Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:43 AM EDT

PDB ID	:	3UR0
Title	:	Crystal structures of murine norovirus RNA-dependent RNA polymerase in complex with Suramin
Authors	:	Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on	:	2011-11-21
Resolution	:	2.45 Å(reported)

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

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

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

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

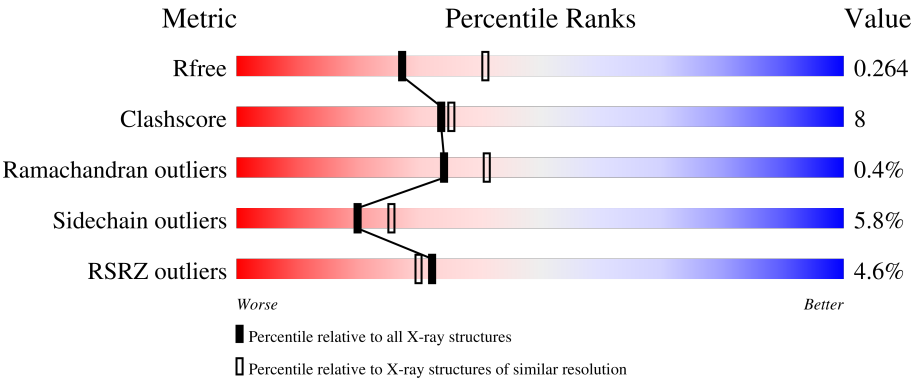
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.45 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	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (2.48-2.44)

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

Mol	Chain	Length	Quality of chain
1	A	515	6% 74% 16% • 8%
1	B	515	5% 74% 17% • 8%
1	C	515	2% 75% 15% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12050 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	475	Total	C	N	O	S	0	1	0
			3785	2395	666	699	25			
1	B	476	Total	C	N	O	S	0	2	0
			3792	2402	665	700	25			
1	C	474	Total	C	N	O	S	0	2	0
			3776	2388	663	700	25			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	EXPRESSION TAG	UNP Q80J95
A	509	GLU	-	EXPRESSION TAG	UNP Q80J95
A	510	HIS	-	EXPRESSION TAG	UNP Q80J95
A	511	HIS	-	EXPRESSION TAG	UNP Q80J95
A	512	HIS	-	EXPRESSION TAG	UNP Q80J95
A	513	HIS	-	EXPRESSION TAG	UNP Q80J95
A	514	HIS	-	EXPRESSION TAG	UNP Q80J95
A	515	HIS	-	EXPRESSION TAG	UNP Q80J95
B	508	LEU	-	EXPRESSION TAG	UNP Q80J95
B	509	GLU	-	EXPRESSION TAG	UNP Q80J95
B	510	HIS	-	EXPRESSION TAG	UNP Q80J95
B	511	HIS	-	EXPRESSION TAG	UNP Q80J95
B	512	HIS	-	EXPRESSION TAG	UNP Q80J95
B	513	HIS	-	EXPRESSION TAG	UNP Q80J95
B	514	HIS	-	EXPRESSION TAG	UNP Q80J95
B	515	HIS	-	EXPRESSION TAG	UNP Q80J95
C	508	LEU	-	EXPRESSION TAG	UNP Q80J95
C	509	GLU	-	EXPRESSION TAG	UNP Q80J95
C	510	HIS	-	EXPRESSION TAG	UNP Q80J95
C	511	HIS	-	EXPRESSION TAG	UNP Q80J95
C	512	HIS	-	EXPRESSION TAG	UNP Q80J95
C	513	HIS	-	EXPRESSION TAG	UNP Q80J95
C	514	HIS	-	EXPRESSION TAG	UNP Q80J95

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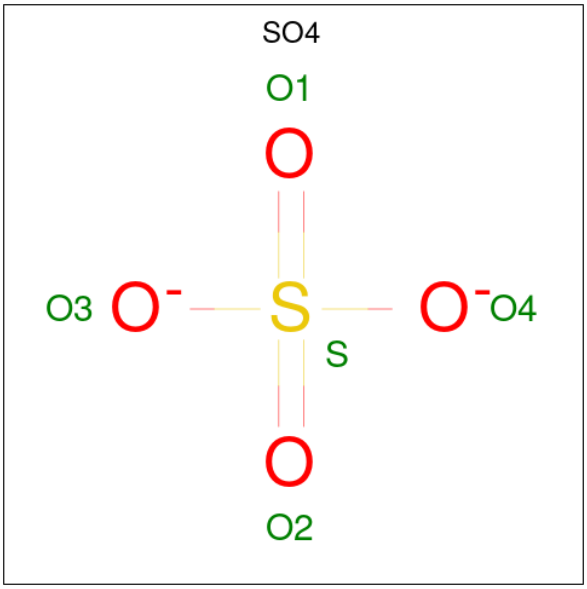
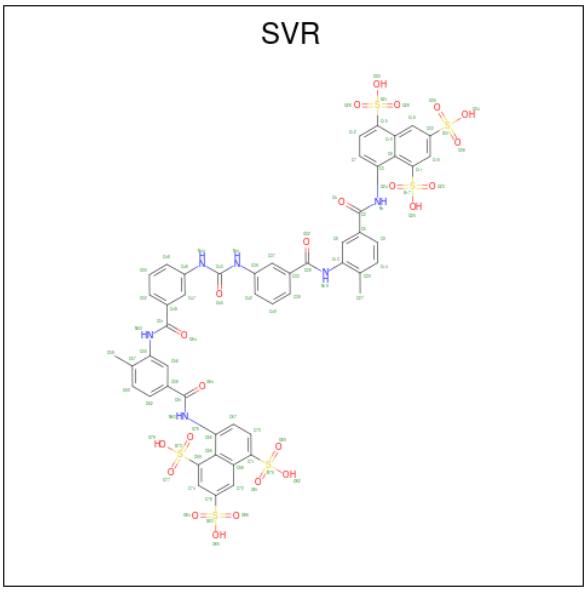
Chain	Residue	Modelled	Actual	Comment	Reference
C	515	HIS	-	EXPRESSION TAG	UNP Q80J95

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is 8,8'-[CARBONYLBIS[IMINO-3,1-PHENYLENECARBONYLIMINO(4-METHYL-3,1-PHENYLENE)CARBONYLIMINO]]BIS-1,3,5-NAPHTHALENETRISULFONIC ACID (three-letter code: SVR) (formula: $C_{51}H_{40}N_6O_{23}S_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O S 26 12 1 10 3	0	0
3	C	1	Total C N O S 26 12 1 10 3	0	0
3	C	1	Total C N O S 54 33 5 13 3	0	0

- Molecule 4 is water.

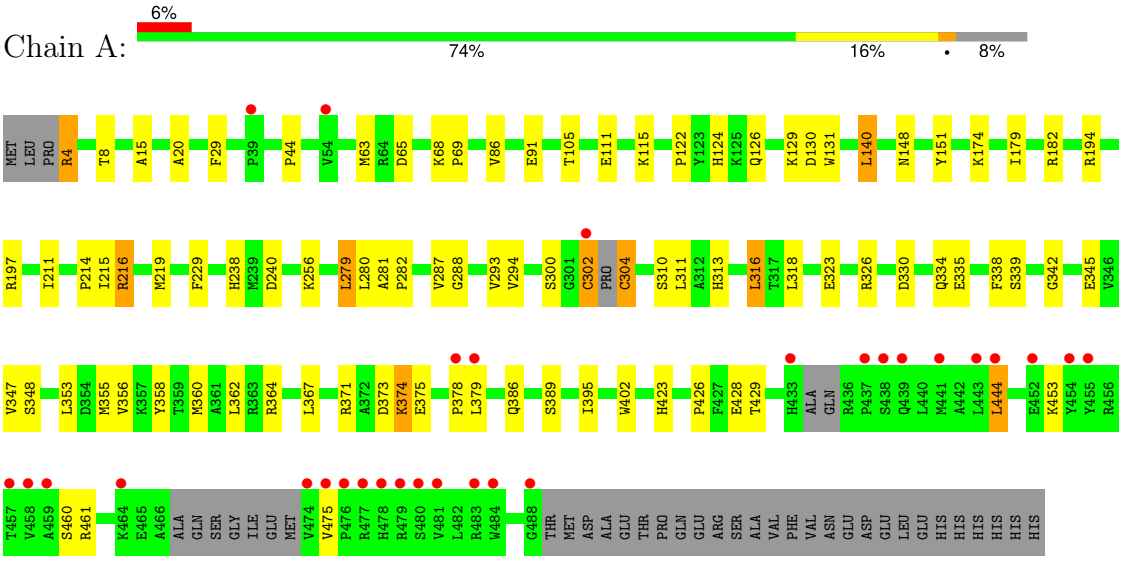
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	173	Total O 173 173	0	0
4	B	166	Total O 166 166	0	0
4	C	217	Total O 217 217	0	0

