Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 07:05 PM BST

PDB ID	:	4O4R
Title	:	Murine Norovirus RdRp in complex with PPNDS
Authors	:	Croci, R.; Tarantino, D.; Milani, M.; Pezzullo, M.; Bolognesi, M.; Mastrangelo, E.
Deposited on	:	2013-12-19
Resolution	:	2.40 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:

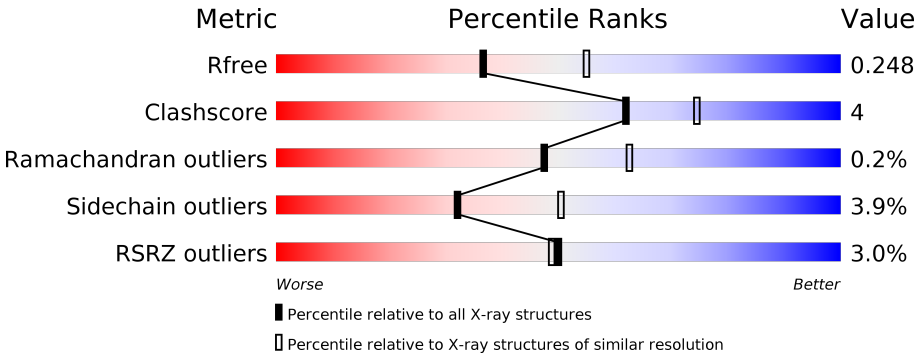
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	83% 9% • 8%
1	B	515	3% 82% 10% • 7%
1	C	515	4% 79% 13% • 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12407 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	476	Total	C	N	O	S	0	0	0
			3784	2394	668	698	24			
1	B	480	Total	C	N	O	S	0	2	0
			3822	2419	673	706	24			
1	C	474	Total	C	N	O	S	0	1	0
			3765	2383	663	695	24			

There are 24 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
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

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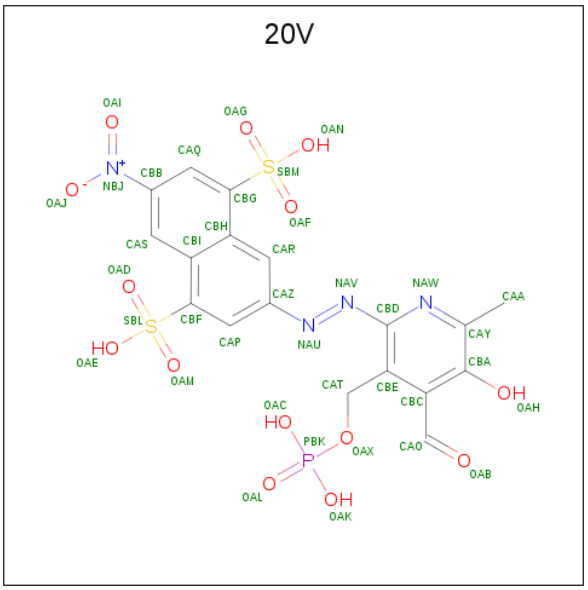
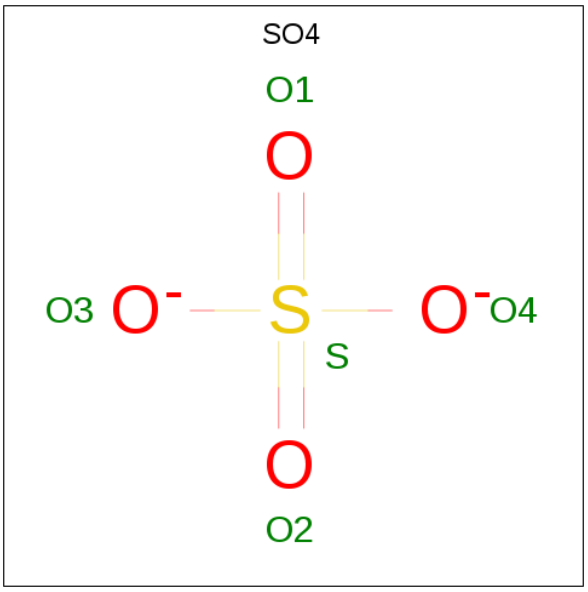
Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	EXPRESSION TAG	UNP S4V9Y7

- Molecule 2 is 3-[(E)-{4-formyl-5-hydroxy-6-methyl-3-[(phosphonooxy)methyl]pyridin-2-yl}diazenyl]-7-nitronaphthalene-1,5-disulfonic acid (three-letter code: 20V) (formula: $C_{18}H_{15}N_4O_{14}PS_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		
2	A	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		
2	B	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		
2	B	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		
2	C	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		
2	C	1	Total	C	N	O	P	S	0	0
			39	18	4	14	1	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	272	Total O 275 275	0	6
4	B	259	Total O 260 260	0	1

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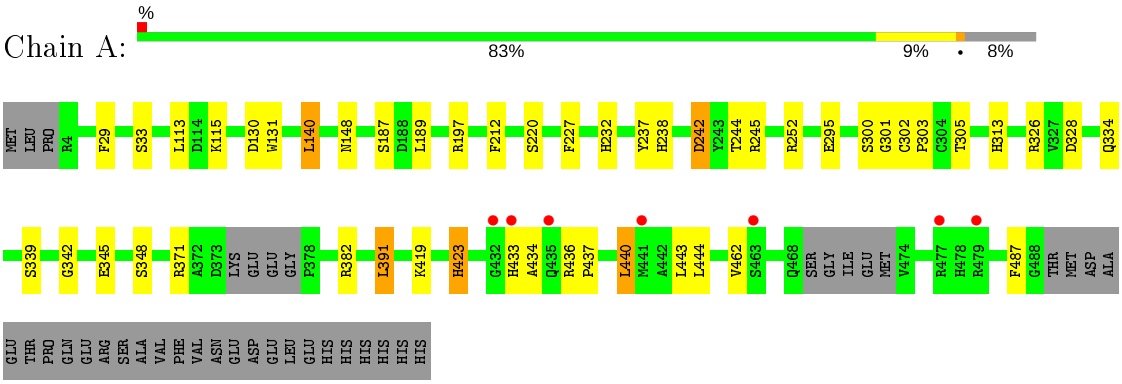
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	217	Total	O	0	1
			217	217		

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.

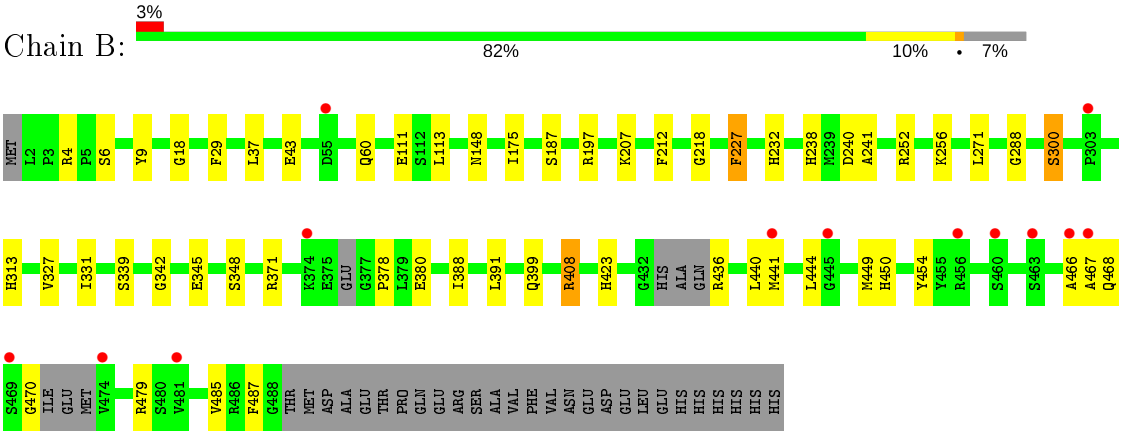
- Molecule 1: RNA-dependent-RNA-polymerase

Chain A:



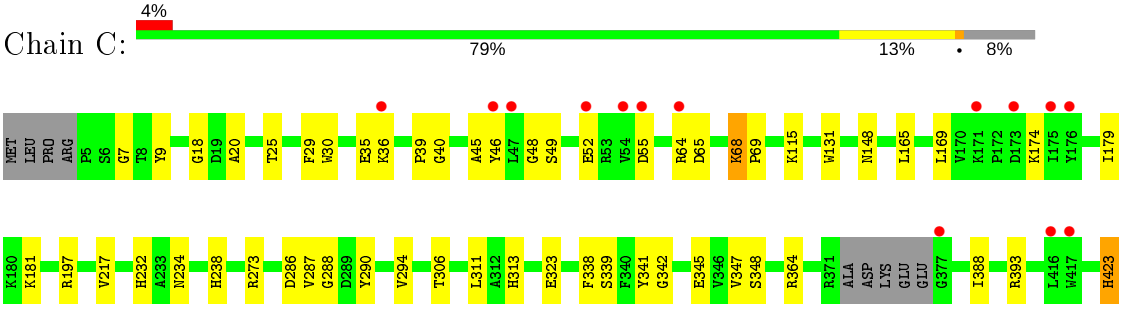
- Molecule 1: RNA-dependent-RNA-polymerase

