.45
1:E:116:ASN:HA	1:E:126:GLN:HE21	1.82	0.45
1:E:148:ASN:HD21	1:E:197:ARG:HH11	1.65	0.45
1:C:68:LYS:HB2	1:C:69:PRO:HD3	1.99	0.45
1:F:10:ALA:HB2	1:F:64:ARG:HG2	1.99	0.45
1:A:392:ARG:HD3	2:A:1101:2NG:H11	1.99	0.45
1:D:211:ILE:HG21	1:D:227:PHE:CD2	2.52	0.44
1:E:339:SER:O	1:E:345:GLU:HA	2.18	0.44
1:B:93:ARG:NH2	1:B:212:PHE:O	2.50	0.44
1:D:232:HIS:CE1	1:D:339:SER:OG	2.67	0.44
1:D:423:HIS:HD2	1:D:428:GLU:OE1	2.01	0.44
1:D:436:ARG:N	1:D:437:PRO:CD	2.80	0.44
1:A:464:LYS:HA	1:A:465:GLU:HA	1.77	0.44
1:B:89:ALA:HB1	1:B:333:MET:HE2	2.00	0.44
1:F:232:HIS:HE1	1:F:339:SER:OG	2.01	0.44
1:A:323:GLU:CD	1:A:364[B]:ARG:HH21	2.21	0.44
1:E:130:ASP:HB2	1:E:140:LEU:HD22	2.00	0.44
1:A:238:HIS:HD2	1:A:348:SER:OG	2.00	0.44
1:A:27:THR:O	1:A:422:ASN:HA	2.17	0.43
1:C:399:GLN:HB3	1:D:334:GLN:HA	2.00	0.43
1:D:313:HIS:CD2	1:D:342:GLY:O	2.67	0.43
1:B:207:LYS:HG3	1:B:218:GLY:HA3	2.00	0.43
1:C:30:TRP:CD2	1:C:430:LEU:HD13	2.53	0.43
1:C:61:GLN:HE21	1:C:64:ARG:HH21	1.66	0.43
1:E:232:HIS:HE1	1:E:339:SER:OG	2.01	0.43
1:F:449:MET:HE3	1:F:485:VAL:HG22	1.99	0.43
1:F:332:VAL:O	1:F:336:SER:HB2	2.19	0.43
1:A:31:ARG:NE	1:A:37:LEU:HD13	2.33	0.43
1:D:214:PRO:HB3	1:D:338:PHE:HB2	1.99	0.43
1:C:234:ASN:OD1	1:D:234:ASN:OD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ASN:OD1	1:B:234:ASN:OD1	2.36	0.43
1:B:232:HIS:CE1	1:B:339:SER:OG	2.67	0.43
1:B:391:LEU:O	1:B:392:ARG:HG2	2.19	0.43
1:F:69:PRO:HB2	1:F:248:SER:HB2	2.01	0.43
1:D:202:PHE:CE2	1:D:262:MET:HG2	2.54	0.43
1:F:68:LYS:HB2	1:F:69:PRO:HD3	2.01	0.43
1:B:313:HIS:HE1	1:B:345:GLU:OE2	2.02	0.42
1:B:382:ARG:NH2	1:B:386:GLN:O	2.52	0.42
1:F:391:LEU:O	1:F:392:ARG:HG3	2.19	0.42
1:E:17:TYR:HB3	4:E:1405:HOH:O	2.18	0.42
1:E:328:ASP:HA	2:E:1102:2NG:OAJ	2.19	0.42
1:C:354:ASP:OD2	1:C:357:LYS:HD2	2.19	0.42
1:E:48:GLY:O	1:E:49:SER:C	2.58	0.42
1:A:252:ARG:HG3	1:A:295:GLU:O	2.19	0.42
1:D:475:VAL:HG13	1:D:475:VAL:O	2.19	0.42
1:F:407:ASP:OD2	1:F:409:ALA:HB3	2.19	0.42
1:A:436:ARG:NH1	2:A:1101:2NG:OAE	2.48	0.42
1:C:435:GLN:HB3	1:C:436:ARG:CB	2.47	0.42
1:C:323:GLU:OE2	1:C:364:ARG:NH2	2.53	0.41
1:F:200:GLY:N	1:F:201:PRO:CD	2.83	0.41
1:F:78:PRO:O	1:F:79:PRO:C	2.58	0.41
1:D:68:LYS:N	1:D:69:PRO:HD2	2.36	0.41
1:F:44:PRO:O	1:F:53:ARG:NH1	2.48	0.41
1:D:284:LEU:HA	1:D:284:LEU:HD12	1.94	0.41
1:E:140:LEU:HG	1:E:189:LEU:HD22	2.02	0.41
1:F:281:ALA:O	1:F:282:PRO:C	2.58	0.41
1:F:69:PRO:HA	1:F:72:GLU:HG2	2.02	0.41
1:A:439:GLN:HG2	2:A:1101:2NG:OAE	2.19	0.41
1:E:238:HIS:CD2	1:E:348:SER:OG	2.60	0.41
1:E:237:TYR:O	1:E:348:SER:HA	2.19	0.41
1:E:4:ARG:HA	4:E:1401:HOH:O	2.21	0.41
1:F:202:PHE:CE2	1:F:206:LEU:HD22	2.55	0.41
1:F:252:ARG:HG3	1:F:295:GLU:O	2.19	0.41
1:A:281:ALA:O	1:A:282:PRO:C	2.58	0.41
1:F:339:SER:O	1:F:345:GLU:HA	2.21	0.41
2:B:1101:2NG:OAH	2:B:1101:2NG:H3	2.21	0.41
1:E:69:PRO:HB2	1:E:248:SER:HB2	2.03	0.41
1:F:151:TYR:HA	4:F:1248:HOH:O	2.20	0.41
1:A:287:VAL:HG22	1:A:290:TYR:O	2.21	0.41
1:C:232:HIS:HD2	1:C:348:SER:OG	2.03	0.41
1:D:31:ARG:HD3	1:D:37:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:LEU:HD13	4:E:1416:HOH:O	2.21	0.41
1:E:408:ARG:HG2	1:E:454:TYR:CZ	2.55	0.41
1:E:440:LEU:HG	1:E:462:VAL:HG13	2.02	0.41
1:D:313:HIS:HE1	1:D:345:GLU:OE2	2.04	0.40
1:E:475:VAL:HA	1:E:476:PRO:HD3	1.97	0.40
1:F:373:ASP:O	1:F:374:LYS:HB2	2.21	0.40
1:E:436:ARG:O	1:E:440:LEU:HB2	2.21	0.40
1:F:225:GLY:N	1:F:226:PRO:CD	2.84	0.40
1:A:458:VAL:O	1:A:462:VAL:HG23	2.22	0.40
1:B:455:TYR:CE1	1:B:481:VAL:HG11	2.57	0.40
1:D:327:VAL:HG12	1:D:331:ILE:HB	2.03	0.40
1:E:432:GLY:HA3	1:E:433:HIS:HA	1.89	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	475/515 (92%)	465 (98%)	10 (2%)	0	100	100
1	B	477/515 (93%)	465 (98%)	12 (2%)	0	100	100
1	C	474/515 (92%)	465 (98%)	8 (2%)	1 (0%)	47	58
1	D	475/515 (92%)	463 (98%)	11 (2%)	1 (0%)	47	58
1	E	473/515 (92%)	460 (97%)	12 (2%)	1 (0%)	47	58
1	F	467/515 (91%)	448 (96%)	19 (4%)	0	100	100
All	All	2841/3090 (92%)	2766 (97%)	72 (2%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	436	ARG

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Mol	Chain	Res	Type
1	D	436	ARG
1	E	38	PRO

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	412/441 (93%)	408 (99%)	4 (1%)	76	87
1	B	412/441 (93%)	396 (96%)	16 (4%)	32	46
1	C	409/441 (93%)	387 (95%)	22 (5%)	22	30
1	D	411/441 (93%)	386 (94%)	25 (6%)	18	25
1	E	410/441 (93%)	387 (94%)	23 (6%)	21	29
1	F	405/441 (92%)	384 (95%)	21 (5%)	23	32
All	All	2459/2646 (93%)	2348 (96%)	111 (4%)	27	39