3 Residue-property plots (i)

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

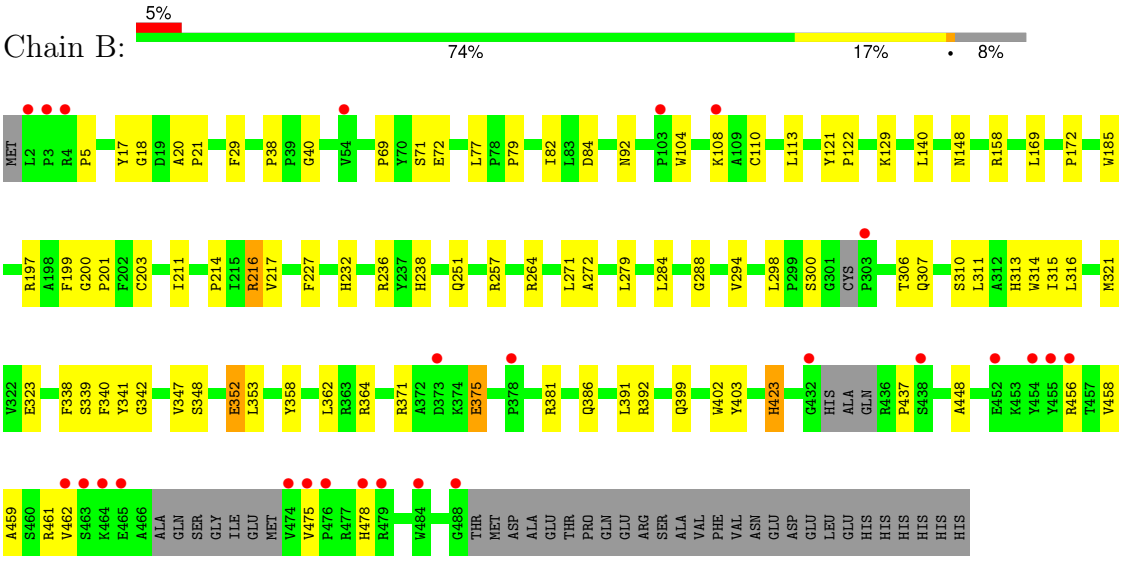
• Molecule 1: RNA-dependent RNA polymerase

Chain A:



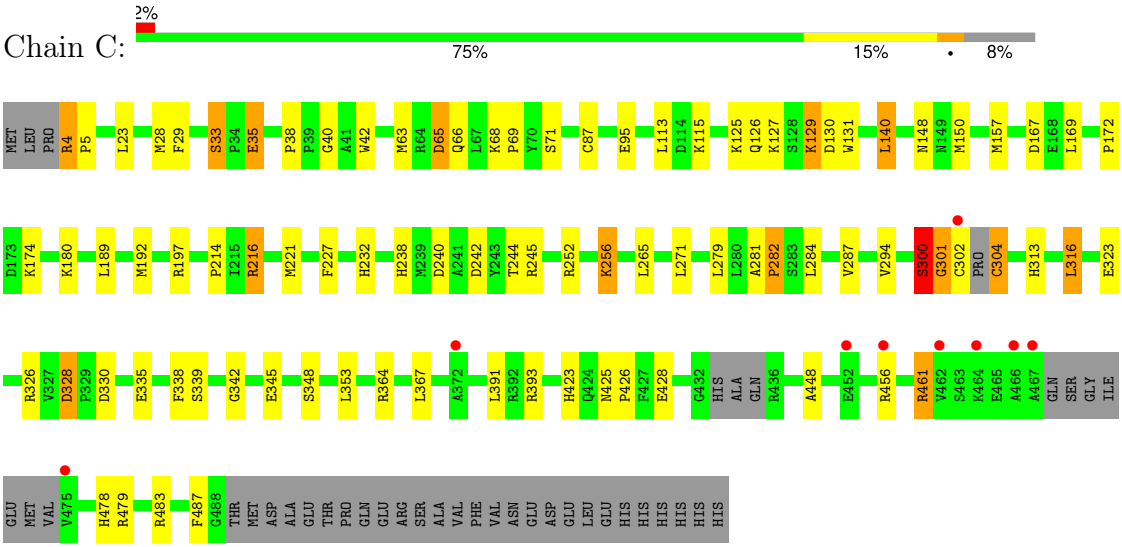
• Molecule 1: RNA-dependent RNA polymerase

Chain B:



• Molecule 1: RNA-dependent RNA polymerase

Chain C:


2%
75%
15%
8%
MET LEU PRO R4 P5 L23 M28 F29 S33 P34 E35 P38 P39 G40 A41 W42 M63 R64 D65 Q66 L67 K68 P69 Y70 S71 C87 E95 L113 D114 K115 K125 Q126 K127 S128 K129 D130 W131 L140 N148 N149 M150 M157 D167 E168 L169 P172
D173 K174 K180 L189 M192 R197 P214 I215 R216 M221 F227 H232 H238 M239 D240 A241 D242 Y243 T244 R245 R252 K256 L265 L271 L279 L280 A281 P282 S283 L284 V287 V294 S300 G301 C302 PRO C304 H313 L316 E323
R326 V327 D328 P329 D330 E335 F338 S339 G342 E345 S348 L353 R364 L367 A372 L391 R392 R393 H423 Q424 N425 P426 F427 E428 G432 HIS ALA GLN R436 A448 E452 R456 R461 V462 S463 K464 E465 A466 A467 GLN SER GLY ILE
GLU MET VAL V475 H478 R479 R483 F487 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	120.84Å 196.51Å 109.07Å 90.00° 114.55° 90.00°	Depositor
Resolution (Å)	48.00 – 2.45 48.08 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (48.00-2.45) 97.4 (48.08-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.268 0.199 , 0.264	Depositor DCC
R_{free} test set	4102 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	47.8	Xtriage
Anisotropy	0.095	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	12050	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.00% 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, SVR

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	0.58	0/3879	0.71	2/5250 (0.0%)
1	B	0.54	0/3890	0.64	0/5267
1	C	0.62	0/3872	0.71	1/5241 (0.0%)
All	All	0.58	0/11641	0.69	3/15758 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	LEU	CA-CB-CG	5.86	128.78	115.30
1	A	65	ASP	CB-CG-OD1	5.26	123.03	118.30
1	C	65	ASP	CB-CG-OD1	5.06	122.85	118.30

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	3785	0	3745	66	0
1	B	3792	0	3760	51	0
1	C	3776	0	3734	68	0
2	A	15	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	0	0	0
3	B	26	0	6	2	0
3	C	80	0	31	17	0
4	A	173	0	0	6	0
4	B	166	0	0	2	0
4	C	217	0	0	3	0
All	All	12050	0	11276	192	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 8.