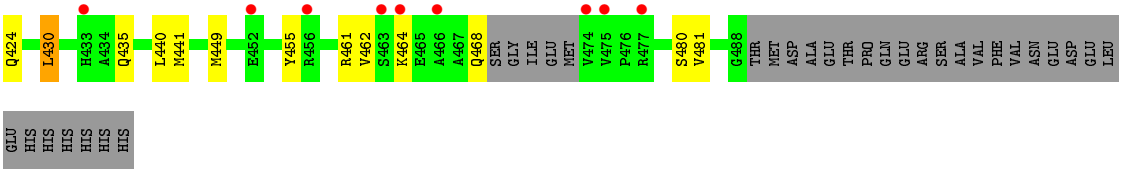
Chain B:



- Molecule 1: RNA-dependent-RNA-polymerase

Chain C:




Q424
L430
H433
A434
Q435
L440
M441
M449
E452
Y455
R456
R461
V462
S463
K464
E465
A466
A467
Q468
SER
GLY
ILE
GLU
MET
V474
V475
P476
R477
S480
V481
G488
THR
MET
ASP
ALA
GLU
THR
PRO
GLN
GLU
ARG
SER
ALA
VAL
PHE
VAL
ASN
GLU
ASP
GLU
LEU
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	119.71Å 197.43Å 109.57Å 90.00° 114.06° 90.00°	Depositor
Resolution (Å)	59.36 – 2.40 59.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	100.0 (59.36-2.40) 100.0 (59.36-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.192 , 0.249 0.195 , 0.248	Depositor DCC
R_{free} test set	4532 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	39.2	Xtriage
Anisotropy	0.265	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 61.4	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	12407	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 3.81% 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: SO4, 20V

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	0.49	0/3877	0.70	2/5252 (0.0%)
1	B	0.49	0/3917	0.68	0/5303
1	C	0.48	0/3863	0.69	0/5233
All	All	0.49	0/11657	0.69	2/15788 (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	A	382	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	326	ARG	NE-CZ-NH1	5.06	122.83	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	3784	0	3743	32	0
1	B	3822	0	3789	29	0
1	C	3765	0	3725	40	1
2	A	78	0	28	3	0
2	B	78	0	28	0	0
2	C	78	0	28	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	0	0	0
3	B	20	0	0	1	0
4	A	275	0	0	1	0
4	B	260	0	0	1	0
4	C	217	0	0	2	0
All	All	12407	0	11341	100	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (100) 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)
2:A:601:20V:NBJ	2:A:601:20V:OAJ	1.59	1.31
1:B:467:ALA:HB3	1:B:468:GLN:NE2	1.82	0.95
1:A:433:HIS:HA	1:A:434:ALA:HB3	1.58	0.85
1:C:238:HIS:HD2	1:C:348:SER:OG	1.62	0.82
1:A:29:PHE:O	1:A:423:HIS:HE1	1.61	0.81
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.30	0.80
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.35	0.74
2:C:601:20V:OAX	2:C:601:20V:CAO	2.35	0.73
1:B:467:ALA:HB3	1:B:468:GLN:HE21	1.54	0.72
1:B:9:TYR:OH	1:B:60:GLN:NE2	2.23	0.72
1:A:313:HIS:HD2	1:A:342:GLY:O	1.72	0.71
1:C:68:LYS:HD2	1:C:69:PRO:HD3	1.77	0.67
1:A:187:SER:HB2	1:A:301:GLY:O	1.97	0.65
1:B:29:PHE:O	1:B:423:HIS:HE1	1.80	0.63
1:A:433:HIS:HA	1:A:434:ALA:CB	2.28	0.62
1:A:148:ASN:HD21	1:A:197:ARG:HH11	1.49	0.60
1:C:7:GLY:HA3	4:C:843:HOH:O	2.01	0.60
1:B:238:HIS:HD2	1:B:348:SER:OG	1.84	0.59
1:B:466:ALA:O	1:B:470:GLY:N	2.35	0.59
1:B:227:PHE:HB2	4:B:717:HOH:O	2.02	0.58
1:A:302:CYS:CB	1:A:305:THR:HB	2.33	0.58
1:A:302:CYS:HB2	1:A:305:THR:HB	1.86	0.58
1:A:238:HIS:HD2	1:A:348:SER:OG	1.85	0.57
1:C:9:TYR:CE1	1:C:64:ARG:HD3	2.39	0.57
1:B:313:HIS:HD2	1:B:342:GLY:O	1.88	0.56
1:A:433:HIS:CA	1:A:434:ALA:HB3	2.31	0.55
1:A:334:GLN:HG2	1:B:399[B]:GLN:HG3	1.89	0.55
1:C:313:HIS:HD2	1:C:342:GLY:O	1.90	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:HIS:HE1	1:C:345:GLU:OE2	1.90	0.54
1:A:313:HIS:HE1	1:A:345:GLU:OE2	1.90	0.54
1:B:467:ALA:HB3	1:B:468:GLN:HE22	1.70	0.54
1:C:148:ASN:ND2	1:C:197:ARG:HH11	2.01	0.53
1:C:30:TRP:CD2	1:C:430:LEU:HD13	2.45	0.52
1:C:9:TYR:OH	1:C:64:ARG:HG3	2.10	0.52
1:B:240:ASP:OD1	1:B:241:ALA:O	2.28	0.52
1:A:302:CYS:HB3	1:A:305:THR:H	1.75	0.51
1:C:148:ASN:HD21	1:C:197:ARG:NH1	2.03	0.51
1:A:130:ASP:HB2	1:A:140:LEU:HD22	1.92	0.50
1:B:207:LYS:HG3	1:B:218:GLY:HA3	1.93	0.50
1:B:327:VAL:HG12	1:B:331:ILE:HB	1.94	0.50
1:A:487:PHE:HB3	1:B:212:PHE:CZ	2.47	0.50
1:A:140:LEU:HG	1:A:189:LEU:HD22	1.94	0.49
1:C:165:LEU:HB3	1:C:181:LYS:HG2	1.94	0.49
1:C:68:LYS:HD2	1:C:69:PRO:CD	2.42	0.49
1:B:232:HIS:HD2	1:B:348:SER:OG	1.95	0.49
1:C:232:HIS:HE1	1:C:339:SER:OG	1.96	0.49
1:C:217:VAL:HG21	1:C:306:THR:HG22	1.95	0.49
1:B:468:GLN:N	1:B:468:GLN:NE2	2.60	0.48
1:C:65:ASP:O	1:C:68:LYS:HG3	2.13	0.48
1:A:29:PHE:O	1:A:423:HIS:CE1	2.54	0.48
1:A:232:HIS:HE1	1:A:339:SER:OG	1.97	0.48
1:C:174:LYS:O	1:C:179:ILE:HA	2.13	0.48
1:B:313:HIS:HE1	1:B:345:GLU:OE2	1.97	0.48
1:C:323:GLU:OE2	1:C:364:ARG:NH2	2.44	0.47
1:A:227:PHE:HB2	4:A:846:HOH:O	2.14	0.47
1:C:18:GLY:HA3	1:C:288:GLY:O	2.15	0.47
1:B:449:MET:HE3	1:B:485:VAL:HG13	1.96	0.47
1:A:242:ASP:HB2	1:A:371:ARG:HG3	1.97	0.46
1:B:252:ARG:O	1:B:256[A]:LYS:HD3	2.16	0.46
1:C:29:PHE:O	1:C:423:HIS:HE1	1.99	0.46
1:C:46:TYR:CE2	1:C:48:GLY:HA2	2.50	0.46
1:C:393:ARG:HD3	2:C:601:20V:OAG	2.15	0.46
1:B:371:ARG:NH1	1:B:378:PRO:O	2.42	0.45
1:A:302:CYS:HB3	1:A:305:THR:HB	1.97	0.45
1:A:419:LYS:HD2	2:A:602:20V:OAE	2.16	0.45
1:B:232:HIS:HE1	1:B:339:SER:OG	2.00	0.45
1:C:338:PHE:CE1	1:C:347:VAL:HG13	2.51	0.45
1:A:115:LYS:HE2	1:A:131:TRP:CD2	2.52	0.44
1:C:449:MET:HE1	4:C:717:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:THR:HG22	1:C:424:GLN:HE22	1.82	0.44
1:A:212:PHE:CZ	1:B:487:PHE:HB3	2.52	0.44
1:C:148:ASN:ND2	1:C:197:ARG:HD2	2.33	0.44
1:C:20:ALA:HB2	1:C:286:ASP:OD1	2.17	0.43
1:B:43:GLU:HB2	1:B:175:ILE:CD1	2.48	0.43
1:B:18:GLY:HA3	1:B:288:GLY:O	2.19	0.43
1:C:287:VAL:HG22	1:C:290:TYR:O	2.18	0.43
1:B:408:ARG:N	3:B:606:SO4:O2	2.45	0.43
1:A:252:ARG:HG3	1:A:295:GLU:O	2.19	0.43
1:C:440:LEU:HG	1:C:462:VAL:HG13	2.01	0.42
1:B:408:ARG:HG3	1:B:454:TYR:CZ	2.54	0.42
1:C:39:PRO:HA	1:C:40:GLY:HA2	1.80	0.42
1:C:20:ALA:CB	1:C:286:ASP:OD1	2.67	0.42
1:C:455:TYR:CE1	1:C:481:VAL:HG11	2.55	0.42
1:A:303:PRO:C	1:A:305:THR:H	2.23	0.42
1:B:408:ARG:HD3	1:B:450:HIS:CE1	2.55	0.42
1:C:68:LYS:N	1:C:69:PRO:CD	2.82	0.42
1:C:148:ASN:HD21	1:C:197:ARG:HD2	1.85	0.42
1:A:237:TYR:O	1:A:348:SER:HA	2.20	0.41
1:B:313:HIS:CD2	1:B:342:GLY:O	2.70	0.41
1:C:273:ARG:O	1:C:273:ARG:HD3	2.20	0.41
1:A:440:LEU:HG	1:A:462:VAL:HG13	2.02	0.41
1:C:30:TRP:CD2	1:C:430:LEU:CD1	3.04	0.41
1:A:244:THR:HG22	1:A:245:ARG:HG3	2.03	0.41
1:A:433:HIS:CA	1:A:434:ALA:CB	2.97	0.41
1:A:391:LEU:HD23	2:A:601:20V:CAQ	2.52	0.40
1:A:436:ARG:N	1:A:437:PRO:HD3	2.36	0.40
1:C:338:PHE:HE1	1:C:347:VAL:HG13	1.87	0.40
1:C:9:TYR:OH	1:C:64:ARG:NH1	2.50	0.40
1:C:115:LYS:HE2	1:C:131:TRP:CE2	2.56	0.40
1:C:238:HIS:CD2	1:C:348:SER:OG	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ASN:OD1	1:C:234:ASN:OD1[2_656]	1.87	0.33