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	37	LEU
1	A	294	VAL
1	A	330	ASP
1	B	52	GLU
1	B	95	GLU
1	B	113	LEU
1	B	140	LEU
1	B	187	SER
1	B	271	LEU
1	B	284	LEU
1	B	305	THR
1	B	423	HIS
1	B	430	LEU
1	B	435	GLN
1	B	439	GLN

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Mol	Chain	Res	Type
1	B	440	LEU
1	B	443	LEU
1	B	444	LEU
1	B	456	ARG
1	C	6	SER
1	C	36	LYS
1	C	49	SER
1	C	113	LEU
1	C	169	LEU
1	C	271	LEU
1	C	294	VAL
1	C	302	CYS
1	C	316	LEU
1	C	330	ASP
1	C	353	LEU
1	C	360	MET
1	C	391	LEU
1	C	399	GLN
1	C	430	LEU
1	C	435	GLN
1	C	436	ARG
1	C	440	LEU
1	C	441	MET
1	C	444	LEU
1	C	453	LYS
1	C	479	ARG
1	D	4	ARG
1	D	6	SER
1	D	33	SER
1	D	71	SER
1	D	97	THR
1	D	113	LEU
1	D	129	LYS
1	D	140	LEU
1	D	169	LEU
1	D	216	ARG
1	D	227	PHE
1	D	271	LEU
1	D	279	LEU
1	D	284	LEU
1	D	294	VAL
1	D	300	SER

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Mol	Chain	Res	Type
1	D	316	LEU
1	D	383	GLN
1	D	391	LEU
1	D	423	HIS
1	D	440	LEU
1	D	443	LEU
1	D	444	LEU
1	D	453	LYS
1	D	481	VAL
1	E	4	ARG
1	E	6	SER
1	E	33	SER
1	E	37	LEU
1	E	55	ASP
1	E	140	LEU
1	E	169	LEU
1	E	197	ARG
1	E	216	ARG
1	E	279	LEU
1	E	294	VAL
1	E	302[A]	CYS
1	E	302[B]	CYS
1	E	316	LEU
1	E	328	ASP
1	E	336	SER
1	E	353	LEU
1	E	360	MET
1	E	383	GLN
1	E	391	LEU
1	E	423	HIS
1	E	435	GLN
1	E	444	LEU
1	F	4	ARG
1	F	6	SER
1	F	93	ARG
1	F	108	LYS
1	F	113	LEU
1	F	140	LEU
1	F	216	ARG
1	F	271	LEU
1	F	279	LEU
1	F	294	VAL

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Mol	Chain	Res	Type
1	F	295	GLU
1	F	302	CYS
1	F	316	LEU
1	F	353	LEU
1	F	364	ARG
1	F	386	GLN
1	F	389	SER
1	F	391	LEU
1	F	418	THR
1	F	429	THR
1	F	463	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	61	GLN
1	A	126	GLN
1	A	148	ASN
1	A	222	ASN
1	A	232	HIS
1	A	234	ASN
1	A	238	HIS
1	A	250	GLN
1	A	313	HIS
1	A	386	GLN
1	A	423	HIS
1	A	478	HIS
1	B	61	GLN
1	B	148	ASN
1	B	232	HIS
1	B	238	HIS
1	B	250	GLN
1	B	313	HIS
1	B	423	HIS
1	B	424	GLN
1	B	435	GLN
1	B	439	GLN
1	B	478	HIS
1	C	60	GLN
1	C	61	GLN
1	C	148	ASN

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Mol	Chain	Res	Type
1	C	232	HIS
1	C	238	HIS
1	C	313	HIS
1	C	423	HIS
1	C	439	GLN
1	C	478	HIS
1	D	60	GLN
1	D	61	GLN
1	D	66	GLN
1	D	148	ASN
1	D	222	ASN
1	D	232	HIS
1	D	238	HIS
1	D	250	GLN
1	D	313	HIS
1	D	334	GLN
1	D	423	HIS
1	E	60	GLN
1	E	126	GLN
1	E	148	ASN
1	E	232	HIS
1	E	238	HIS
1	E	313	HIS
1	E	334	GLN
1	E	383	GLN
1	E	423	HIS
1	E	439	GLN
1	E	478	HIS
1	F	60	GLN
1	F	61	GLN
1	F	66	GLN
1	F	148	ASN
1	F	232	HIS
1	F	238	HIS
1	F	250	GLN
1	F	386	GLN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
2	2NG	B	1101	-	40,43,43	2.98	8 (20%)	56,65,65	1.08	4 (7%)
2	2NG	F	1101	-	40,43,43	3.65	6 (15%)	56,65,65	1.30	5 (8%)
2	2NG	D	1101	-	40,43,43	3.63	8 (20%)	56,65,65	1.17	4 (7%)
2	2NG	A	1101	-	40,43,43	2.90	7 (17%)	56,65,65	1.11	2 (3%)
2	2NG	E	1102	-	40,43,43	3.18	10 (25%)	56,65,65	1.37	9 (16%)
2	2NG	E	1101	-	40,43,43	2.87	7 (17%)	56,65,65	1.14	3 (5%)
2	2NG	C	1101	-	40,43,43	3.05	6 (15%)	56,65,65	1.22	4 (7%)

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	2NG	B	1101	-	-	4/30/32/32	0/4/4/4
2	2NG	F	1101	-	-	2/30/32/32	0/4/4/4
2	2NG	D	1101	-	-	2/30/32/32	0/4/4/4
2	2NG	A	1101	-	-	3/30/32/32	0/4/4/4
2	2NG	E	1102	-	-	2/30/32/32	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2NG	E	1101	-	-	3/30/32/32	0/4/4/4
2	2NG	C	1101	-	-	4/30/32/32	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1101	2NG	OAK-NBL	19.68	1.56	1.22
2	D	1101	2NG	OAK-NBL	19.01	1.55	1.22
2	E	1102	2NG	OAK-NBL	15.55	1.49	1.22
2	C	1101	2NG	OAK-NBL	14.90	1.48	1.22
2	B	1101	2NG	OAK-NBL	14.56	1.47	1.22
2	A	1101	2NG	OAK-NBL	13.96	1.46	1.22
2	E	1101	2NG	OAK-NBL	13.41	1.45	1.22
2	E	1102	2NG	CBG-NBL	-5.61	1.31	1.45
2	D	1101	2NG	CBC-CAZ	-5.27	1.39	1.50
2	E	1101	2NG	CAA-CBB	-5.26	1.40	1.51
2	D	1101	2NG	CBG-NBL	-5.23	1.32	1.45
2	C	1101	2NG	CBC-CAZ	-5.23	1.39	1.50
2	D	1101	2NG	CAA-CBB	-5.23	1.40	1.51
2	C	1101	2NG	CAA-CBB	-5.17	1.40	1.51
2	E	1102	2NG	CAA-CBB	-5.10	1.40	1.51
2	C	1101	2NG	CBG-NBL	-5.08	1.33	1.45
2	F	1101	2NG	CAA-CBB	-5.02	1.41	1.51
2	F	1101	2NG	CBC-CAZ	-5.02	1.39	1.50
2	B	1101	2NG	CAA-CBB	-4.89	1.41	1.51
2	A	1101	2NG	CBG-NBL	-4.87	1.33	1.45
2	B	1101	2NG	CBC-CAZ	-4.87	1.40	1.50
2	A	1101	2NG	CAA-CBB	-4.86	1.41	1.51
2	E	1101	2NG	CBC-CAZ	-4.84	1.40	1.50
2	B	1101	2NG	CBG-NBL	-4.83	1.33	1.45
2	E	1101	2NG	CBG-NBL	-4.60	1.34	1.45
2	F	1101	2NG	CBG-NBL	-4.53	1.34	1.45
2	D	1101	2NG	CBE-NAX	-4.52	1.33	1.41
2	E	1101	2NG	CBD-CBA	-4.43	1.41	1.50
2	A	1101	2NG	CBC-CAZ	-4.38	1.41	1.50
2	F	1101	2NG	CBE-NAX	-4.33	1.33	1.41
2	E	1102	2NG	CBE-NAX	-4.24	1.33	1.41
2	D	1101	2NG	CBD-CBA	-4.23	1.41	1.50
2	E	1102	2NG	CBC-CAZ	-4.22	1.41	1.50
2	F	1101	2NG	CBD-CBA	-4.16	1.41	1.50
2	E	1101	2NG	CBE-NAX	-4.10	1.34	1.41
2	A	1101	2NG	CBE-NAX	-4.08	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	2NG	CBD-CBA	-4.07	1.41	1.50
2	A	1101	2NG	CBD-CBA	-4.01	1.41	1.50
2	E	1102	2NG	CBD-CBA	-3.98	1.41	1.50
2	C	1101	2NG	CBE-NAX	-3.93	1.34	1.41
2	B	1101	2NG	CBD-CBA	-3.91	1.42	1.50
2	B	1101	2NG	CBE-NAX	-3.52	1.35	1.41
2	D	1101	2NG	CBF-NAY	-2.76	1.34	1.41
2	B	1101	2NG	CAR-CBI	2.43	1.40	1.37
2	D	1101	2NG	OAF-SBN	2.36	1.55	1.43
2	E	1101	2NG	CBF-NAY	-2.35	1.35	1.41
2	E	1102	2NG	CAR-CBI	2.22	1.40	1.37
2	E	1102	2NG	CAT-CBH	2.17	1.40	1.37
2	E	1102	2NG	OAF-SBN	2.13	1.54	1.43
2	B	1101	2NG	OAG-SBN	2.12	1.54	1.43
2	A	1101	2NG	CAR-CBI	2.11	1.39	1.37
2	E	1102	2NG	OAG-SBN	2.10	1.54	1.43