All (192) 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:C:301:GLY:HA3	1:C:302:CYS:CB	1.56	1.27
1:C:301:GLY:HA3	1:C:302:CYS:HB3	1.24	1.12
1:C:301:GLY:HA3	1:C:302:CYS:HB2	1.35	1.03
1:A:373:ASP:O	1:A:374:LYS:HB2	1.59	0.97
1:C:301:GLY:CA	1:C:302:CYS:CB	2.44	0.93
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.12	0.91
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.00	0.91
1:A:148:ASN:HD21	1:A:197:ARG:HH11	0.94	0.90
3:C:517:SVR:H42	3:C:517:SVR:H44	1.34	0.88
1:B:232:HIS:HE1	1:B:339:SER:OG	1.59	0.86
1:C:33:SER:OG	1:C:35:GLU:HG2	1.80	0.82
1:A:68:LYS:HB2	1:A:69:PRO:HD3	1.58	0.82
1:B:29:PHE:O	1:B:423:HIS:HE1	1.62	0.82
1:A:360[B]:MET:HE3	1:A:360[B]:MET:HA	1.61	0.80
1:A:371:ARG:HD3	1:A:375:GLU:O	1.81	0.80
1:C:301:GLY:CA	1:C:302:CYS:HB3	2.06	0.80
1:B:77:LEU:HD23	1:B:251:GLN:NE2	1.97	0.80
3:C:517:SVR:H271	3:C:517:SVR:C26	2.10	0.80
1:B:203[B]:CYS:SG	1:B:307:GLN:NE2	2.57	0.77
1:A:360[B]:MET:HA	1:A:360[B]:MET:CE	2.14	0.77
1:A:148:ASN:HD21	1:A:197:ARG:NH1	1.78	0.77
1:C:180:LYS:HB3	3:C:517:SVR:C27	2.15	0.77
1:C:238:HIS:HD2	1:C:348:SER:OG	1.66	0.77
1:C:302:CYS:O	1:C:304:CYS:N	2.18	0.75
1:B:77:LEU:HD23	1:B:251:GLN:HE22	1.51	0.75
1:C:216:ARG:N	1:C:216:ARG:HD2	2.02	0.75
1:A:148:ASN:ND2	1:A:197:ARG:HH11	1.78	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ASN:ND2	1:C:197:ARG:HH11	1.82	0.74
1:B:232:HIS:CE1	1:B:339:SER:OG	2.39	0.74
1:A:313:HIS:HD2	1:A:342:GLY:O	1.73	0.72
1:B:29:PHE:O	1:B:423:HIS:CE1	2.44	0.71
1:B:313:HIS:HD2	1:B:342:GLY:O	1.74	0.70
1:C:180:LYS:HB3	3:C:517:SVR:H272	1.72	0.69
1:B:238:HIS:HD2	1:B:348:SER:OG	1.74	0.69
1:A:124:HIS:HE1	4:A:597:HOH:O	1.73	0.69
1:C:323:GLU:CD	1:C:364:ARG:HH22	1.96	0.69
1:C:95:GLU:HG2	1:C:265:LEU:HD21	1.75	0.68
1:C:328:ASP:HB3	1:C:330[A]:ASP:OD1	1.94	0.68
1:C:301:GLY:CA	1:C:302:CYS:HB2	2.20	0.67
1:C:244:THR:HG22	1:C:245:ARG:HG3	1.74	0.67
1:B:110:CYS:SG	4:B:617:HOH:O	2.52	0.67
1:A:335:GLU:OE1	1:C:326:ARG:NH1	2.29	0.65
1:C:28:MET:HG2	1:C:167:ASP:OD2	1.96	0.65
1:A:238:HIS:HD2	1:A:348:SER:OG	1.82	0.63
1:A:356:VAL:HG22	1:A:378:PRO:HB3	1.81	0.63
1:C:313:HIS:HD2	1:C:342:GLY:O	1.83	0.62
1:B:311:LEU:O	1:B:315:ILE:HG13	1.99	0.61
1:A:355:MET:HB3	1:A:379:LEU:O	2.00	0.61
1:A:68:LYS:HB2	1:A:69:PRO:CD	2.29	0.61
1:B:353:LEU:H	1:B:381:ARG:NH1	1.98	0.61
1:C:66:GLN:HE22	3:C:517:SVR:H37	1.65	0.61
1:A:182:ARG:HG3	4:A:541:HOH:O	2.02	0.60
1:B:40:GLY:HA2	1:B:172:PRO:HG3	1.84	0.59
1:B:69:PRO:HA	1:B:72:GLU:HG2	1.83	0.59
1:A:356:VAL:HA	1:A:378:PRO:HB3	1.85	0.59
3:C:517:SVR:H44	3:C:517:SVR:C42	2.12	0.58
1:A:214:PRO:HB3	1:A:338:PHE:HB2	1.84	0.58
3:C:516:SVR:S73	3:C:516:SVR:N63	2.70	0.58
1:A:313:HIS:HE1	1:A:345:GLU:OE2	1.87	0.58
1:C:238:HIS:CD2	1:C:348:SER:OG	2.55	0.58
1:B:84:ASP:OD1	1:B:257:ARG:NH2	2.35	0.57
1:B:371:ARG:HD3	1:B:375:GLU:O	2.04	0.57
1:C:180:LYS:CB	3:C:517:SVR:H272	2.35	0.57
1:B:214:PRO:HB3	1:B:338:PHE:HB2	1.86	0.56
1:A:371:ARG:NH2	1:A:373:ASP:OD1	2.27	0.56
1:B:211:ILE:O	1:B:216:ARG:NH2	2.38	0.56
1:C:339:SER:O	1:C:345:GLU:HA	2.05	0.56
1:A:86:VAL:HG13	1:A:318:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:HG3	1:A:402:TRP:HZ3	1.71	0.56
3:C:517:SVR:H16	3:C:517:SVR:O30	2.05	0.56
1:A:373:ASP:OD2	1:A:375:GLU:N	2.29	0.56
1:C:148:ASN:HD21	1:C:197:ARG:NH1	1.85	0.56
1:B:321:MET:HG2	1:B:353:LEU:HD11	1.88	0.55
1:C:232:HIS:HD2	1:C:348:SER:OG	1.90	0.55
1:C:448:ALA:O	1:C:478:HIS:HE1	1.89	0.55
1:C:323:GLU:OE2	1:C:364:ARG:NH2	2.31	0.55
1:C:180:LYS:HB3	3:C:517:SVR:H271	1.88	0.54
1:B:79:PRO:HG2	1:B:82:ILE:HB	1.88	0.54
1:A:326:ARG:NH1	1:C:335:GLU:OE1	2.40	0.54
1:B:217:VAL:HA	1:B:341:TYR:CE1	2.43	0.54
1:A:339:SER:O	1:A:345:GLU:HA	2.10	0.52
1:C:40:GLY:HA2	1:C:172:PRO:HG3	1.92	0.52
1:C:316:LEU:HG	1:C:367:LEU:HD11	1.92	0.52
3:C:516:SVR:H67	3:C:516:SVR:O64	2.09	0.52
1:B:104:TRP:CG	1:B:201:PRO:HD3	2.44	0.52
1:B:40:GLY:CA	1:B:172:PRO:HG3	2.40	0.52
1:B:201:PRO:HG2	4:B:532:HOH:O	2.08	0.52
1:B:458:VAL:O	1:B:462:VAL:HG23	2.09	0.52
1:C:29:PHE:O	1:C:423:HIS:HE1	1.91	0.52
3:C:517:SVR:N1	3:C:517:SVR:O25	2.43	0.52
1:C:216:ARG:NH1	1:C:339:SER:OG	2.41	0.52
3:C:517:SVR:H42	3:C:517:SVR:N44	2.11	0.52
1:A:373:ASP:O	1:A:374:LYS:CB	2.40	0.52
1:B:448:ALA:O	1:B:478:HIS:HE1	1.93	0.51
1:B:353:LEU:H	1:B:381:ARG:HH12	1.57	0.51
1:B:5:PRO:HD3	1:B:17:TYR:CE2	2.46	0.51
1:C:126:GLN:O	1:C:129:LYS:HB2	2.12	0.50
1:B:200:GLY:N	1:B:201:PRO:HD2	2.26	0.50
1:B:456:ARG:HA	1:B:459:ALA:HB3	1.94	0.50
1:C:214:PRO:HB3	1:C:338:PHE:HB2	1.94	0.50
1:A:4:ARG:HA	4:A:538:HOH:O	2.12	0.49