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	470/515 (91%)	453 (96%)	17 (4%)	0	100	100
1	B	474/515 (92%)	460 (97%)	13 (3%)	1 (0%)	47	62
1	C	469/515 (91%)	439 (94%)	28 (6%)	2 (0%)	34	48
All	All	1413/1545 (92%)	1352 (96%)	58 (4%)	3 (0%)	47	62

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	45	ALA
1	C	35	GLU
1	B	300	SER

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	406/441 (92%)	394 (97%)	12 (3%)	41	61
1	B	411/441 (93%)	393 (96%)	18 (4%)	28	45
1	C	405/441 (92%)	387 (96%)	18 (4%)	28	45
All	All	1222/1323 (92%)	1174 (96%)	48 (4%)	32	50

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	SER
1	A	113	LEU
1	A	140	LEU
1	A	220	SER
1	A	242	ASP
1	A	300	SER
1	A	328	ASP
1	A	391	LEU
1	A	423	HIS
1	A	440	LEU
1	A	443	LEU
1	A	444	LEU
1	B	4	ARG
1	B	6	SER
1	B	37	LEU
1	B	111	GLU
1	B	113	LEU
1	B	187	SER
1	B	227	PHE
1	B	271	LEU
1	B	300	SER
1	B	380	GLU
1	B	388	ILE
1	B	391	LEU
1	B	408	ARG
1	B	436	ARG
1	B	440	LEU
1	B	441	MET
1	B	444	LEU
1	B	479	ARG
1	C	36	LYS
1	C	49	SER
1	C	52	GLU
1	C	55	ASP
1	C	68	LYS
1	C	169	LEU
1	C	294	VAL
1	C	311	LEU
1	C	341	TYR
1	C	388	ILE
1	C	423	HIS
1	C	430	LEU
1	C	435	GLN

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Mol	Chain	Res	Type
1	C	441	MET
1	C	461	ARG
1	C	464	LYS
1	C	468	GLN
1	C	480	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	124	HIS
1	A	146	HIS
1	A	148	ASN
1	A	232	HIS
1	A	238	HIS
1	A	250	GLN
1	A	313	HIS
1	A	423	HIS
1	B	60	GLN
1	B	66	GLN
1	B	148	ASN
1	B	232	HIS
1	B	238	HIS
1	B	313	HIS
1	B	334	GLN
1	B	423	HIS
1	B	468	GLN
1	C	66	GLN
1	C	148	ASN
1	C	232	HIS
1	C	238	HIS
1	C	250	GLN
1	C	313	HIS
1	C	334	GLN
1	C	423	HIS
1	C	468	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	SO4	A	607	-	4,4,4	0.39	0	6,6,6	0.30	0
3	SO4	A	603	-	4,4,4	0.40	0	6,6,6	0.35	0
3	SO4	A	608	-	4,4,4	0.58	0	6,6,6	0.56	0
3	SO4	B	604	-	4,4,4	0.40	0	6,6,6	0.39	0
2	20V	A	602	-	37,41,41	2.92	11 (29%)	49,64,64	1.48	8 (16%)
2	20V	C	602	-	37,41,41	2.40	12 (32%)	49,64,64	1.36	4 (8%)
3	SO4	A	605	-	4,4,4	0.33	0	6,6,6	0.11	0
2	20V	B	601	-	37,41,41	3.00	13 (35%)	49,64,64	1.47	6 (12%)
2	20V	C	601	-	37,41,41	3.11	11 (29%)	49,64,64	1.39	7 (14%)
3	SO4	A	606	-	4,4,4	0.39	0	6,6,6	0.25	0
2	20V	A	601	-	37,41,41	3.10	9 (24%)	49,64,64	1.50	7 (14%)
3	SO4	B	606	-	4,4,4	0.37	0	6,6,6	0.17	0
3	SO4	A	604	-	4,4,4	0.33	0	6,6,6	0.15	0
3	SO4	B	605	-	4,4,4	0.43	0	6,6,6	0.38	0
2	20V	B	602	-	37,41,41	2.74	12 (32%)	49,64,64	1.46	7 (14%)
3	SO4	B	603	-	4,4,4	0.37	0	6,6,6	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	20V	A	602	-	-	13/27/29/29	0/3/3/3
2	20V	C	602	-	-	12/27/29/29	0/3/3/3
2	20V	B	601	-	-	4/27/29/29	0/3/3/3
2	20V	C	601	-	-	7/27/29/29	0/3/3/3
2	20V	A	601	-	-	6/27/29/29	0/3/3/3
2	20V	B	602	-	-	10/27/29/29	0/3/3/3