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1101	2NG	CAU-CBJ-CBH	-4.41	117.82	123.60
2	C	1101	2NG	CAP-CBG-NBL	3.80	122.24	119.38
2	A	1101	2NG	CAU-CBJ-CBH	-3.72	118.72	123.60
2	C	1101	2NG	CAU-CBJ-CBH	-3.63	118.84	123.60
2	E	1101	2NG	CAU-CBJ-CBH	-3.63	118.84	123.60
2	B	1101	2NG	CAU-CBJ-CBH	-3.51	119.00	123.60
2	E	1102	2NG	CBF-NAY-CBA	-3.49	118.30	128.64
2	F	1101	2NG	CAW-CBG-NBL	3.48	121.81	118.75
2	D	1101	2NG	CAU-CBJ-CBH	-3.34	119.22	123.60
2	C	1101	2NG	CBE-NAX-CAZ	-3.12	118.38	126.93
2	E	1101	2NG	CBE-NAX-CAZ	-3.06	118.53	126.93
2	D	1101	2NG	CAP-CBG-NBL	3.05	121.67	119.38
2	E	1102	2NG	CAU-CBJ-CBH	-2.95	119.73	123.60
2	D	1101	2NG	CBE-NAX-CAZ	-2.88	119.04	126.93
2	E	1101	2NG	CBF-NAY-CBA	-2.71	120.60	128.64
2	E	1102	2NG	CAW-CBG-NBL	-2.57	116.48	118.75
2	B	1101	2NG	CBF-NAY-CBA	-2.51	121.20	128.64
2	E	1102	2NG	OAH-SBM-CBH	2.50	113.89	106.43
2	C	1101	2NG	CBF-NAY-CBA	-2.45	121.39	128.64
2	E	1102	2NG	CBE-NAX-CAZ	-2.44	120.24	126.93
2	F	1101	2NG	CBE-NAX-CAZ	-2.40	120.33	126.93
2	D	1101	2NG	CBF-NAY-CBA	-2.37	121.63	128.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1102	2NG	CAS-CAT-CBH	-2.33	118.85	121.66
2	E	1102	2NG	CAP-CBG-CAW	2.25	122.94	120.09
2	F	1101	2NG	CBB-CBE-NAX	-2.24	115.32	118.81
2	F	1101	2NG	CBH-CBJ-CBK	2.24	121.59	118.01
2	B	1101	2NG	CBE-NAX-CAZ	-2.14	121.07	126.93
2	E	1102	2NG	CAL-CAN-CBC	2.13	122.87	120.34
2	B	1101	2NG	CAW-CBG-NBL	2.11	120.61	118.75
2	E	1102	2NG	CAN-CBC-CAW	-2.10	116.75	119.24
2	A	1101	2NG	CBE-NAX-CAZ	-2.07	121.25	126.93

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	2NG	CAW-CBG-NBL-OAK
2	B	1101	2NG	CAP-CBG-NBL-OAK
2	C	1101	2NG	CAW-CBG-NBL-OAK
2	C	1101	2NG	CAP-CBG-NBL-OAK
2	A	1101	2NG	CAV-CBE-NAX-CAZ
2	F	1101	2NG	CAV-CBE-NAX-CAZ
2	A	1101	2NG	CBB-CBE-NAX-CAZ
2	C	1101	2NG	CAV-CBE-NAX-CAZ
2	D	1101	2NG	CAV-CBE-NAX-CAZ
2	F	1101	2NG	CBB-CBE-NAX-CAZ
2	B	1101	2NG	CAV-CBE-NAX-CAZ
2	E	1101	2NG	CAV-CBE-NAX-CAZ
2	A	1101	2NG	CAS-CBF-NAY-CBA
2	E	1102	2NG	CAV-CBE-NAX-CAZ
2	D	1101	2NG	CBB-CBE-NAX-CAZ
2	C	1101	2NG	CBB-CBE-NAX-CAZ
2	B	1101	2NG	CBB-CBE-NAX-CAZ
2	E	1101	2NG	CBB-CBE-NAX-CAZ
2	E	1101	2NG	CAS-CBF-NAY-CBA
2	E	1102	2NG	CBB-CBE-NAX-CAZ

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1101	2NG	2	0
2	F	1101	2NG	3	0