1:A:229:PHE:CZ	1:A:395:ILE:HG12	2.48	0.49
1:A:29:PHE:O	1:A:423:HIS:HE1	1.95	0.49
1:A:216:ARG:HD3	1:A:339:SER:OG	2.13	0.48
1:B:338:PHE:HE1	1:B:347:VAL:HG13	1.79	0.48
1:A:256:LYS:HA	1:A:280:LEU:CD1	2.43	0.48
1:C:300:SER:O	1:C:301:GLY:O	2.31	0.47
1:A:20:ALA:HB3	1:A:288:GLY:HA2	1.96	0.47
1:C:125:LYS:HD3	1:C:129:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:MET:CE	1:A:379:LEU:HB3	2.44	0.47
1:C:232:HIS:HE1	1:C:339:SER:OG	1.97	0.47
1:A:174:LYS:O	1:A:179:ILE:HA	2.15	0.47
1:A:355:MET:HE3	1:A:379:LEU:CB	2.45	0.47
1:C:38:PRO:HG2	3:C:516:SVR:O77	2.14	0.47
1:A:130:ASP:HB2	1:A:140:LEU:HD22	1.97	0.47
3:C:517:SVR:N1	3:C:517:SVR:S17	2.88	0.47
1:A:386:GLN:HG3	1:A:402:TRP:CZ3	2.50	0.46
1:B:158:ARG:NH2	1:B:284:LEU:HD13	2.30	0.46
1:B:310:SER:O	1:B:313:HIS:HB3	2.14	0.46
1:A:115:LYS:HE2	1:A:131:TRP:CD2	2.50	0.46
1:A:345:GLU:OE2	4:A:653:HOH:O	2.21	0.46
1:A:323:GLU:OE2	1:A:364:ARG:NH2	2.49	0.46
1:B:338:PHE:CE1	1:B:347:VAL:HG13	2.51	0.46
1:C:40:GLY:CA	1:C:172:PRO:HG3	2.45	0.46
1:C:63:MET:HE3	1:C:287:VAL:HB	1.98	0.46
1:A:215:ILE:HG12	1:A:310:SER:HB3	1.98	0.45
1:B:148:ASN:ND2	1:B:197:ARG:HH11	1.95	0.45
1:C:33:SER:OG	1:C:35:GLU:CG	2.59	0.45
1:C:65:ASP:O	1:C:68:LYS:HB2	2.16	0.45
1:B:199:PHE:CE1	1:B:272:ALA:HB1	2.50	0.45
1:C:23:LEU:HD11	1:C:63:MET:HE2	1.98	0.45
1:A:63:MET:HE1	1:A:287:VAL:HB	1.98	0.45
1:C:4:ARG:HA	1:C:5:PRO:C	2.37	0.45
1:A:15:ALA:HB2	1:A:293:VAL:HG23	1.99	0.45
1:B:104:TRP:CD1	1:B:201:PRO:HD3	2.52	0.45
1:C:130:ASP:HB2	1:C:140:LEU:HB2	1.98	0.45
1:C:150:MET:HG3	1:C:157:MET:SD	2.56	0.45
1:A:338:PHE:CE1	1:A:347:VAL:HG13	2.53	0.44
1:A:373:ASP:OD2	1:A:375:GLU:HB2	2.15	0.44
1:C:252:ARG:O	1:C:256:LYS:HB2	2.17	0.44
1:A:374:LYS:HD3	1:A:374:LYS:HA	1.54	0.44
1:A:316:LEU:HG	1:A:367:LEU:HD11	1.98	0.44
1:A:358:TYR:CE2	1:A:362:LEU:HD11	2.53	0.44
1:C:68:LYS:N	1:C:69:PRO:CD	2.81	0.44
3:B:516:SVR:S73	3:B:516:SVR:N63	2.91	0.43
1:C:115:LYS:HE2	1:C:131:TRP:CD2	2.53	0.43
1:A:444:LEU:HD21	1:A:475:VAL:HG23	2.00	0.43
1:A:423:HIS:HD2	1:A:428:GLU:OE1	2.01	0.43
1:C:240:ASP:OD1	1:C:240:ASP:C	2.57	0.43
1:A:229:PHE:CE2	1:A:395:ILE:HG12	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASP:OD1	1:A:240:ASP:C	2.56	0.43
1:C:221:MET:HG2	1:C:393:ARG:HG3	2.01	0.43
1:A:105:THR:HB	4:A:680:HOH:O	2.18	0.43
1:B:38:PRO:HG2	3:B:516:SVR:O77	2.18	0.43
1:A:313:HIS:CD2	1:A:342:GLY:O	2.62	0.43
1:C:127:LYS:HE2	1:C:192:MET:SD	2.59	0.43
1:C:174:LYS:HE2	3:C:517:SVR:O24	2.19	0.43
1:A:44:PRO:HG2	1:A:426:PRO:HB3	2.00	0.42
1:C:425:ASN:HA	1:C:426:PRO:HD2	1.82	0.42
1:A:330:ASP:N	1:A:330:ASP:OD1	2.52	0.42
1:C:313:HIS:HE1	1:C:345:GLU:OE2	2.02	0.42
1:C:87:CYS:SG	4:C:682:HOH:O	2.62	0.42
1:B:185:TRP:CD1	1:B:300:SER:HB2	2.54	0.42
1:B:358:TYR:CZ	1:B:362:LEU:HD11	2.55	0.42
1:C:281:ALA:O	1:C:282:PRO:C	2.57	0.42
1:C:42:TRP:HH2	3:C:517:SVR:C16	2.33	0.42
1:C:483:ARG:NH2	4:C:630:HOH:O	2.53	0.42
1:A:281:ALA:O	1:A:282:PRO:C	2.57	0.42
1:C:423:HIS:HD2	1:C:428:GLU:OE1	2.03	0.42
1:B:121:TYR:HA	1:B:122:PRO:HA	1.84	0.41
1:C:425:ASN:HB3	1:C:428:GLU:OE2	2.20	0.41
1:A:151:TYR:HB2	1:A:194:ARG:HG2	2.02	0.41
1:A:238:HIS:HD2	1:A:348:SER:CB	2.33	0.41
1:B:18:GLY:HA3	1:B:288:GLY:O	2.20	0.41
1:B:352:GLU:HA	1:B:381:ARG:HH12	1.86	0.41
1:C:232:HIS:HD2	1:C:348:SER:CB	2.34	0.41
1:A:126:GLN:HB3	1:A:129:LYS:HD2	2.01	0.41
1:B:386:GLN:HG3	1:B:402:TRP:CZ3	2.56	0.41
1:C:35:GLU:HG2	1:C:35:GLU:H	1.55	0.41
1:A:122:PRO:O	1:A:124:HIS:CD2	2.74	0.41
1:A:151:TYR:HA	4:A:598:HOH:O	2.21	0.41
1:B:391:LEU:O	1:B:392:ARG:HB2	2.21	0.41
1:A:334:GLN:HG2	1:B:399:GLN:CG	2.51	0.40
1:C:461:ARG:NH2	4:C:706:HOH:O	2.54	0.40
1:B:314:TRP:HA	1:B:340:PHE:CE2	2.56	0.40
1:B:323:GLU:CD	1:B:364:ARG:HH22	2.24	0.40
1:B:386:GLN:HG3	1:B:402:TRP:HZ3	1.86	0.40
1:A:219:MET:O	1:A:219:MET:HG3	2.21	0.40
1:A:302:CYS:HG	1:A:304:CYS:HG	1.40	0.40
1:A:211:ILE:O	1:A:216:ARG:NH2	2.54	0.40
1:B:20:ALA:HB3	1:B:288:GLY:HA2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/515 (91%)	451 (96%)	16 (3%)	1 (0%)	47	57
1	B	470/515 (91%)	449 (96%)	20 (4%)	1 (0%)	47	57
1	C	468/515 (91%)	452 (97%)	12 (3%)	4 (1%)	17	19
All	All	1406/1545 (91%)	1352 (96%)	48 (3%)	6 (0%)	34	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	301	GLY
1	A	300	SER
1	B	437	PRO
1	C	242	ASP
1	C	300	SER
1	C	282	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	407/441 (92%)	387 (95%)	20 (5%)	25	32
1	B	409/441 (93%)	385 (94%)	24 (6%)	19	25
1	C	406/441 (92%)	380 (94%)	26 (6%)	17	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1222/1323 (92%)	1152 (94%)	70 (6%)	20 26