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	20V	OAI-NBJ	12.68	1.44	1.22
2	C	601	20V	OAI-NBJ	12.08	1.43	1.22
2	B	601	20V	OAI-NBJ	12.03	1.43	1.22
2	A	602	20V	OAI-NBJ	11.35	1.42	1.22
2	B	602	20V	OAI-NBJ	9.26	1.38	1.22
2	C	601	20V	CAA-CAY	-6.58	1.39	1.50
2	C	601	20V	CAT-CBE	-6.46	1.39	1.51
2	A	601	20V	CAA-CAY	-6.30	1.39	1.50
2	C	602	20V	CAA-CAY	-6.24	1.39	1.50
2	B	602	20V	CAA-CAY	-6.16	1.39	1.50
2	B	601	20V	CAA-CAY	-6.02	1.40	1.50
2	A	602	20V	CAT-CBE	-5.99	1.40	1.51
2	A	601	20V	CAT-CBE	-5.93	1.40	1.51
2	B	602	20V	CAT-CBE	-5.64	1.40	1.51
2	A	602	20V	CAA-CAY	-5.62	1.40	1.50
2	C	602	20V	CAT-CBE	-5.59	1.41	1.51
2	A	601	20V	CBD-NAV	-5.45	1.33	1.41
2	B	602	20V	CBB-NBJ	-5.35	1.32	1.45
2	B	601	20V	CAT-CBE	-5.31	1.41	1.51
2	C	602	20V	CBB-NBJ	-5.06	1.33	1.45
2	A	602	20V	CBD-NAV	-4.92	1.34	1.41
2	B	601	20V	CBD-NAV	-4.81	1.34	1.41
2	C	601	20V	PBK-OAL	4.80	1.66	1.50
2	B	601	20V	CBB-NBJ	-4.63	1.34	1.45
2	B	602	20V	CBD-NAV	-4.62	1.34	1.41
2	C	601	20V	CBD-NAV	-4.55	1.34	1.41
2	A	602	20V	CBB-NBJ	-4.52	1.34	1.45
2	C	602	20V	OAI-NBJ	4.30	1.30	1.22
2	C	602	20V	CBD-NAV	-4.29	1.35	1.41
2	C	601	20V	CBB-NBJ	-4.27	1.34	1.45
2	C	602	20V	PBK-OAL	4.23	1.64	1.50
2	A	602	20V	PBK-OAL	4.08	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	20V	PBK-OAL	4.04	1.63	1.50
2	A	601	20V	CBB-NBJ	-4.00	1.35	1.45
2	A	601	20V	PBK-OAL	3.67	1.62	1.50
2	B	601	20V	PBK-OAL	3.54	1.62	1.50
2	A	601	20V	CBC-CAO	-3.11	1.39	1.46
2	C	601	20V	CAR-CAZ	3.10	1.40	1.37
2	B	601	20V	CAR-CAZ	2.90	1.40	1.37
2	C	602	20V	PBK-OAK	2.87	1.65	1.54
2	C	601	20V	CBC-CAO	-2.83	1.39	1.46
2	A	602	20V	CAZ-NAU	-2.68	1.32	1.44
2	B	601	20V	CBC-CAO	-2.61	1.40	1.46
2	A	602	20V	PBK-OAK	2.49	1.64	1.54
2	A	601	20V	CAZ-NAU	-2.48	1.33	1.44
2	B	601	20V	CAZ-NAU	-2.48	1.33	1.44
2	C	601	20V	PBK-OAK	2.45	1.64	1.54
2	C	602	20V	CAZ-NAU	-2.43	1.33	1.44
2	C	602	20V	CAR-CAZ	2.38	1.39	1.37
2	A	602	20V	CAR-CAZ	2.38	1.39	1.37
2	A	602	20V	CBC-CAO	-2.33	1.41	1.46
2	C	602	20V	OAM-SBL	2.31	1.55	1.43
2	B	601	20V	PBK-OAK	2.27	1.63	1.54
2	B	602	20V	CAR-CAZ	2.24	1.39	1.37
2	B	602	20V	CAZ-NAU	-2.22	1.34	1.44
2	B	602	20V	OAF-SBM	2.17	1.54	1.43
2	C	601	20V	CAZ-NAU	-2.16	1.35	1.44
2	C	601	20V	OAM-SBL	2.12	1.54	1.43
2	B	601	20V	OAM-SBL	2.11	1.54	1.43
2	B	602	20V	PBK-OAK	2.11	1.63	1.54
2	B	601	20V	CBF-CBI	-2.10	1.39	1.43
2	C	602	20V	CBC-CAO	-2.09	1.41	1.46
2	A	601	20V	CAR-CAZ	2.08	1.39	1.37
2	B	601	20V	OAG-SBM	2.08	1.54	1.43
2	B	602	20V	CBC-CAO	-2.07	1.41	1.46
2	A	602	20V	OAF-SBM	2.07	1.54	1.43
2	C	602	20V	OAD-SBL	2.06	1.54	1.43
2	B	602	20V	OAM-SBL	2.03	1.54	1.43

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	602	20V	CBC-CBA-CAY	5.08	123.33	120.19
2	B	601	20V	CAQ-CBB-NBJ	4.78	122.95	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	602	20V	CBC-CBA-CAY	4.60	123.03	120.19
2	A	602	20V	CAS-CBB-NBJ	4.57	122.77	118.75
2	A	602	20V	CBC-CBA-CAY	4.31	122.86	120.19
2	C	601	20V	CBD-NAV-NAU	4.00	123.34	113.94
2	A	601	20V	CAQ-CBB-NBJ	3.99	122.26	118.75
2	B	601	20V	CBD-NAV-NAU	3.90	123.09	113.94
2	A	601	20V	CBD-NAV-NAU	3.79	122.83	113.94
2	A	602	20V	CAA-CAY-CBA	3.27	124.93	120.89
2	B	602	20V	CBA-CBC-CBE	-3.23	116.19	119.50
2	B	601	20V	CBB-CAS-CBI	3.15	121.28	119.02
2	B	602	20V	CAZ-CAP-CBF	3.15	121.77	119.21
2	B	602	20V	OAM-SBL-CBF	3.08	115.64	106.43
2	B	601	20V	CBC-CBA-CAY	3.07	122.09	120.19
2	A	601	20V	CBB-CAS-CBI	3.06	121.22	119.02
2	C	601	20V	CAQ-CBB-NBJ	3.06	121.44	118.75
2	C	602	20V	CBA-CBC-CBE	-3.04	116.38	119.50
2	A	601	20V	OAC-PBK-OAX	2.89	114.43	106.73
2	C	602	20V	CAA-CAY-NAW	2.75	120.74	116.49
2	C	602	20V	CBD-NAV-NAU	2.74	120.36	113.94
2	B	602	20V	CBD-NAV-NAU	2.72	120.33	113.94
2	A	602	20V	CBB-CAS-CBI	2.71	120.97	119.02
2	C	601	20V	CBC-CBA-CAY	2.67	121.84	120.19
2	A	601	20V	CAZ-CAP-CBF	2.61	121.34	119.21
2	B	602	20V	CBB-CAS-CBI	2.56	120.86	119.02
2	C	601	20V	CAA-CAY-NAW	2.56	120.44	116.49
2	B	601	20V	CAA-CAY-NAW	2.49	120.34	116.49
2	A	602	20V	OAC-PBK-OAX	2.45	113.24	106.73
2	A	602	20V	CBD-NAV-NAU	2.44	119.66	113.94
2	A	602	20V	CBA-CAY-NAW	-2.35	118.03	120.81
2	C	601	20V	CBB-CAS-CBI	2.29	120.67	119.02
2	B	601	20V	CBF-CBI-CBH	2.29	120.83	117.94
2	A	602	20V	CBA-CBC-CBE	-2.29	117.15	119.50
2	C	601	20V	OAB-CAO-CBC	-2.19	120.14	124.91
2	C	601	20V	OAF-SBM-CBG	2.08	112.64	106.43
2	A	601	20V	CBC-CBA-CAY	2.01	121.43	120.19
2	A	601	20V	OAB-CAO-CBC	-2.00	120.54	124.91
2	B	602	20V	CBF-CBI-CBH	2.00	120.47	117.94

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	602	20V	CAT-OAX-PBK-OAK
2	A	602	20V	CAT-OAX-PBK-OAC
2	A	602	20V	OAB-CAO-CBC-CBA
2	A	602	20V	CBH-CBG-SBM-OAF
2	C	602	20V	CAT-OAX-PBK-OAL
2	C	602	20V	CAQ-CBB-NBJ-OAI
2	C	602	20V	CAS-CBB-NBJ-OAI
2	C	601	20V	CAT-OAX-PBK-OAK
2	C	601	20V	OAX-CAT-CBE-CBD
2	C	601	20V	OAB-CAO-CBC-CBE
2	C	601	20V	OAB-CAO-CBC-CBA
2	A	601	20V	CAT-OAX-PBK-OAK
2	A	601	20V	OAB-CAO-CBC-CBE
2	B	602	20V	CAT-OAX-PBK-OAK
2	B	602	20V	CAT-OAX-PBK-OAL
2	B	602	20V	CAT-OAX-PBK-OAC
2	A	601	20V	OAB-CAO-CBC-CBA
2	A	602	20V	CAR-CAZ-NAU-NAV
2	A	602	20V	CAP-CAZ-NAU-NAV
2	C	601	20V	OAX-CAT-CBE-CBC
2	B	601	20V	OAB-CAO-CBC-CBA
2	B	602	20V	OAB-CAO-CBC-CBA
2	B	601	20V	OAB-CAO-CBC-CBE
2	A	602	20V	CBH-CBG-SBM-OAG
2	C	602	20V	CBH-CBG-SBM-OAG
2	B	602	20V	CBI-CBF-SBL-OAM
2	A	602	20V	CAT-OAX-PBK-OAL
2	A	602	20V	CAQ-CBG-SBM-OAF
2	B	602	20V	CAP-CBF-SBL-OAM
2	C	602	20V	CAT-OAX-PBK-OAC
2	A	601	20V	CAT-OAX-PBK-OAC
2	B	601	20V	OAX-CAT-CBE-CBD
2	A	602	20V	OAB-CAO-CBC-CBE
2	C	602	20V	CBH-CBG-SBM-OAF
2	C	602	20V	CBI-CBF-SBL-OAD
2	B	602	20V	CBI-CBF-SBL-OAD
2	A	602	20V	CAQ-CBG-SBM-OAG
2	C	602	20V	CAQ-CBG-SBM-OAG
2	B	602	20V	CAP-CBF-SBL-OAD
2	A	602	20V	NAW-CBD-NAV-NAU
2	B	601	20V	NAW-CBD-NAV-NAU
2	B	602	20V	OAB-CAO-CBC-CBE
2	C	602	20V	CBI-CBF-SBL-OAM