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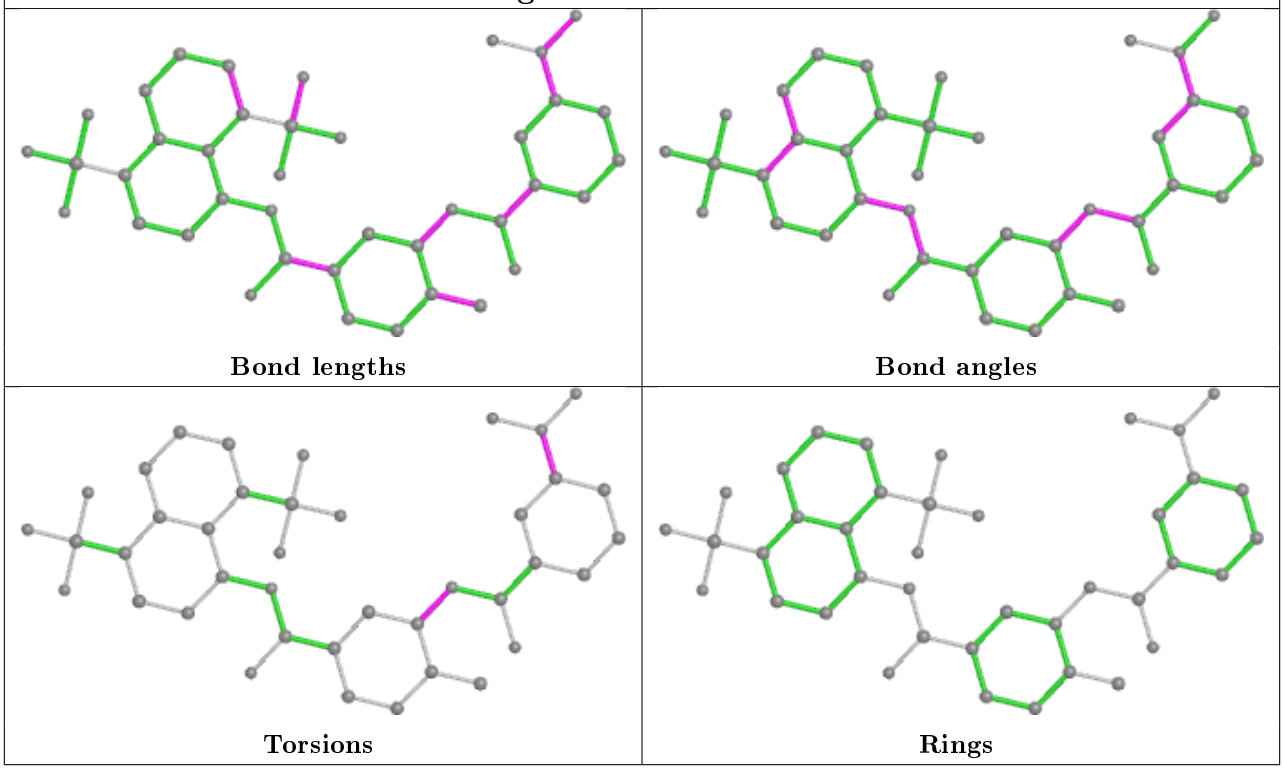
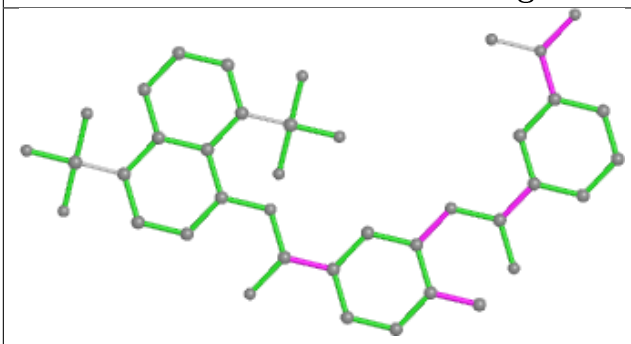
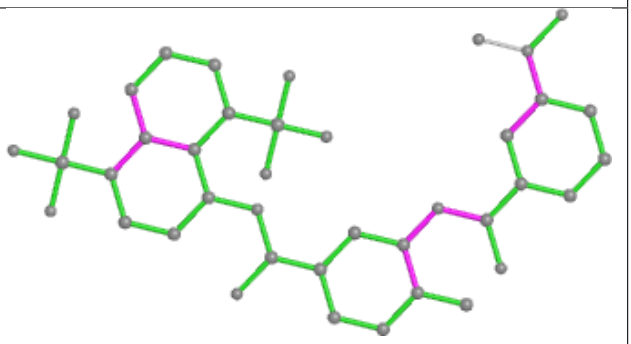
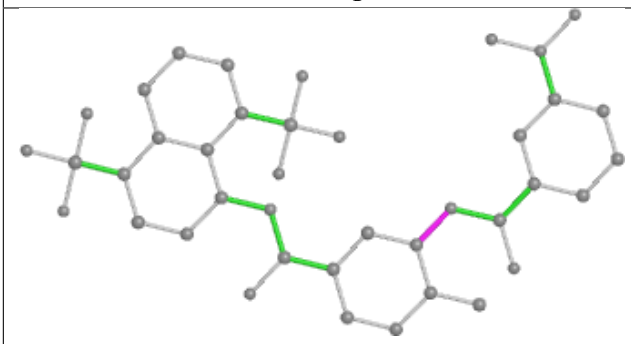
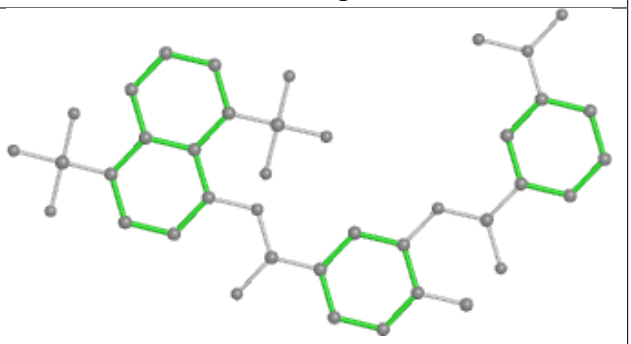
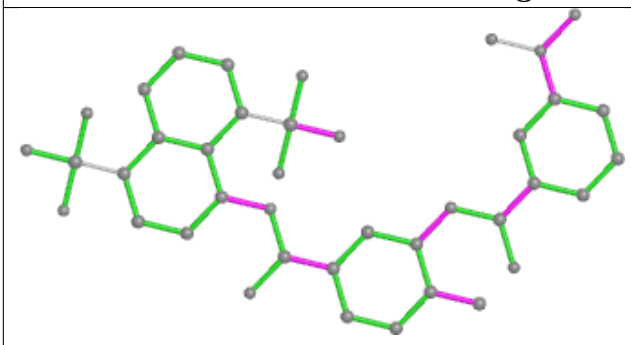
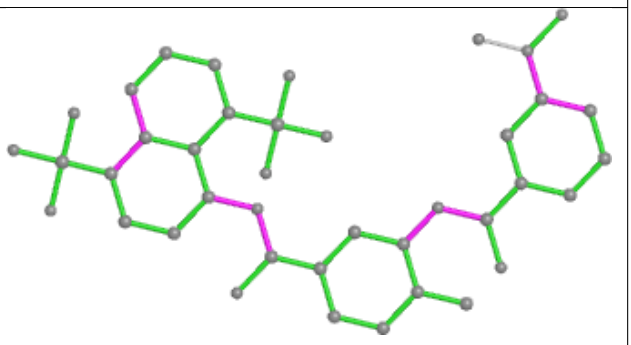
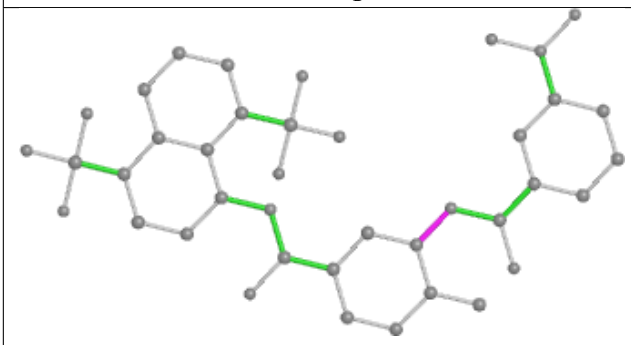
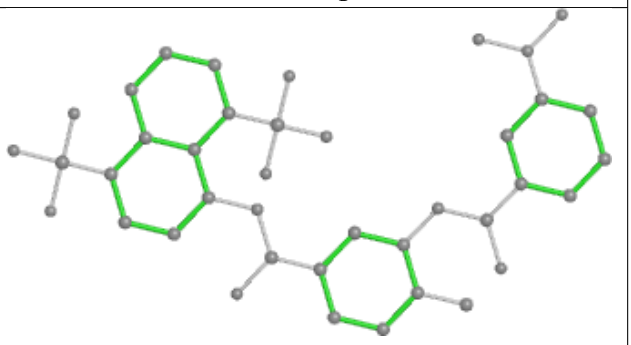
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	2NG	1	0
2	A	1101	2NG	5	0
2	E	1102	2NG	2	0
2	E	1101	2NG	3	0
2	C	1101	2NG	2	0