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

Mol	Chain	Res	Type
1	A	4	ARG
1	A	8	THR
1	A	91	GLU
1	A	111	GLU
1	A	140	LEU
1	A	216	ARG
1	A	279	LEU
1	A	294	VAL
1	A	302	CYS
1	A	304	CYS
1	A	311	LEU
1	A	316	LEU
1	A	353	LEU
1	A	374	LYS
1	A	389	SER
1	A	429	THR
1	A	444	LEU
1	A	453	LYS
1	A	460	SER
1	A	461	ARG
1	B	21	PRO
1	B	71	SER
1	B	92	ASN
1	B	108	LYS
1	B	113	LEU
1	B	129	LYS
1	B	140	LEU
1	B	169	LEU
1	B	216	ARG
1	B	227	PHE
1	B	236	ARG
1	B	264	ARG
1	B	271	LEU
1	B	279	LEU
1	B	294	VAL
1	B	298	LEU
1	B	306	THR

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Mol	Chain	Res	Type
1	B	316	LEU
1	B	352	GLU
1	B	375	GLU
1	B	403	TYR
1	B	423	HIS
1	B	461	ARG
1	B	475	VAL
1	C	4	ARG
1	C	33	SER
1	C	35	GLU
1	C	71	SER
1	C	113	LEU
1	C	129	LYS
1	C	140	LEU
1	C	169	LEU
1	C	189	LEU
1	C	216	ARG
1	C	227	PHE
1	C	256	LYS
1	C	271	LEU
1	C	279	LEU
1	C	284	LEU
1	C	294	VAL
1	C	300	SER
1	C	304	CYS
1	C	316	LEU
1	C	328	ASP
1	C	353	LEU
1	C	391	LEU
1	C	456	ARG
1	C	461	ARG
1	C	479	ARG
1	C	487	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	92	ASN
1	A	124	HIS
1	A	148	ASN
1	A	222	ASN

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Mol	Chain	Res	Type
1	A	232	HIS
1	A	234	ASN
1	A	238	HIS
1	A	313	HIS
1	A	334	GLN
1	A	399	GLN
1	A	423	HIS
1	B	80	GLN
1	B	148	ASN
1	B	232	HIS
1	B	238	HIS
1	B	251	GLN
1	B	307	GLN
1	B	313	HIS
1	B	423	HIS
1	B	478	HIS
1	C	60	GLN
1	C	66	GLN
1	C	124	HIS
1	C	148	ASN
1	C	232	HIS
1	C	238	HIS
1	C	251	GLN
1	C	313	HIS
1	C	423	HIS
1	C	478	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 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	SVR	C	516	-	25,27,93	1.20	2 (8%)	38,44,145	1.00	0
2	SO4	A	518	-	4,4,4	0.25	0	6,6,6	0.15	0
3	SVR	B	516	-	25,27,93	1.10	0	38,44,145	1.19	4 (10%)
2	SO4	C	519	-	4,4,4	0.46	0	6,6,6	0.16	0
2	SO4	C	518	-	4,4,4	0.32	0	6,6,6	0.49	0
2	SO4	C	520	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SVR	C	517	-	56,58,93	2.96	14 (25%)	82,88,145	1.58	11 (13%)
2	SO4	A	517	-	4,4,4	0.22	0	6,6,6	0.18	0
2	SO4	A	516	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	B	517	-	4,4,4	0.26	0	6,6,6	0.17	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
3	SVR	C	516	-	-	0/22/22/76	0/2/2/8
3	SVR	C	517	-	-	17/46/46/76	0/5/5/8
3	SVR	B	516	-	-	0/22/22/76	0/2/2/8

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	517	SVR	O54-C51	15.99	1.53	1.24
3	C	517	SVR	C27-C20	-7.70	1.36	1.51
3	C	517	SVR	C49-C51	-6.65	1.40	1.50
3	C	517	SVR	C5-C2	-4.98	1.39	1.50
3	C	517	SVR	C33-C26	-4.20	1.41	1.50
3	C	517	SVR	C39-N41	-3.10	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	517	SVR	C46-N44	-3.06	1.35	1.41
3	C	517	SVR	C3-N1	-2.77	1.33	1.41
3	C	517	SVR	C13-N19	-2.40	1.37	1.41
3	C	516	SVR	C58-C61	2.18	1.55	1.50
3	C	517	SVR	O28-S21	2.17	1.54	1.43
3	C	517	SVR	O29-S21	2.13	1.54	1.43
3	C	516	SVR	C65-N63	-2.08	1.35	1.41
3	C	517	SVR	O24-S17	2.05	1.53	1.43
3	C	517	SVR	O36-S31	2.05	1.53	1.43
3	C	517	SVR	O35-S31	2.02	1.53	1.43

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	517	SVR	C3-N1-C2	-5.71	110.40	128.32
3	C	517	SVR	C14-C20-C13	5.52	122.67	117.50
3	C	517	SVR	N44-C43-N41	4.71	121.55	112.44
3	C	517	SVR	O45-C43-N41	-3.21	117.94	123.64
3	C	517	SVR	C46-N44-C43	-3.02	120.44	126.61
3	C	517	SVR	C49-C51-N53	2.64	120.99	117.74
3	B	516	SVR	C72-C76-S83	2.52	124.13	119.89
3	B	516	SVR	C67-C65-N63	-2.36	116.91	123.50
3	B	516	SVR	C66-C65-N63	2.35	123.72	120.33
3	C	517	SVR	O54-C51-N53	-2.33	119.24	122.62
3	B	516	SVR	C74-C69-S73	-2.33	111.65	118.42
3	C	517	SVR	C7-C12-C15	-2.30	118.86	121.66
3	C	517	SVR	O34-S31-C22	2.29	112.56	106.64
3	C	517	SVR	C15-C10-C6	2.20	121.81	118.16
3	C	517	SVR	C11-C6-C10	2.07	117.92	116.78

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	517	SVR	N44-C43-N41-C39
3	C	517	SVR	O45-C43-N41-C39
3	C	517	SVR	C7-C3-N1-C2
3	C	517	SVR	N19-C26-C33-C37
3	C	517	SVR	C6-C11-S17-O23
3	C	517	SVR	C6-C11-S17-O24
3	C	517	SVR	C10-C15-S21-O28
3	C	517	SVR	C10-C15-S21-O29

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Mol	Chain	Res	Type	Atoms
3	C	517	SVR	O32-C26-C33-C37
3	C	517	SVR	N19-C26-C33-C38
3	C	517	SVR	O32-C26-C33-C38
3	C	517	SVR	O4-C2-C5-C8
3	C	517	SVR	N1-C2-C5-C8
3	C	517	SVR	O4-C2-C5-C9
3	C	517	SVR	N1-C2-C5-C9
3	C	517	SVR	C6-C3-N1-C2
3	C	517	SVR	C20-C13-N19-C26

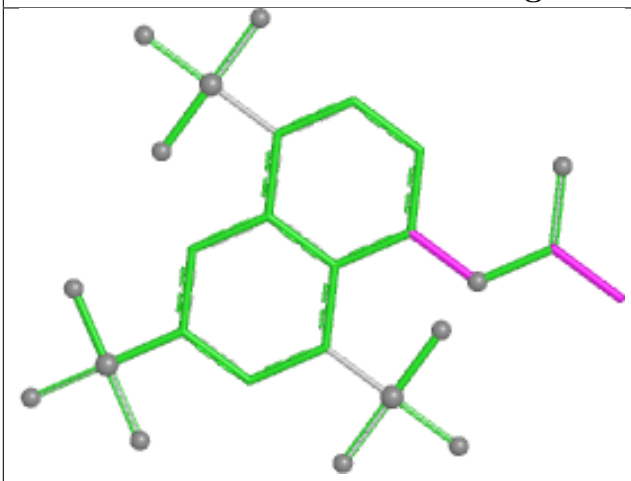
There are no ring outliers.