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Mol	Chain	Res	Type	Atoms
2	A	602	20V	CBE-CBD-NAV-NAU
2	C	602	20V	CAT-OAX-PBK-OAK
2	C	601	20V	CBE-CBD-NAV-NAU
2	A	601	20V	CBE-CBD-NAV-NAU
2	B	602	20V	OAX-CAT-CBE-CBD
2	C	602	20V	CAQ-CBG-SBM-OAF
2	C	602	20V	CAP-CBF-SBL-OAD
2	C	601	20V	NAW-CBD-NAV-NAU
2	A	601	20V	NAW-CBD-NAV-NAU

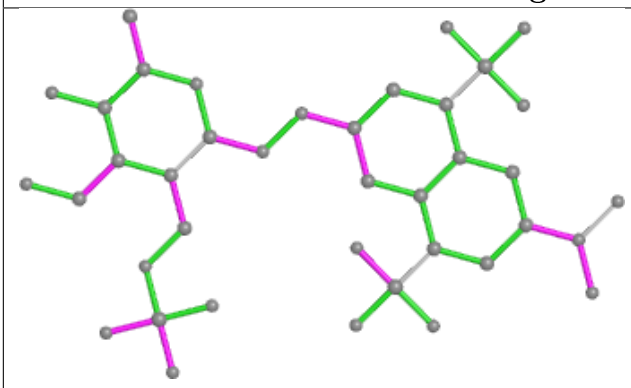
There are no ring outliers.

4 monomers are involved in 6 short contacts:

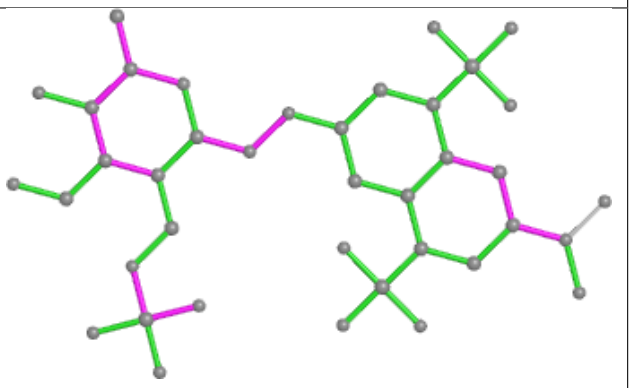
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	602	20V	1	0
2	C	601	20V	2	0
2	A	601	20V	2	0
3	B	606	SO4	1	0