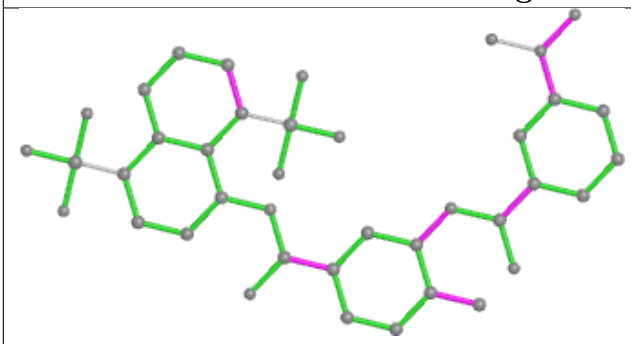
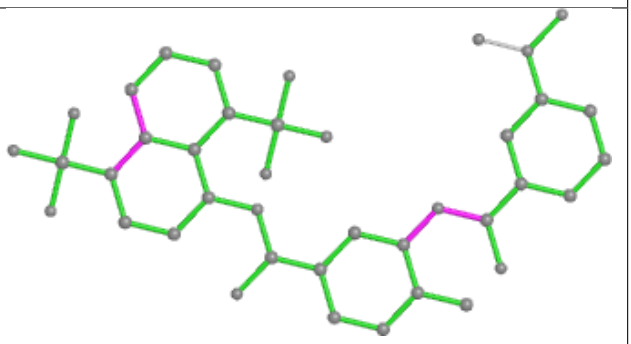
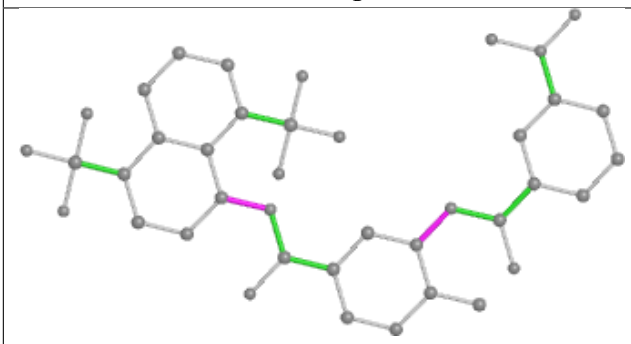
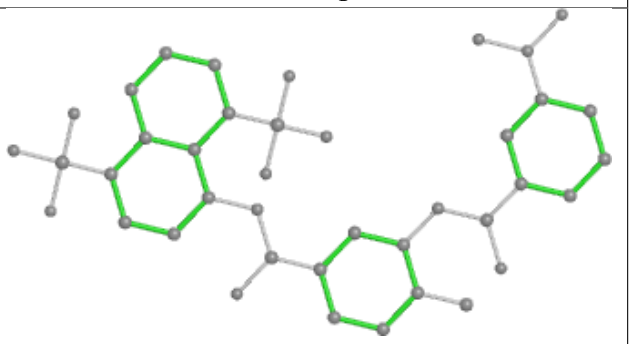
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

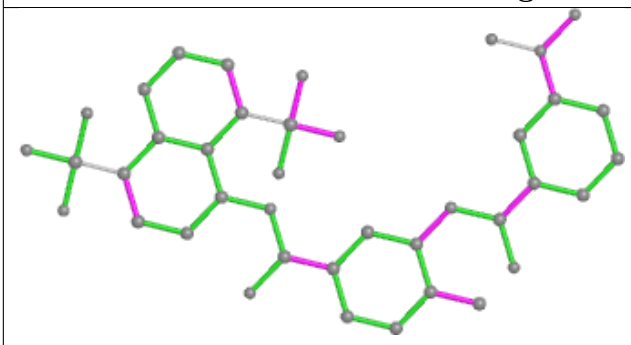
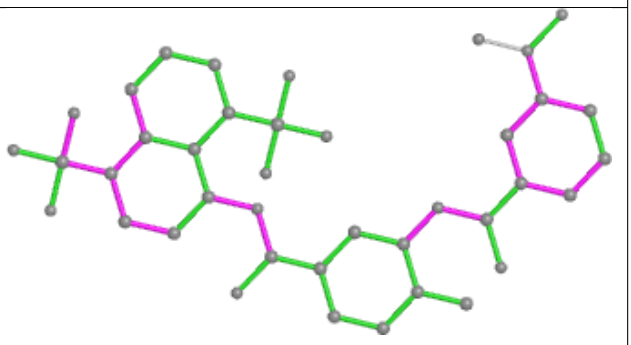
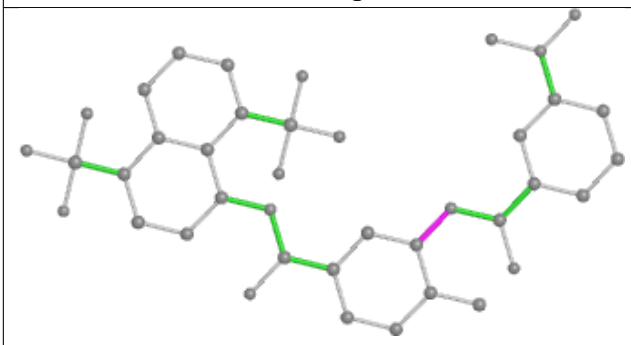
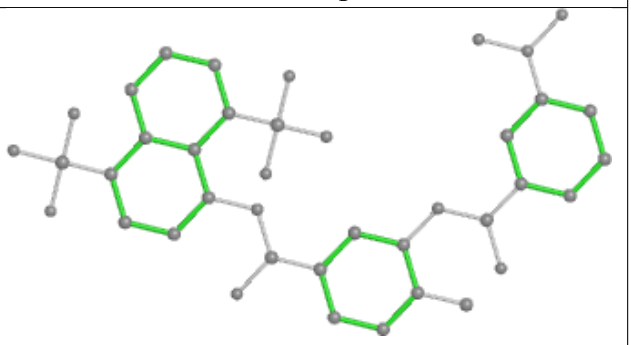
Ligand 2NG B 1101



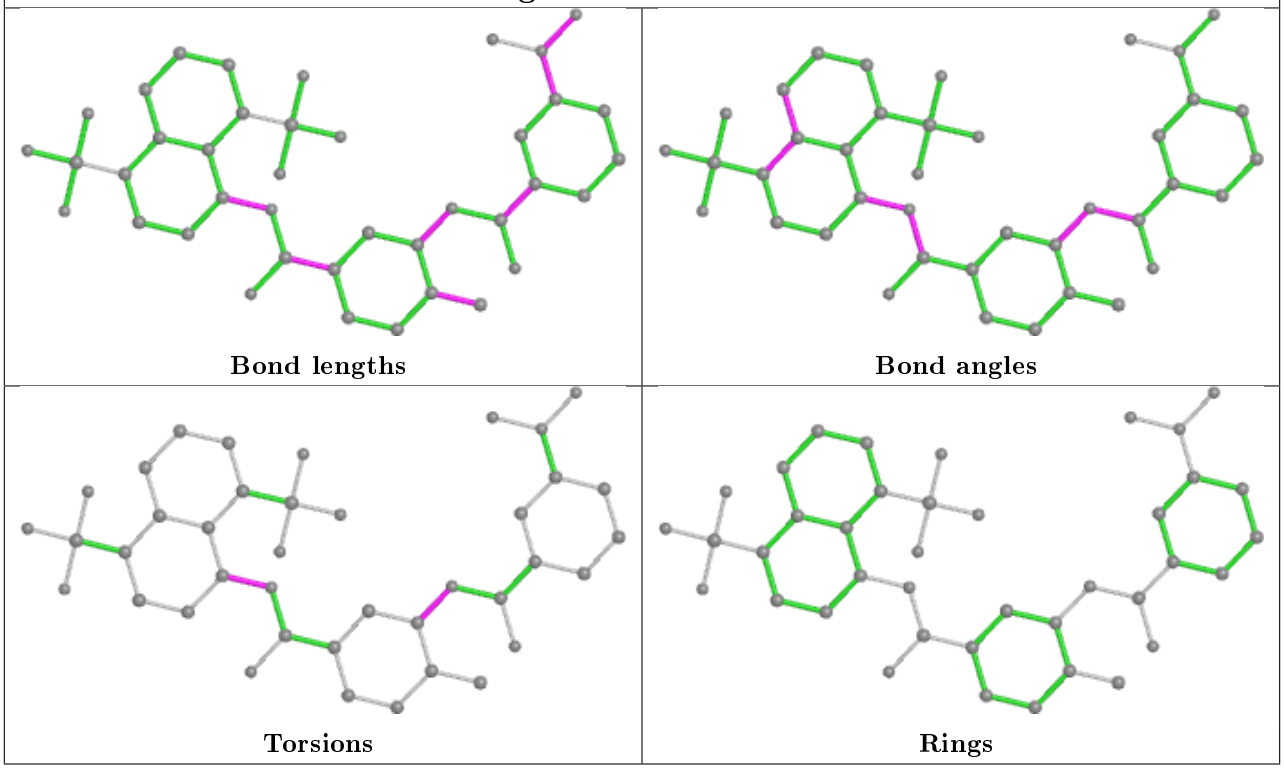
Ligand 2NG F 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 2NG D 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