3 monomers are involved in 19 short contacts:

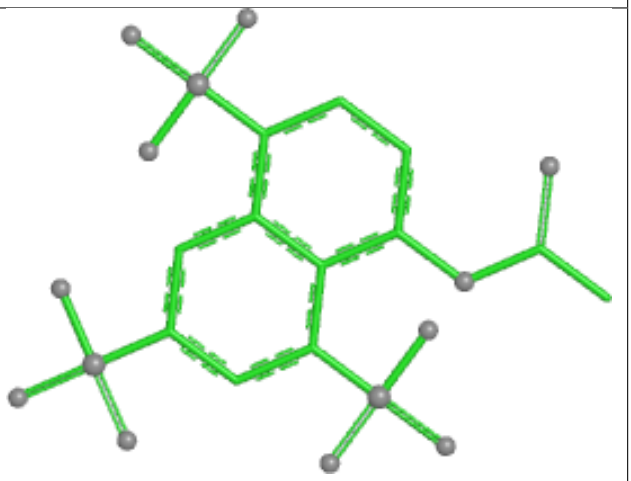
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	516	SVR	3	0
3	B	516	SVR	2	0
3	C	517	SVR	14	0

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.

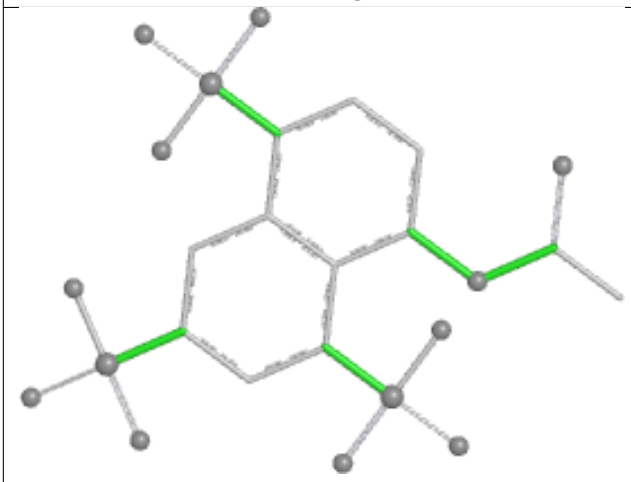
Ligand SVR C 516



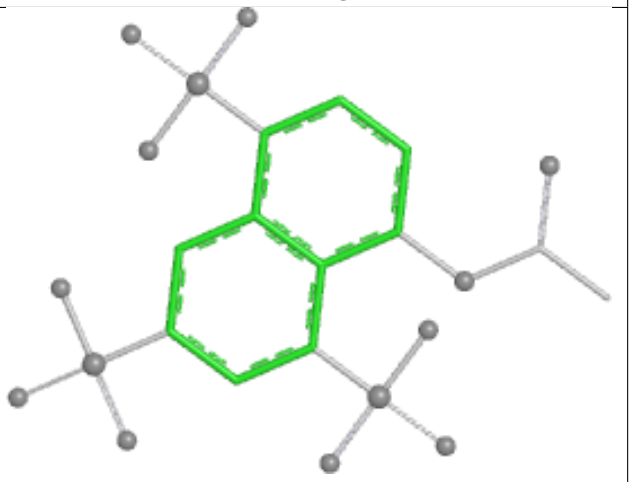
Bond lengths



Bond angles

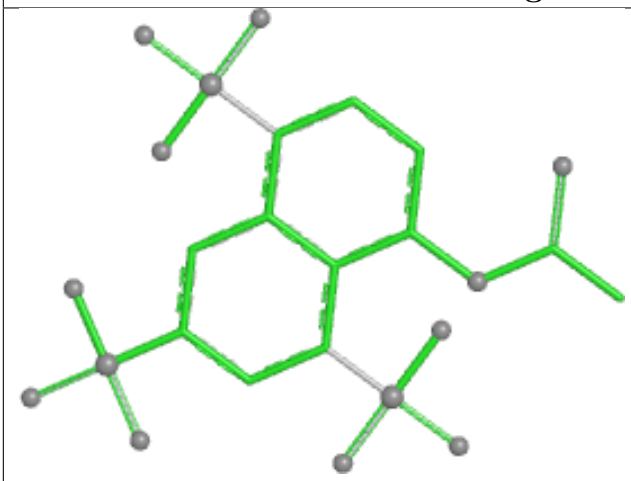


Torsions

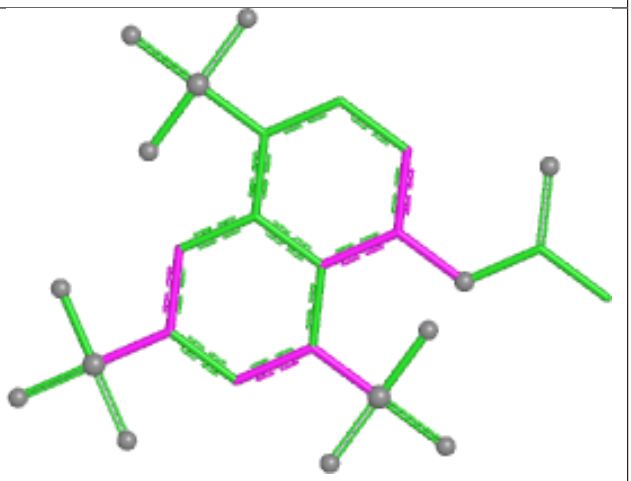


Rings

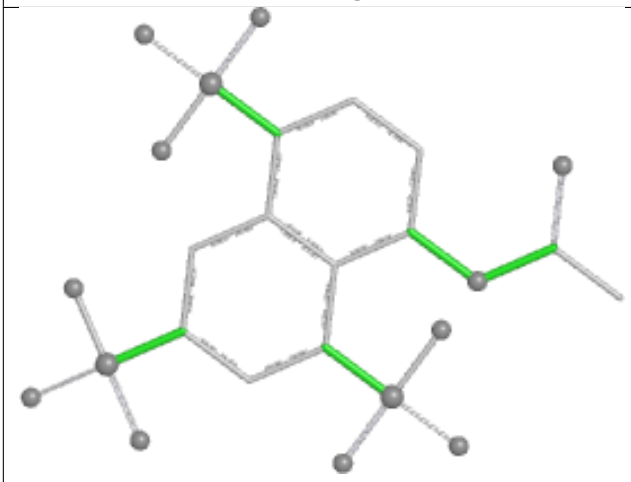
Ligand SVR B 516



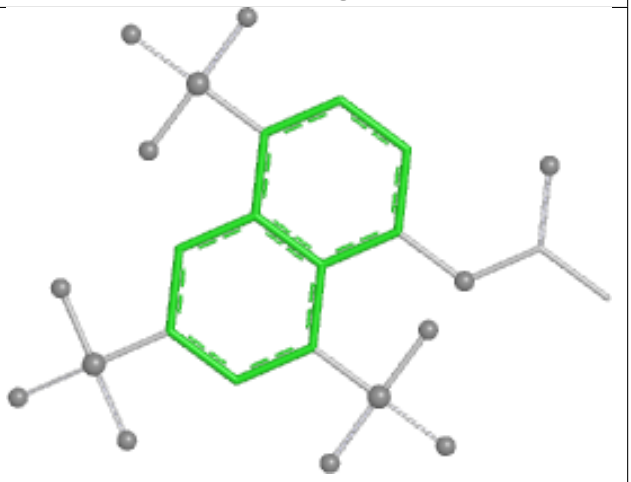
Bond lengths



Bond angles

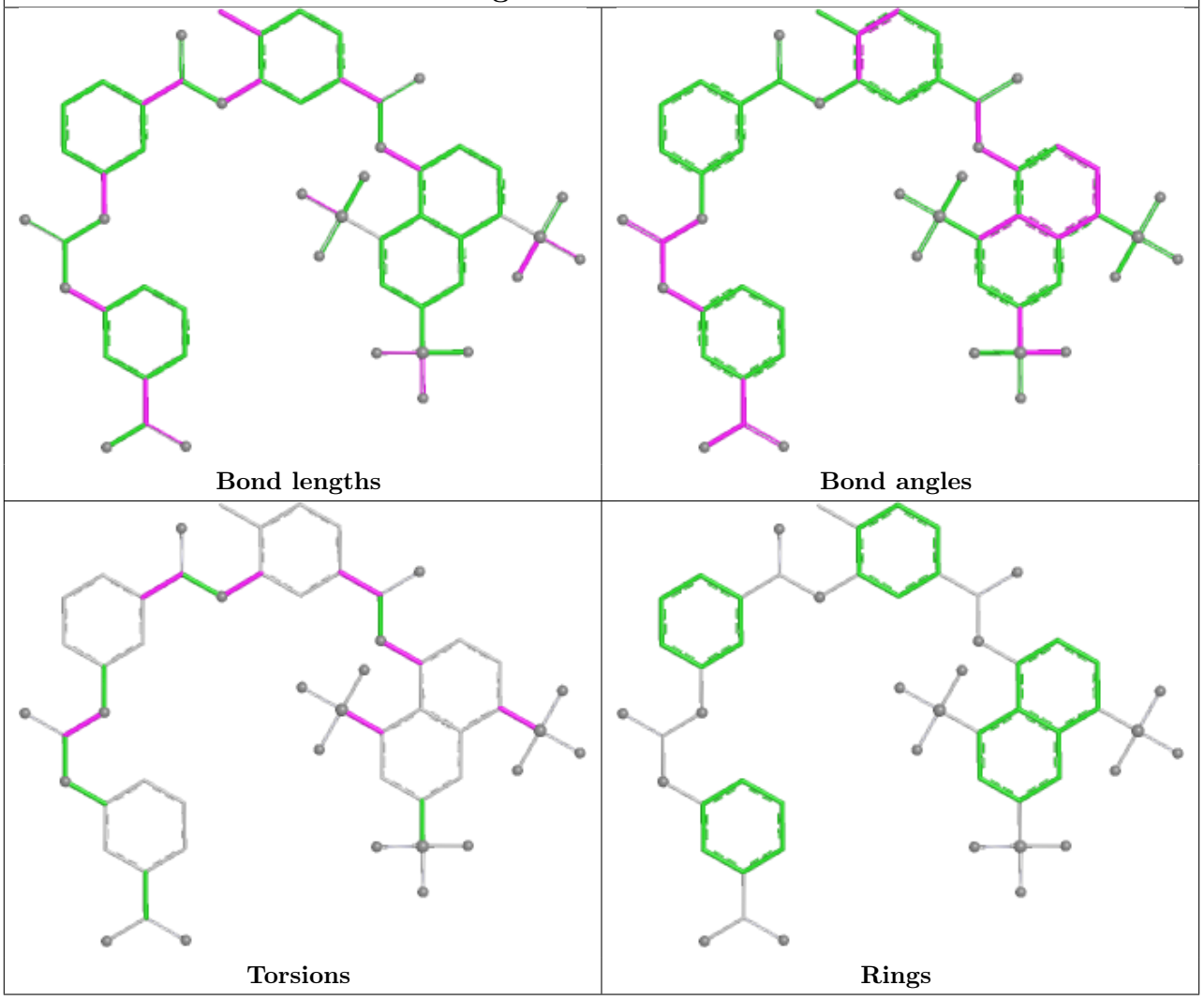


Torsions



Rings

Ligand SVR C 517



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	475/515 (92%)	0.13	30 (6%)	20	16	30, 50, 105, 124	7 (1%)
1	B	476/515 (92%)	0.17	26 (5%)	25	22	36, 58, 102, 124	7 (1%)
1	C	474/515 (92%)	-0.06	9 (1%)	66	64	25, 44, 83, 120	7 (1%)
All	All	1425/1545 (92%)	0.08	65 (4%)	32	30	25, 51, 99, 124	21 (1%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	454	TYR	6.6
1	A	481	VAL	6.6
1	A	474	VAL	5.8
1	B	378	PRO	5.7
1	A	39	PRO	5.7
1	B	479	ARG	5.4
1	A	476	PRO	5.4
1	A	475	VAL	5.2
1	B	2	LEU	5.0
1	A	478	HIS	4.8
1	A	480	SER	4.8
1	B	303	PRO	4.7
1	A	484	TRP	4.6
1	A	444	LEU	4.3
1	A	455	TYR	4.3
1	B	103	PRO	4.2
1	B	464	LYS	4.1
1	B	484	TRP	4.1
1	A	443	LEU	3.9
1	C	302	CYS	3.8
1	A	479	ARG	3.8