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

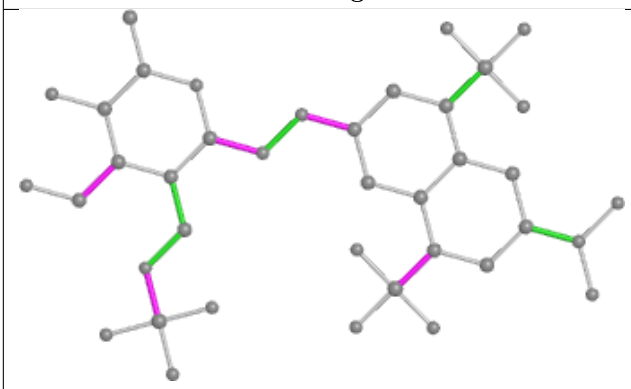
Ligand 20V A 602



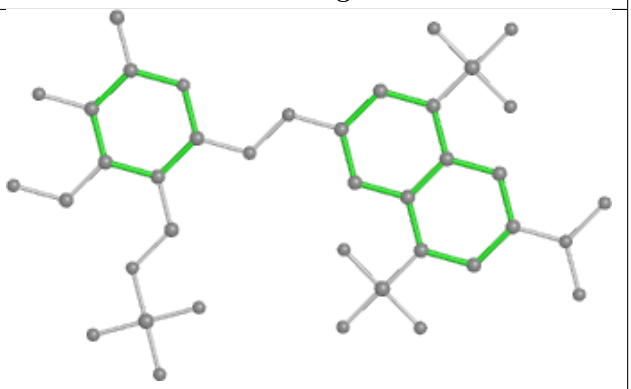
Bond lengths



Bond angles

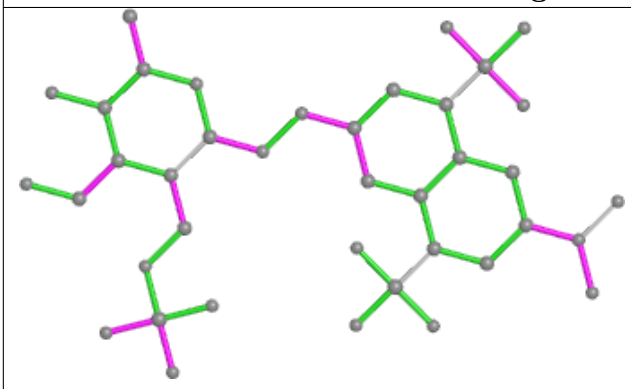


Torsions

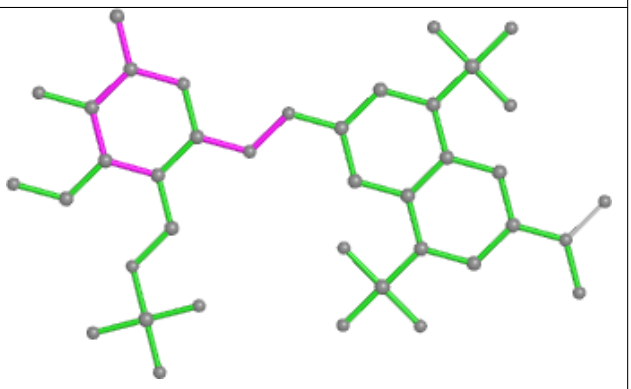


Rings

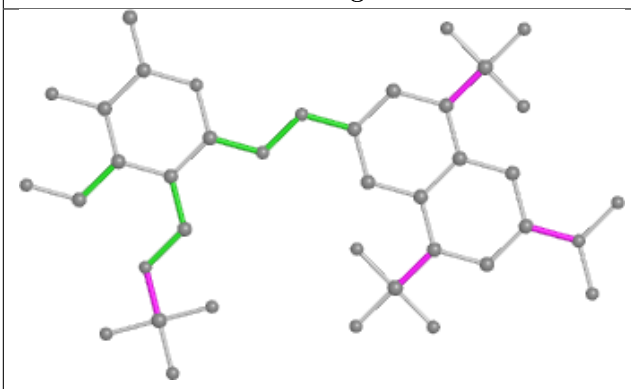
Ligand 20V C 602



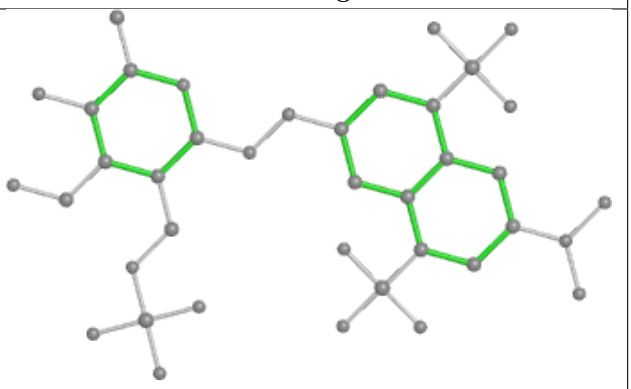
Bond lengths



Bond angles

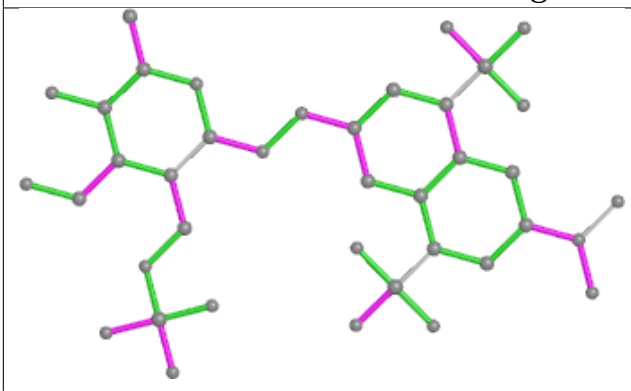


Torsions

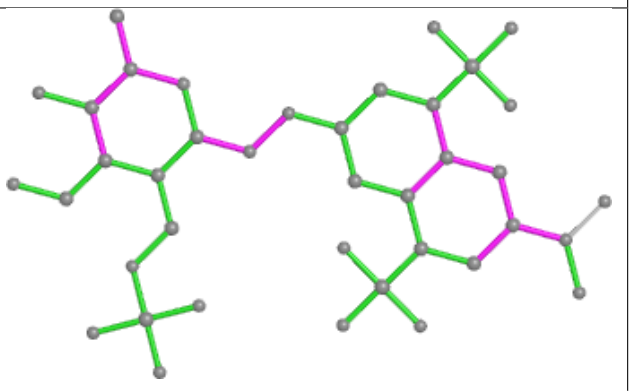


Rings

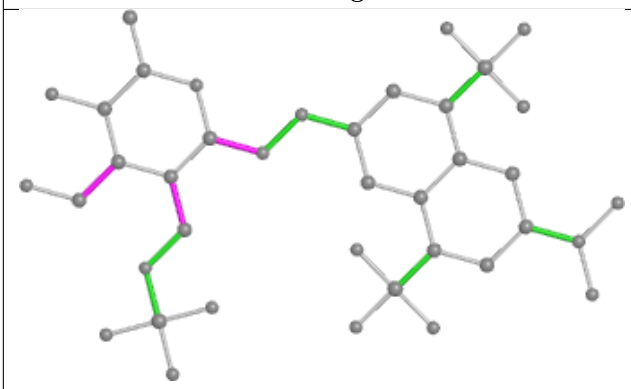
Ligand 20V B 601



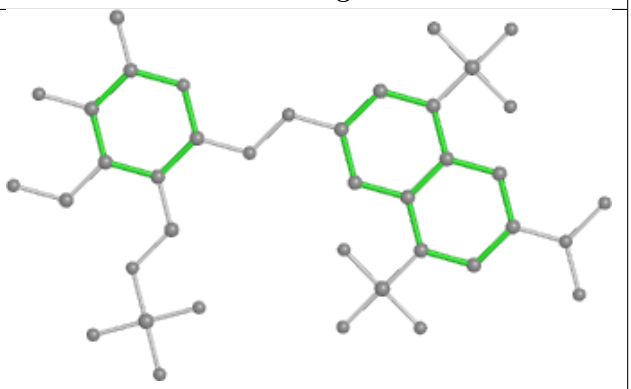
Bond lengths



Bond angles

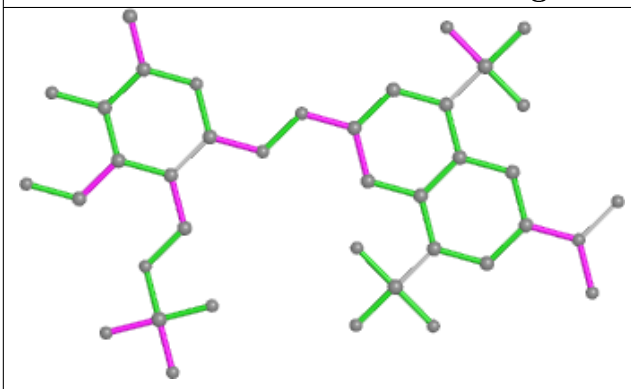


Torsions

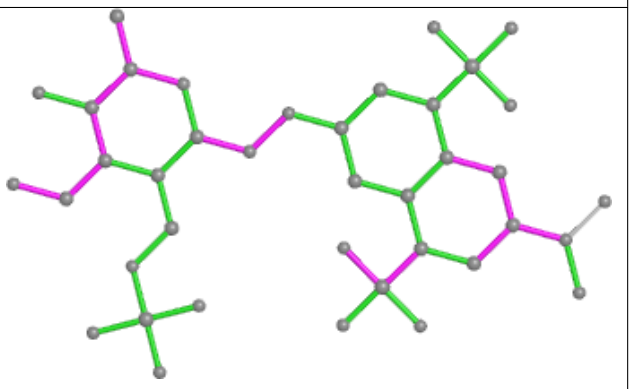


Rings

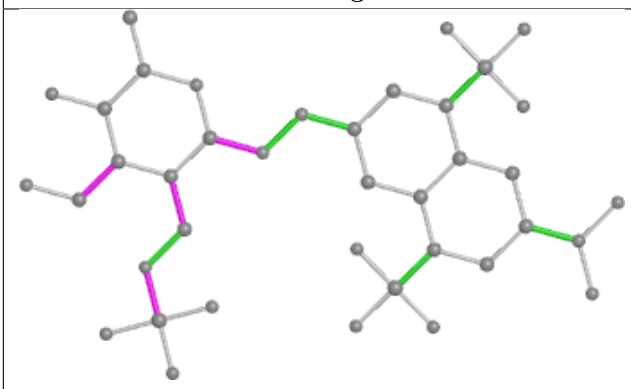
Ligand 20V C 601



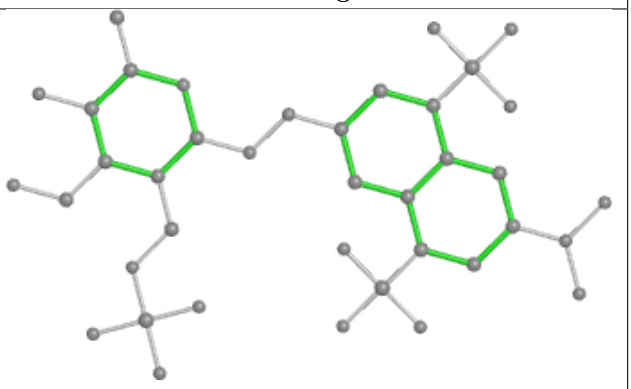
Bond lengths



Bond angles

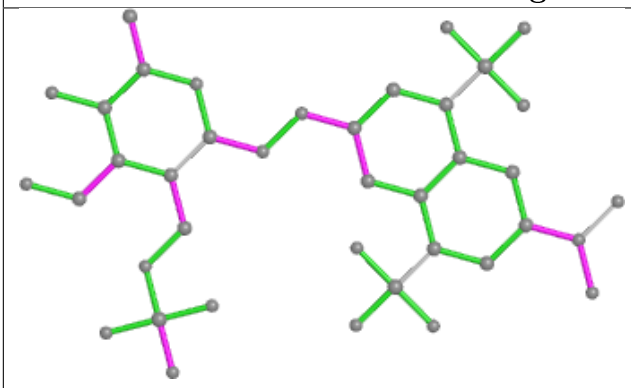


Torsions

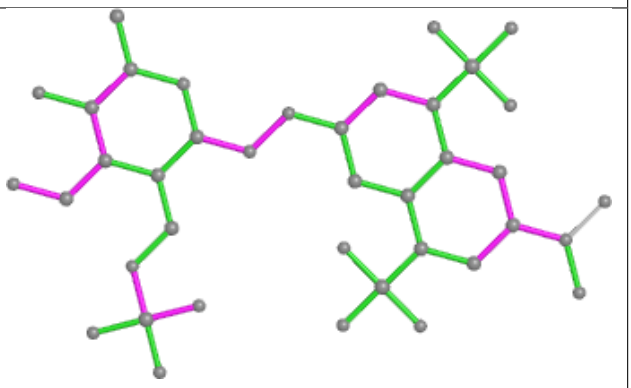


Rings

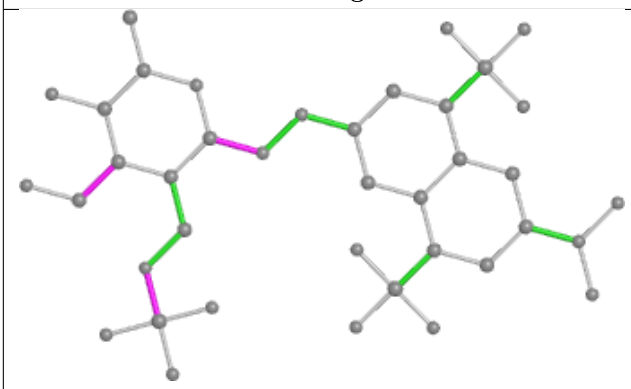
Ligand 20V A 601



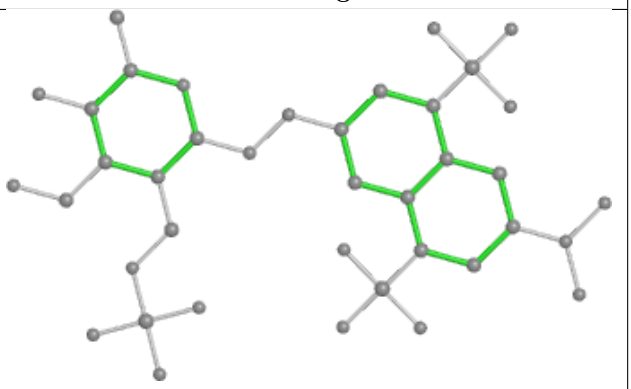
Bond lengths



Bond angles

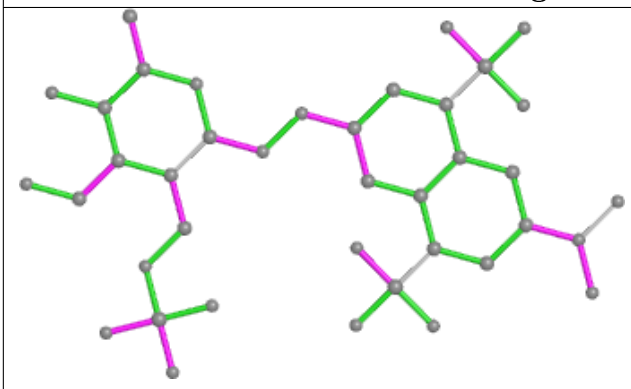


Torsions

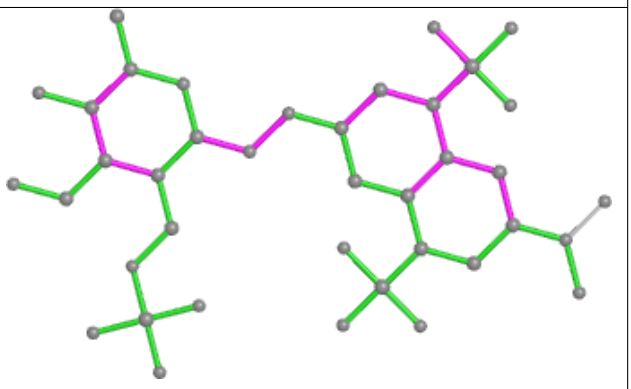


Rings

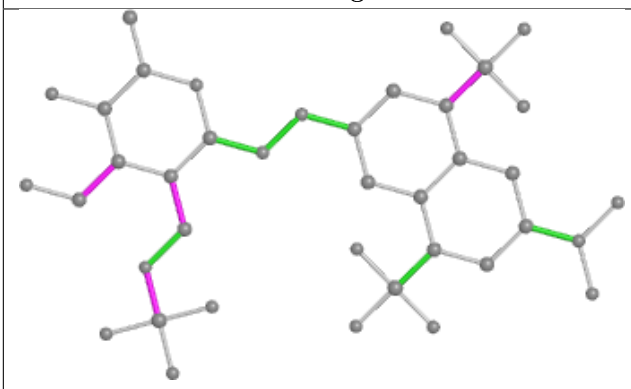
Ligand 20V B 602



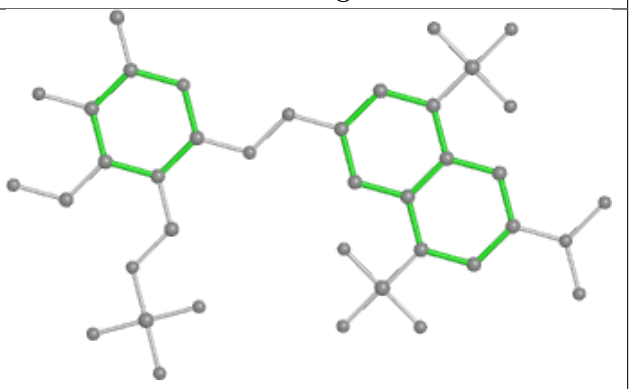
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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	476/515 (92%)	-0.06	7 (1%)	73	72	20, 35, 77, 126	5 (1%)
1	B	480/515 (93%)	-0.05	13 (2%)	54	52	21, 37, 86, 118	2 (0%)
1	C	474/515 (92%)	0.26	23 (4%)	29	28	20, 46, 84, 117	5 (1%)
All	All	1430/1545 (92%)	0.05	43 (3%)	50	49	20, 39, 83, 126	12 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	GLY	5.9
1	B	467	ALA	5.5
1	C	475	VAL	5.1
1	A	433	HIS	4.0
1	C	463	SER	3.8
1	C	477	ARG	3.5
1	C	54	VAL	3.5
1	C	46	TYR	3.4
1	C	433	HIS	3.3