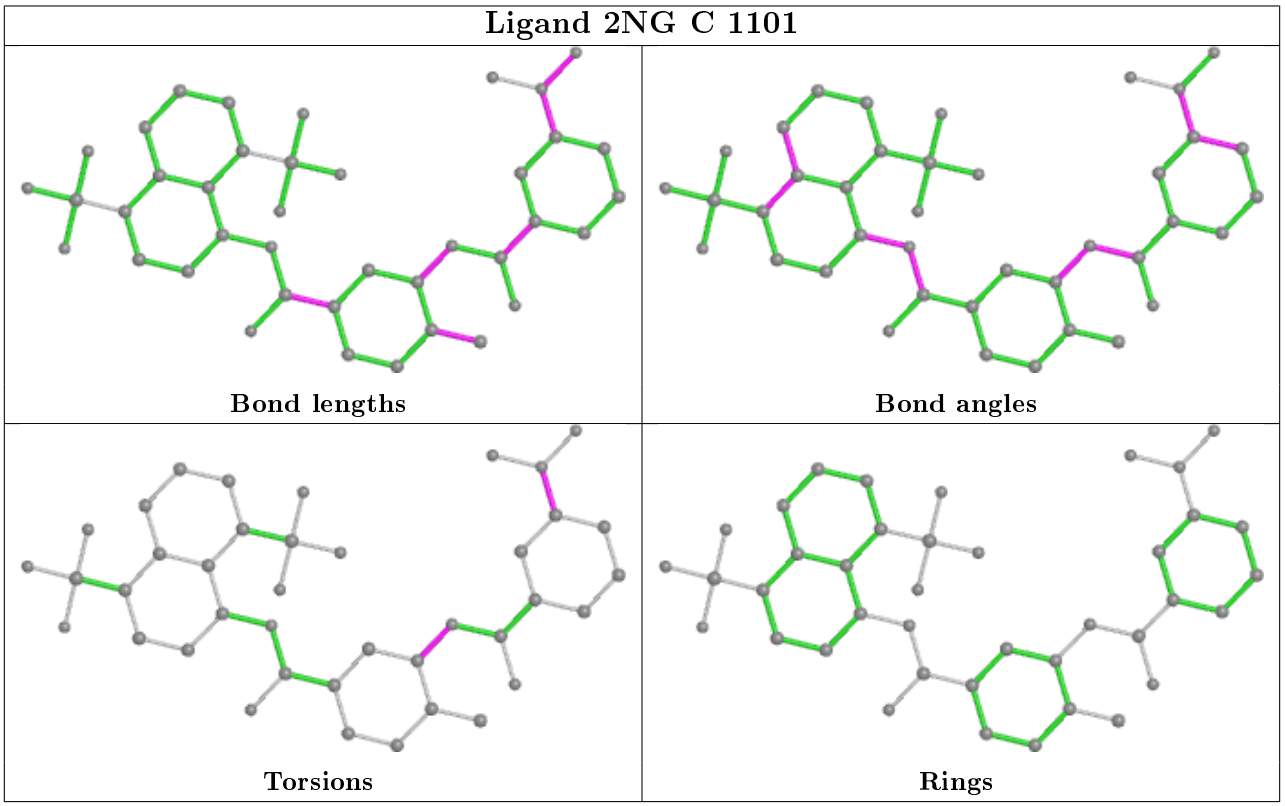
Ligand 2NG A 1101	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 2NG E 1102	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 2NG E 1101



Ligand 2NG C 1101



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	477/515 (92%)	0.26	15 (3%) 49 56	20, 33, 74, 113	6 (1%)
1	B	482/515 (93%)	-0.03	4 (0%) 86 89	21, 36, 66, 101	8 (1%)
1	C	478/515 (92%)	0.04	10 (2%) 63 70	23, 37, 75, 106	9 (1%)
1	D	479/515 (93%)	0.00	9 (1%) 66 73	25, 39, 71, 101	7 (1%)
1	E	477/515 (92%)	0.24	15 (3%) 49 56	27, 44, 88, 111	5 (1%)
1	F	473/515 (91%)	0.54	30 (6%) 20 25	33, 54, 94, 116	7 (1%)
All	All	2866/3090 (92%)	0.18	83 (2%) 51 58	20, 40, 80, 116	42 (1%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	462	VAL	6.3
1	F	456	ARG	5.1
1	F	474	VAL	5.1
1	F	475	VAL	5.0
1	F	463	SER	5.0
1	F	459	ALA	4.4
1	A	463	SER	4.2
1	A	474	VAL	4.1
1	F	455	TYR	3.9
1	C	435	GLN	3.9
1	A	3	PRO	3.9
1	F	46	TYR	3.7
1	F	34	PRO	3.5
1	D	469	SER	3.4
1	E	439	GLN	3.4
1	F	441	MET	3.4
1	F	54	VAL	3.3
1	E	441	MET	3.2
1	F	457	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	431	PRO	3.2
1	C	433	HIS	3.1
1	C	441	MET	3.0
1	A	433	HIS	3.0
1	E	462	VAL	3.0
1	B	469	SER	2.9
1	F	439	GLN	2.9
1	F	294	VAL	2.9
1	F	458	VAL	2.9
1	F	484	TRP	2.8
1	C	477	ARG	2.8
1	D	326	ARG	2.7
1	A	475	VAL	2.7
1	E	475	VAL	2.7
1	B	475	VAL	2.7
1	D	484	TRP	2.7
1	E	432	GLY	2.6
1	E	444	LEU	2.6
1	C	382	ARG	2.6
1	F	417	TRP	2.6
1	F	37	LEU	2.6
1	D	468	GLN	2.6
1	E	437	PRO	2.6
1	F	464	LYS	2.6
1	A	432	GLY	2.5
1	C	376	GLU	2.5
1	A	459	ALA	2.5
1	E	290	TYR	2.5
1	D	475	VAL	2.5
1	A	462	VAL	2.4
1	E	484	TRP	2.4
1	F	465	GLU	2.4
1	E	456	ARG	2.4
1	E	271	LEU	2.3
1	C	484	TRP	2.3
1	F	460	SER	2.3
1	F	76	LEU	2.3
1	D	379	LEU	2.2
1	A	456	ARG	2.2
1	F	295	GLU	2.2
1	D	435	GLN	2.2
1	A	231[A]	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	477	ARG	2.2
1	F	323	GLU	2.2
1	C	192	MET	2.2
1	C	456	ARG	2.2
1	A	441	MET	2.2
1	F	41	ALA	2.2
1	F	13	PRO	2.2
1	F	290	TYR	2.1
1	F	430	LEU	2.1
1	D	474	VAL	2.1
1	E	433	HIS	2.1
1	A	399	GLN	2.1
1	F	326	ARG	2.1
1	B	399	GLN	2.1
1	A	360	MET	2.1
1	C	479	ARG	2.1
1	A	430	LEU	2.0
1	B	435	GLN	2.0
1	A	484	TRP	2.0
1	E	463	SER	2.0
1	E	4	ARG	2.0
1	F	315	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 carbohydrates 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, 95^{th} 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
3	MG	E	1103	1/1	0.68	0.11	48,48,48,48	0