1	A	477	ARG	3.7
1	B	455	TYR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	379	LEU	3.7
1	B	474	VAL	3.6
1	C	466	ALA	3.6
1	B	3	PRO	3.5
1	B	463	SER	3.5
1	B	488	GLY	3.5
1	B	456	ARG	3.4
1	A	452	GLU	3.3
1	B	475	VAL	3.2
1	C	456	ARG	3.2
1	C	464	LYS	3.2
1	C	475	VAL	3.1
1	A	438	SER	3.1
1	A	459	ALA	3.1
1	B	478	HIS	3.0
1	A	437	PRO	3.0
1	B	476	PRO	3.0
1	B	452	GLU	2.9
1	A	378	PRO	2.9
1	C	467	ALA	2.9
1	B	454	TYR	2.9
1	C	372	ALA	2.8
1	A	433	HIS	2.7
1	A	483	ARG	2.7
1	A	302	CYS	2.7
1	A	458	VAL	2.6
1	A	457	THR	2.5
1	A	488	GLY	2.5
1	B	108	LYS	2.4
1	A	464	LYS	2.3
1	B	465	GLU	2.3
1	B	432	GLY	2.3
1	C	462	VAL	2.2
1	A	441	MET	2.2
1	B	438	SER	2.2
1	B	4	ARG	2.1
1	B	462	VAL	2.1
1	B	54	VAL	2.1
1	A	439	GLN	2.1
1	A	54	VAL	2.0
1	C	452	GLU	2.0
1	B	373	ASP	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)

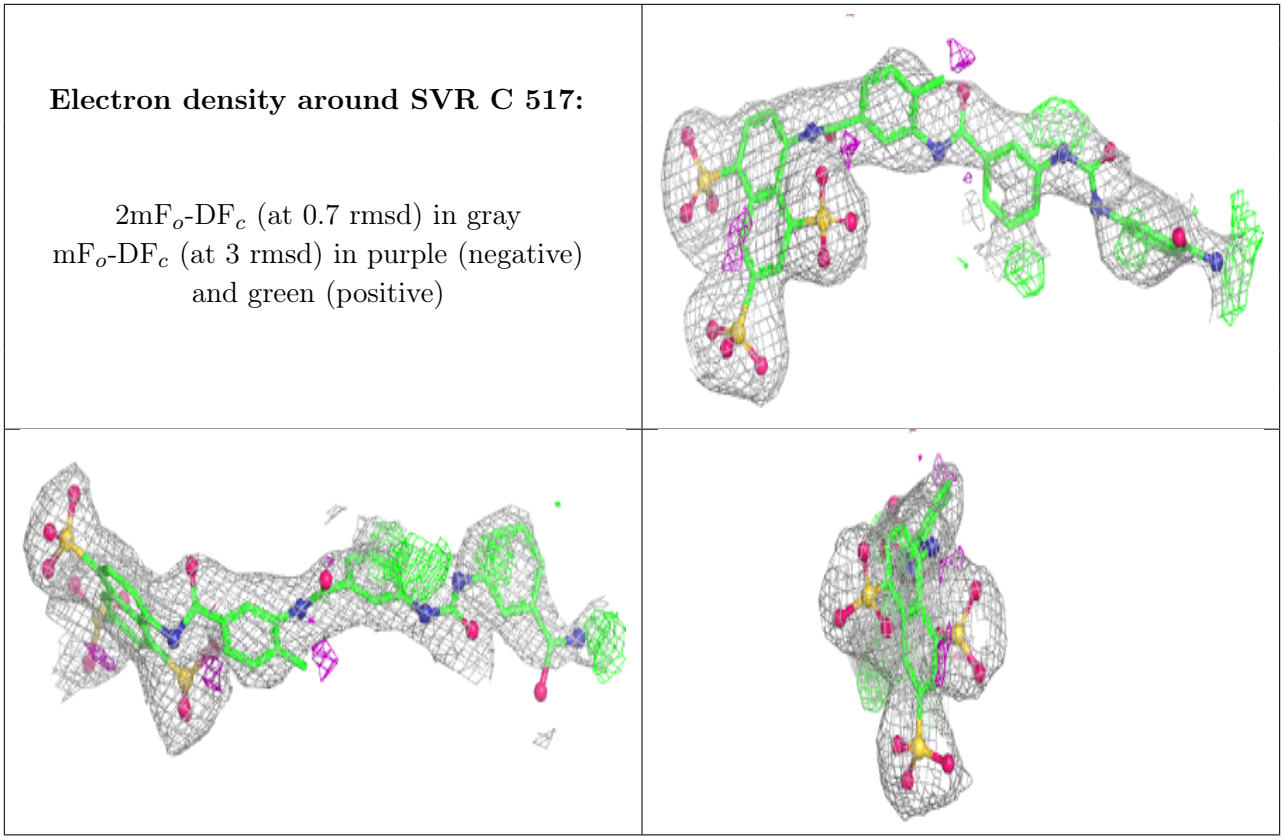
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	SO4	A	517	5/5	0.84	0.18	155,155,155,156	0
3	SVR	C	517	54/86	0.85	0.23	87,95,127,130	0
2	SO4	A	516	5/5	0.86	0.20	112,115,116,116	0
2	SO4	B	517	5/5	0.87	0.18	133,134,135,135	0
3	SVR	B	516	26/86	0.90	0.20	112,121,130,131	0
2	SO4	A	518	5/5	0.94	0.22	124,124,125,127	0
3	SVR	C	516	26/86	0.94	0.19	82,96,102,104	0
2	SO4	C	519	5/5	0.94	0.14	92,94,97,98	0
2	SO4	C	520	5/5	0.95	0.12	93,94,96,96	0
2	SO4	C	518	5/5	0.98	0.12	72,79,86,88	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.