1	C	464	LYS	3.3
1	C	474	VAL	3.2
1	C	171	LYS	3.1
1	A	479	ARG	3.1
1	B	469	SER	3.1
1	A	477	ARG	3.0
1	C	417	TRP	3.0
1	C	176	TYR	2.9
1	A	441	MET	2.9
1	B	466	ALA	2.9
1	C	55	ASP	2.9
1	A	435	GLN	2.9
1	C	456	ARG	2.9
1	B	456	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	416	LEU	2.7
1	C	377	GLY	2.7
1	C	173	ASP	2.7
1	B	463	SER	2.7
1	B	55	ASP	2.6
1	B	460	SER	2.6
1	C	36	LYS	2.5
1	B	445	GLY	2.5
1	C	452	GLU	2.4
1	C	64	ARG	2.4
1	C	466	ALA	2.4
1	C	175	ILE	2.3
1	C	52	GLU	2.3
1	B	474	VAL	2.3
1	B	481	VAL	2.2
1	C	47	LEU	2.2
1	B	303	PRO	2.1
1	B	441	MET	2.0
1	B	374	LYS	2.0
1	A	463	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 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	SO4	A	606	5/5	0.78	0.27	87,110,130,138	0
3	SO4	A	608	5/5	0.85	0.17	45,67,75,85	0
3	SO4	B	606	5/5	0.87	0.21	89,92,108,110	0

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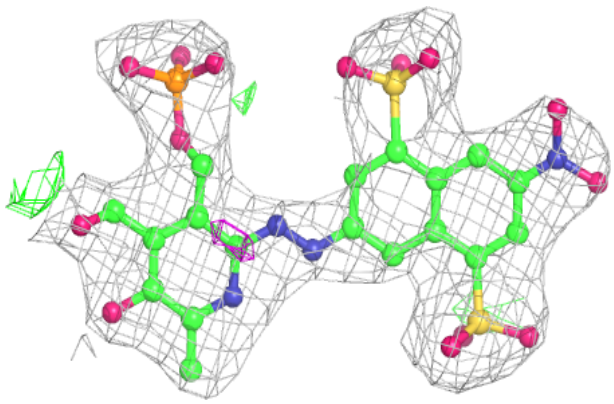
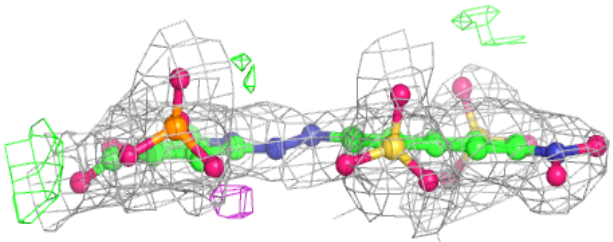
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	20V	B	602	39/39	0.88	0.19	46,70,91,98	0
3	SO4	A	604	5/5	0.89	0.19	112,115,123,151	0
2	20V	C	602	39/39	0.89	0.18	42,65,88,100	0
2	20V	A	602	39/39	0.91	0.20	48,72,99,114	0
3	SO4	B	604	5/5	0.92	0.12	48,59,68,71	0
3	SO4	B	605	5/5	0.94	0.09	47,54,68,73	0
2	20V	A	601	39/39	0.95	0.22	47,57,107,110	0
2	20V	B	601	39/39	0.96	0.18	39,54,103,107	0
2	20V	C	601	39/39	0.96	0.16	35,55,98,99	0
3	SO4	A	607	5/5	0.96	0.10	54,55,66,74	0
3	SO4	A	603	5/5	0.96	0.18	48,63,74,95	0
3	SO4	B	603	5/5	0.96	0.16	50,54,67,68	0
3	SO4	A	605	5/5	0.97	0.19	75,76,98,98	0

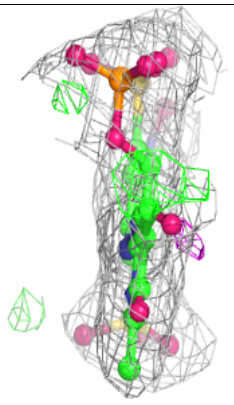
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 20V B 602:

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

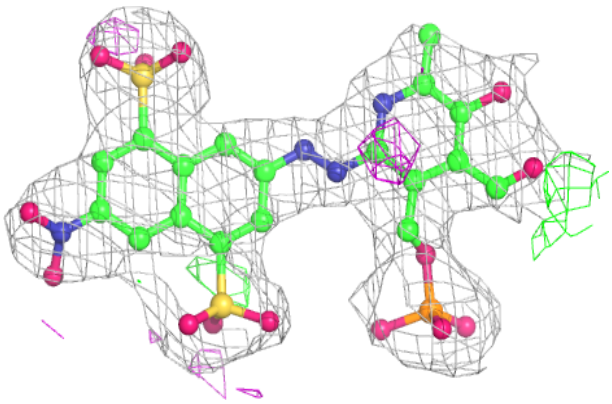


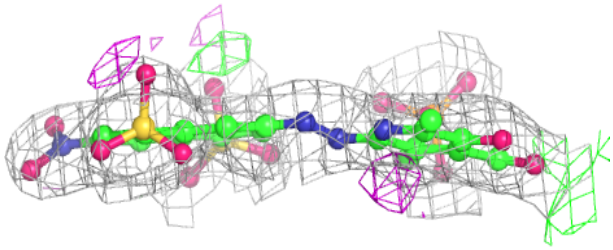


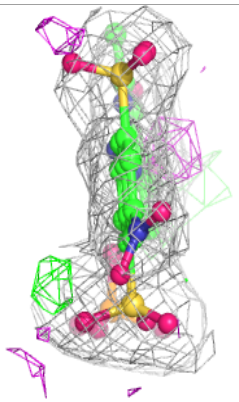


Electron density around 20V C 602:

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

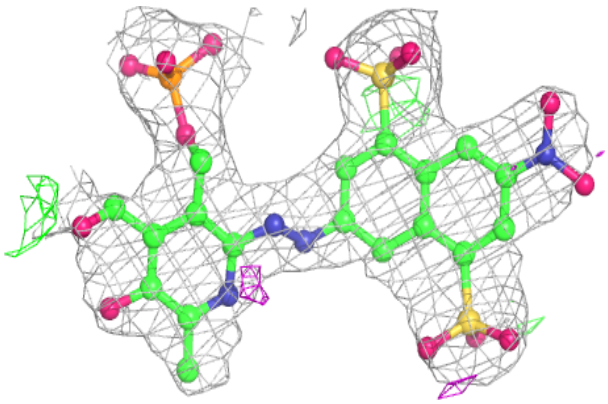


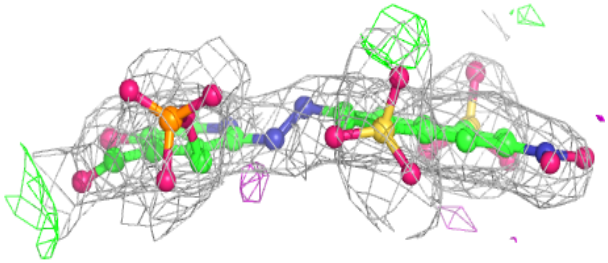


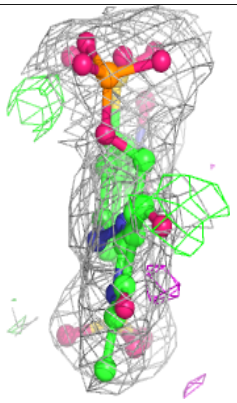


Electron density around 20V A 602:

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

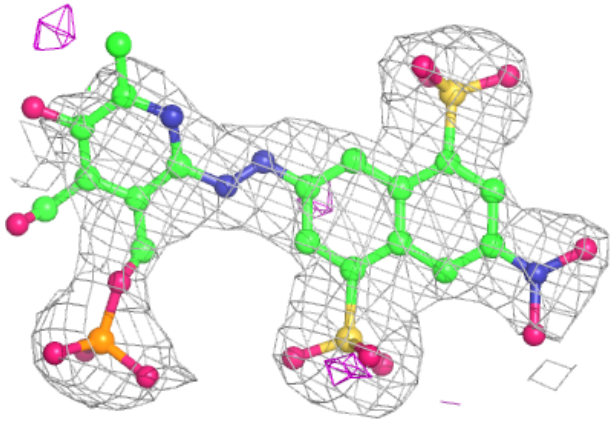


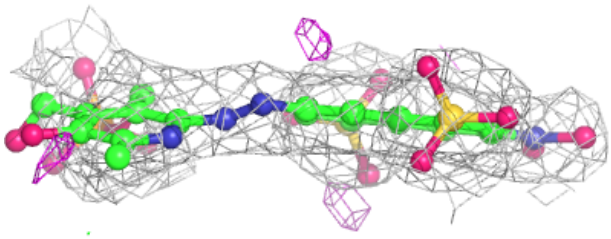


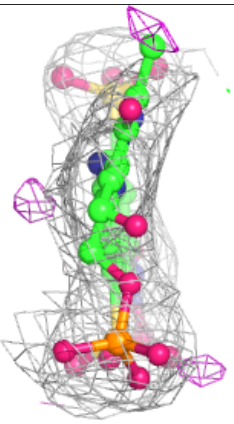


Electron density around 20V A 601:

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

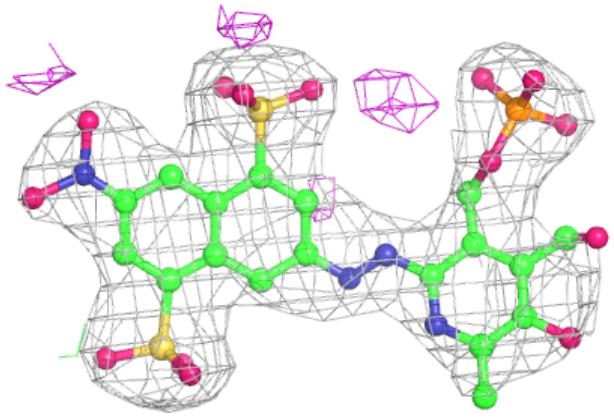


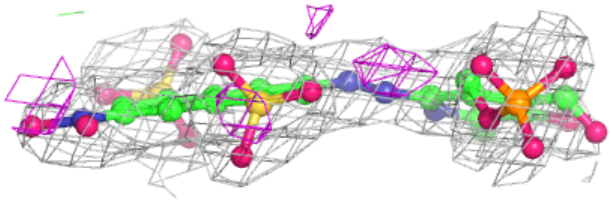


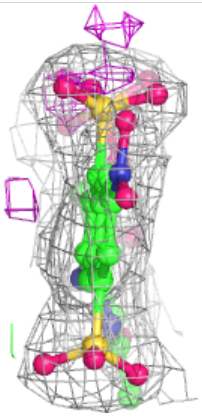


Electron density around 20V B 601:

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

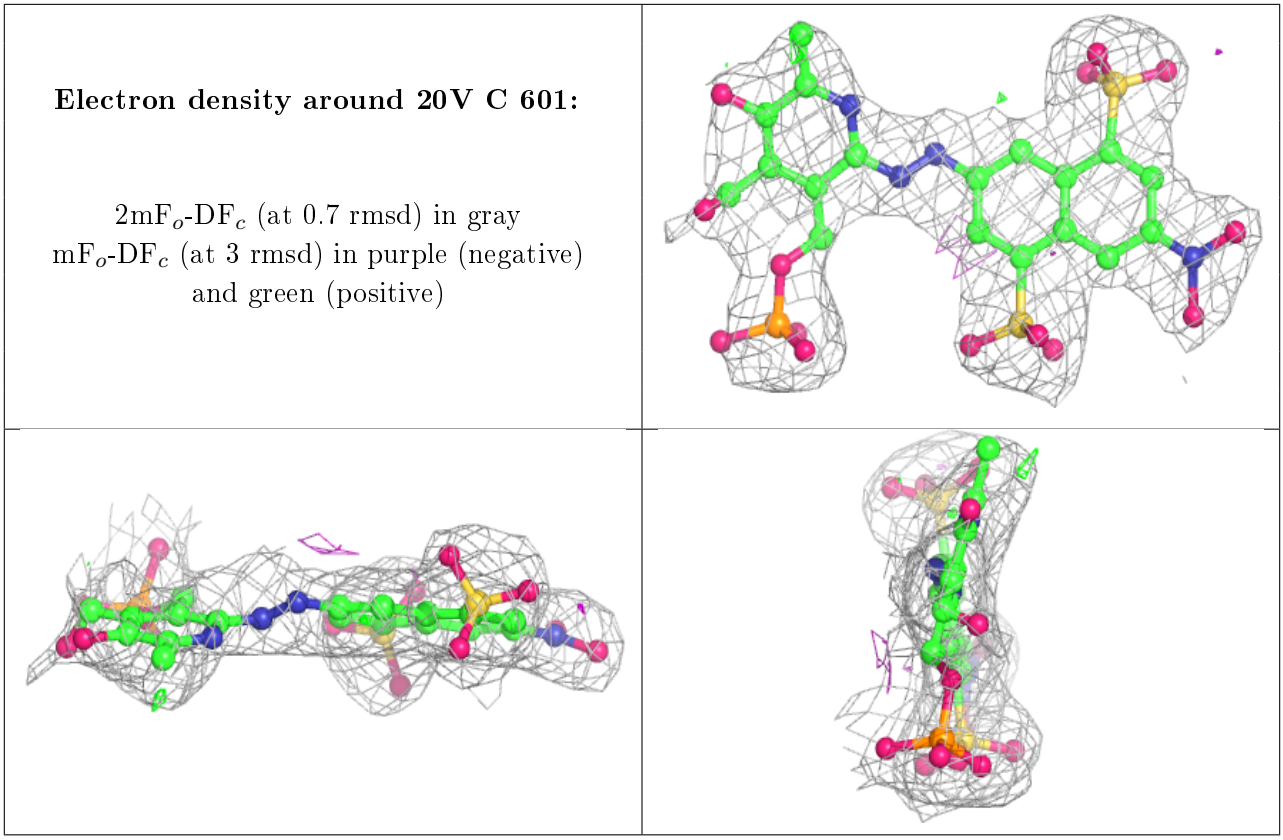






Electron density around 20V C 601:

$2mF_o$-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

There are no such residues in this entry.