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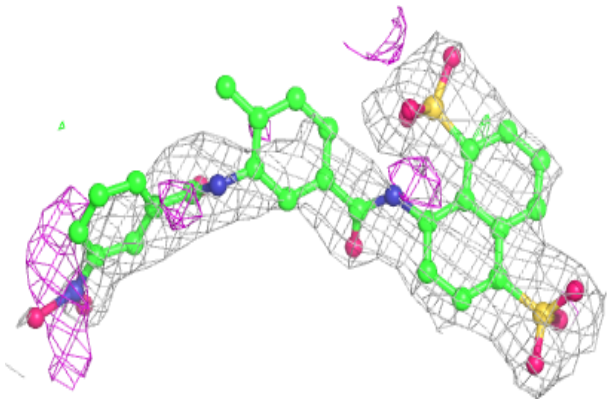
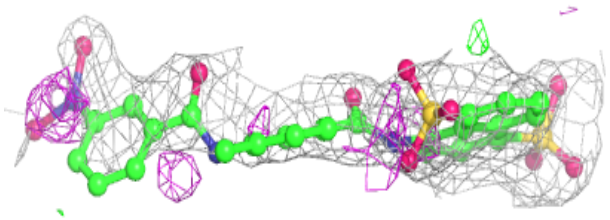
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	F	1102	1/1	0.83	0.08	56,56,56,56	0
2	2NG	F	1101	40/40	0.90	0.28	62,84,112,117	0
2	2NG	A	1101	40/40	0.92	0.22	48,76,111,114	0
2	2NG	E	1102	40/40	0.92	0.17	29,48,70,90	0
2	2NG	E	1101	40/40	0.94	0.23	59,88,103,111	0
3	MG	D	1102	1/1	0.95	0.11	50,50,50,50	0
2	2NG	C	1101	40/40	0.95	0.18	40,71,96,117	0
3	MG	C	1102	1/1	0.95	0.07	37,37,37,37	0
2	2NG	D	1101	40/40	0.96	0.15	39,61,93,100	0
3	MG	A	1102	1/1	0.96	0.15	34,34,34,34	0
2	2NG	B	1101	40/40	0.97	0.15	30,55,80,91	0
3	MG	B	1102	1/1	0.98	0.10	31,31,31,31	0

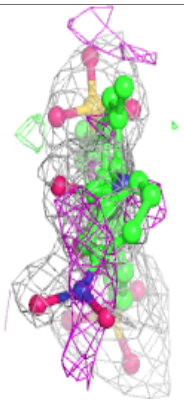
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2NG F 1101:

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

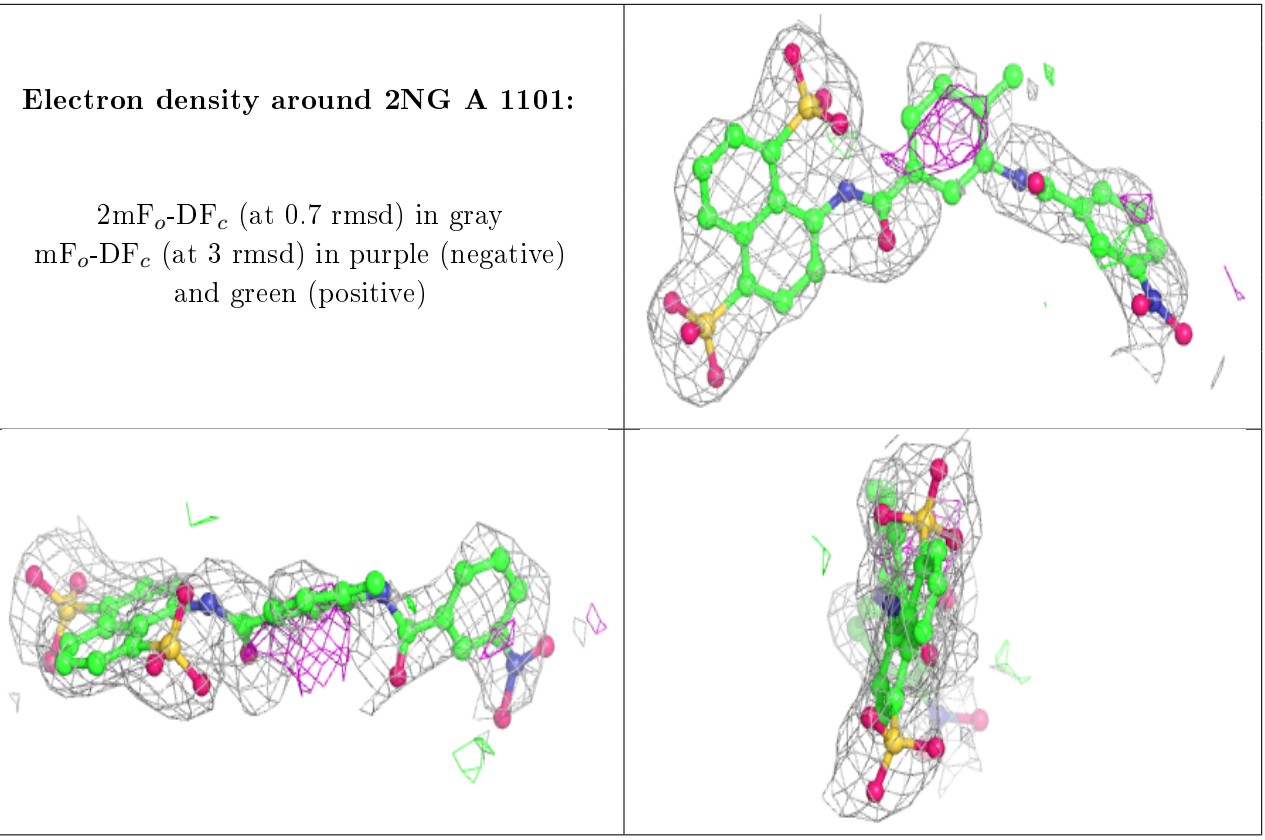






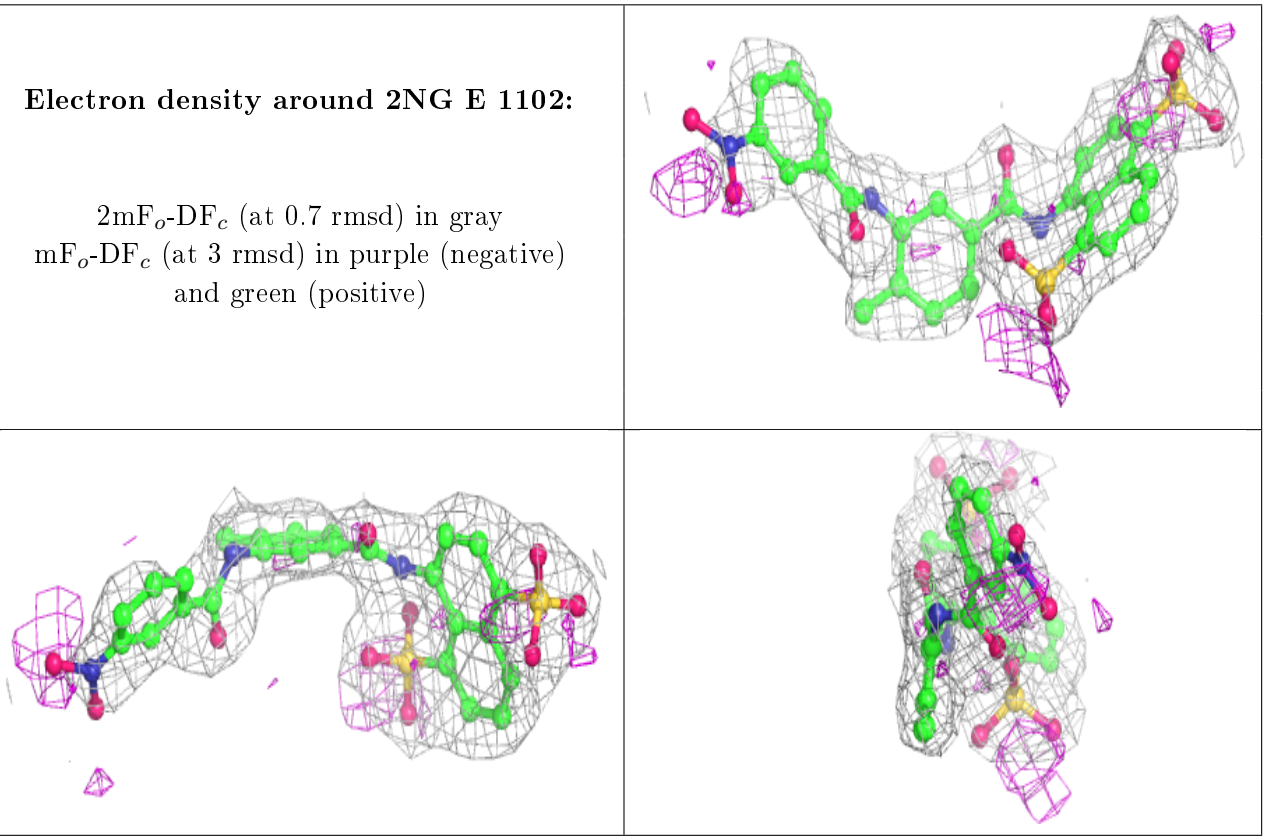
Electron density around 2NG A 1101:

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



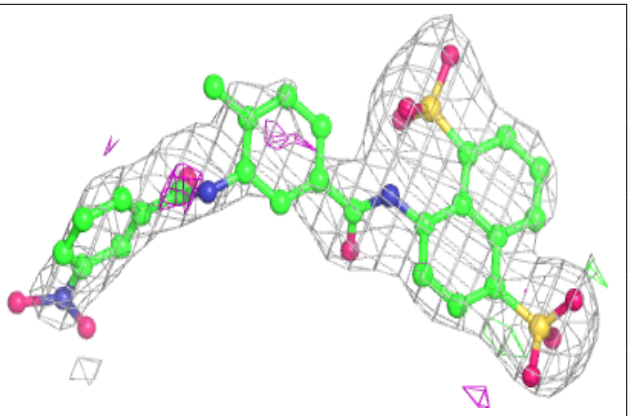
Electron density around 2NG E 1102:

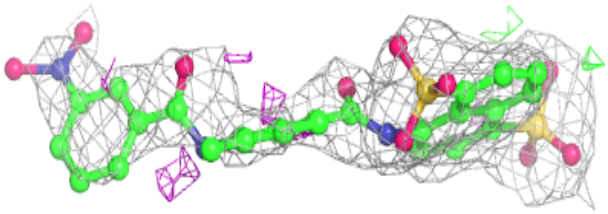
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

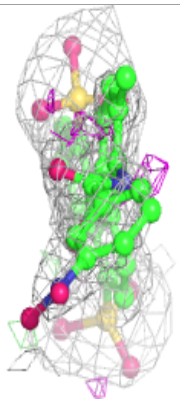


Electron density around 2NG E 1101:

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

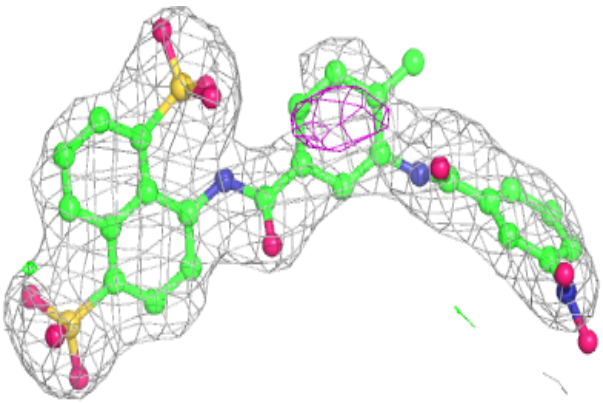


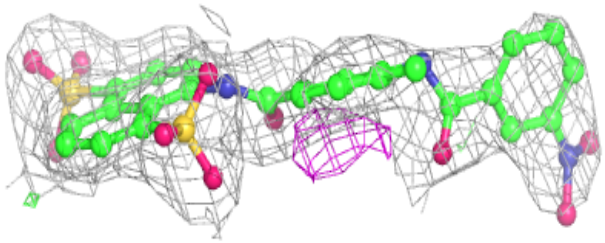


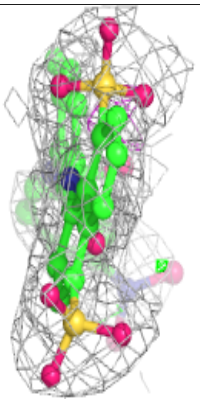


Electron density around 2NG C 1101:

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

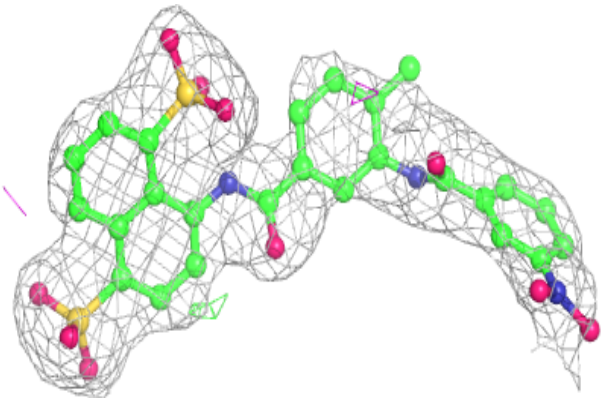


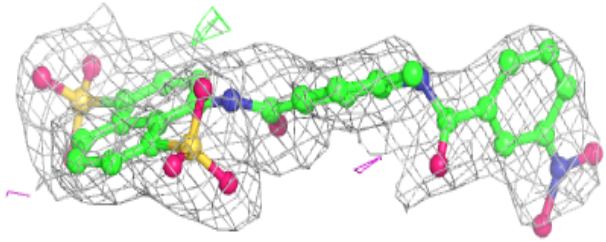


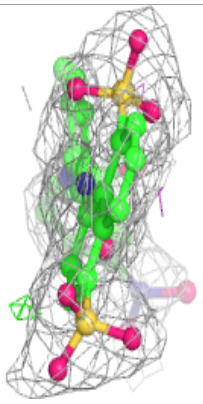


Electron density around 2NG D 1101:

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

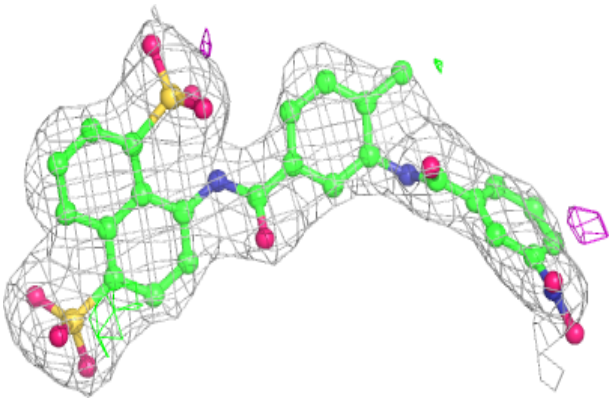


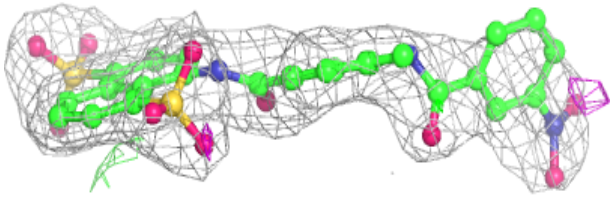


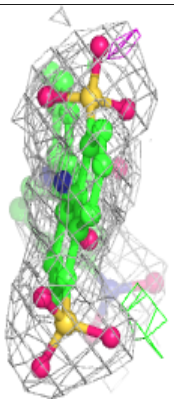


Electron density around 2NG B 1101:

$2mF_o$-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.