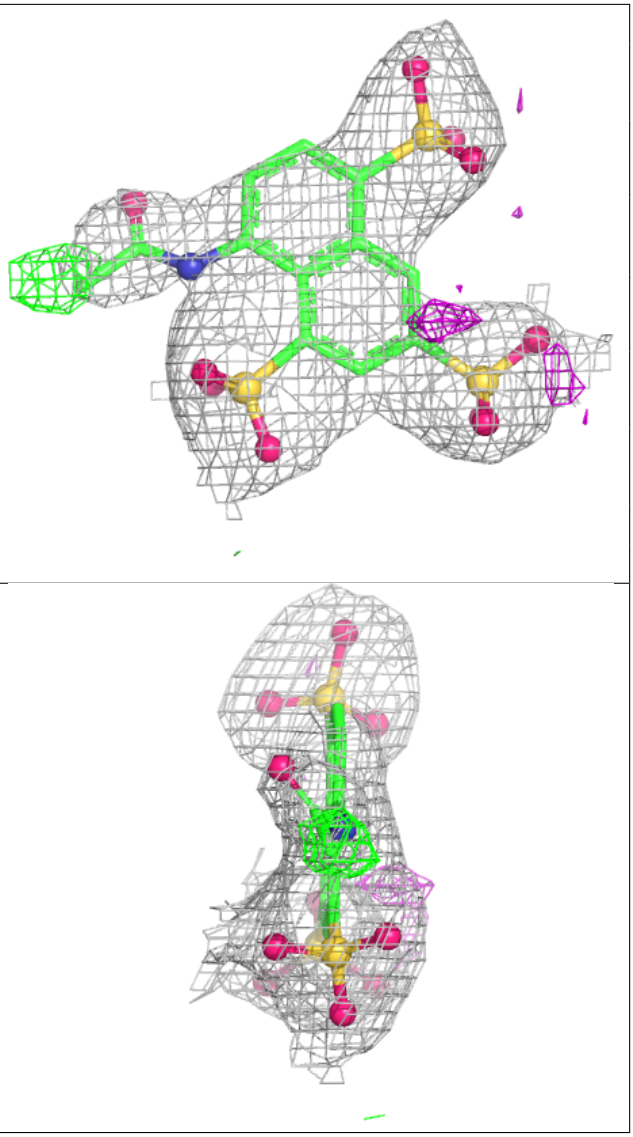
Electron density around SVR C 517:

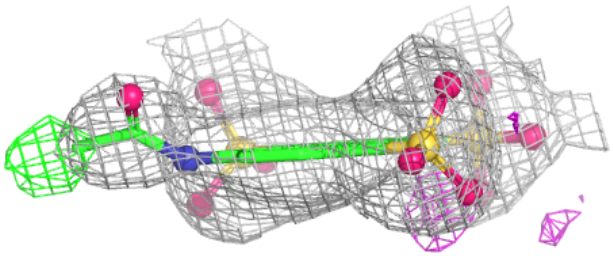
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SVR B 516:

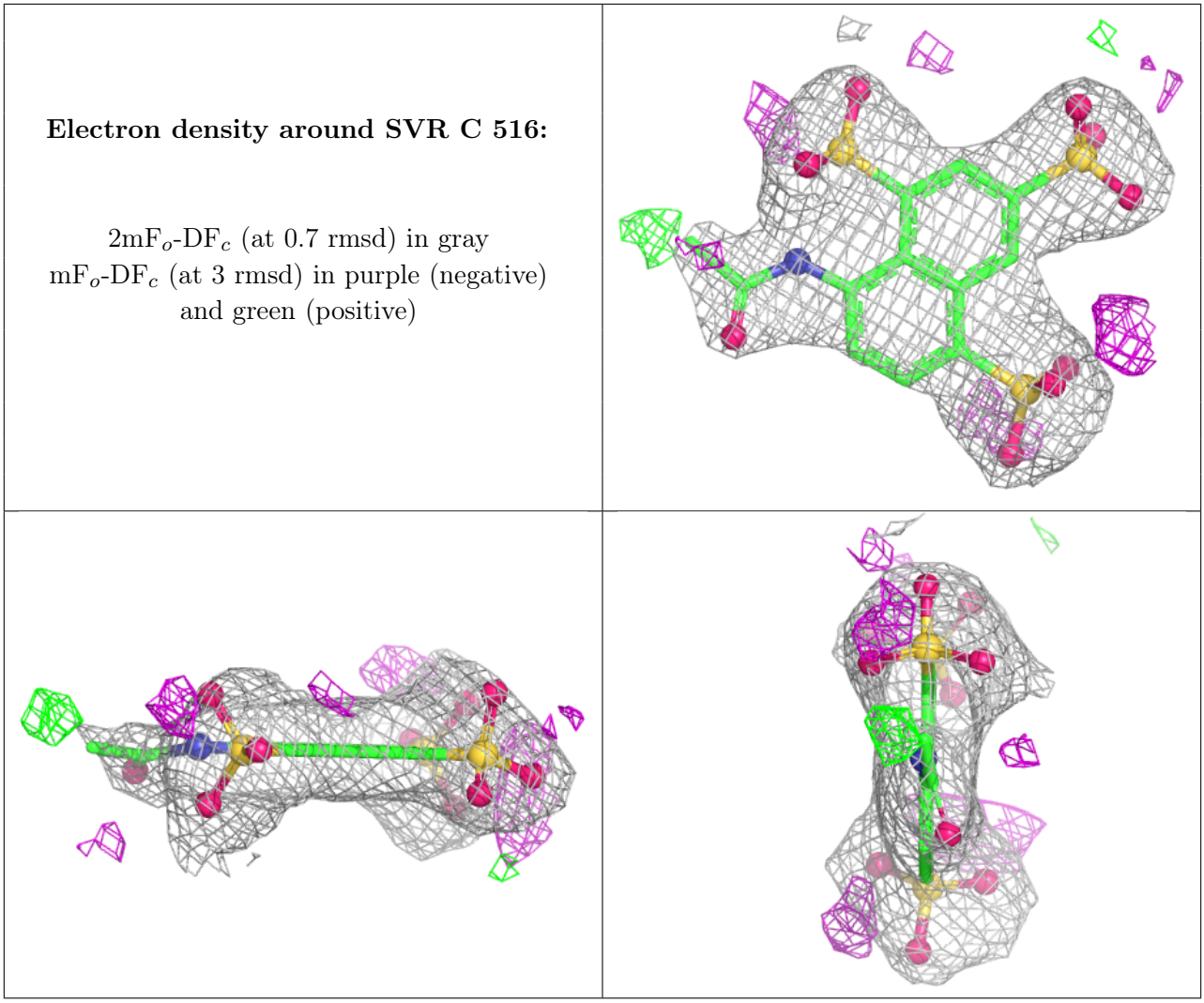
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





Electron density around SVR C 516:

$2mF_o$-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.