



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 17, 2024 – 10:58 PM EST

PDB ID : 3UPF
Title : Crystal structure of murine norovirus RNA-dependent RNA polymerase bound to NF023
Authors : Milani, M.; Mastrangelo, E.; Bolognesi, M.
Deposited on : 2011-11-18
Resolution : 2.60 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

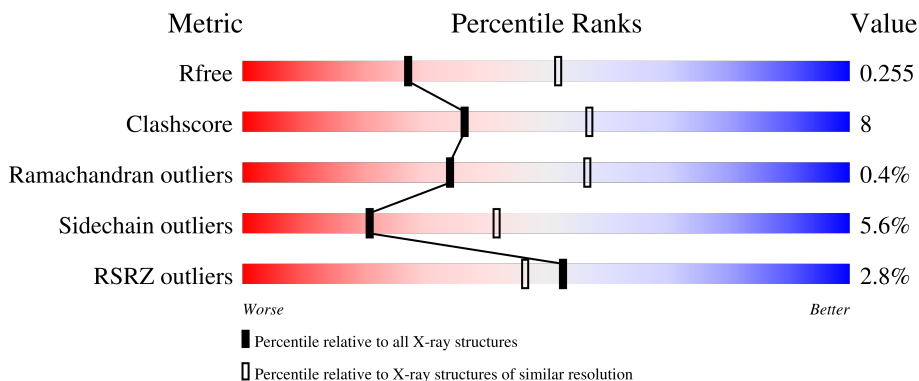
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	525	 3% 74% 15% • 9%
1	B	525	 2% 75% 16% • 8%
1	C	525	 2% 74% 14% • 10%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12242 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
			Total	C	N	O	S			
1	A	476	3801	2408	670	699	24	0	1	0
1	B	483	3833	2423	676	710	24	0	0	0
1	C	471	3750	2373	658	696	23	0	0	0

There are 33 discrepancies between the modelled and reference sequences:

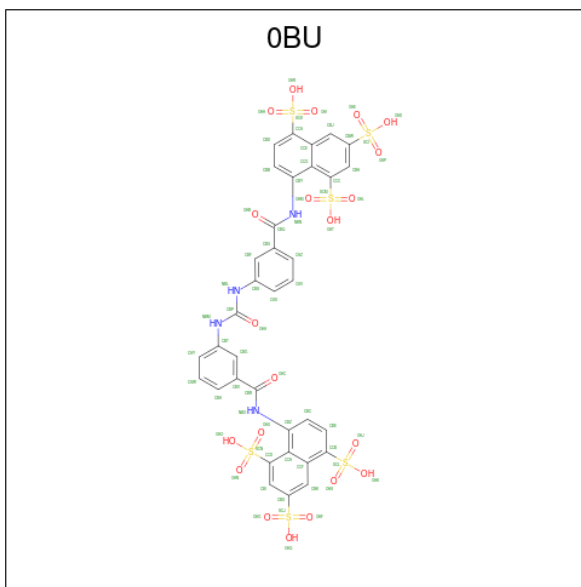
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	expression tag	UNP Q80J95
A	-8	LYS	-	expression tag	UNP Q80J95
A	-7	ALA	-	expression tag	UNP Q80J95
A	508	LEU	-	expression tag	UNP Q80J95
A	509	GLU	-	expression tag	UNP Q80J95
A	510	HIS	-	expression tag	UNP Q80J95
A	511	HIS	-	expression tag	UNP 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	-9	MET	-	expression tag	UNP Q80J95
B	-8	LYS	-	expression tag	UNP Q80J95
B	-7	ALA	-	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	-9	MET	-	expression tag	UNP Q80J95

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	LYS	-	expression tag	UNP Q80J95
C	-7	ALA	-	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
C	515	HIS	-	expression tag	UNP Q80J95

- Molecule 2 is 8-((3-((3-((4,6,8-trisulfonaphthalen-1-yl)carbamoyl]phenyl)carbamoyl)amino]benzoyl)amino)naphthalene-1,3,5-trisulfonic acid (three-letter code: 0BU) (formula: $C_{35}H_{26}N_4O_{21}S_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	N	O	S			
2	A	1	Total	66	35	4	21	6	0	0
2	B	1	Total	66	35	4	21	6	0	0
2	C	1	Total	66	35	4	21	6	0	0

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



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

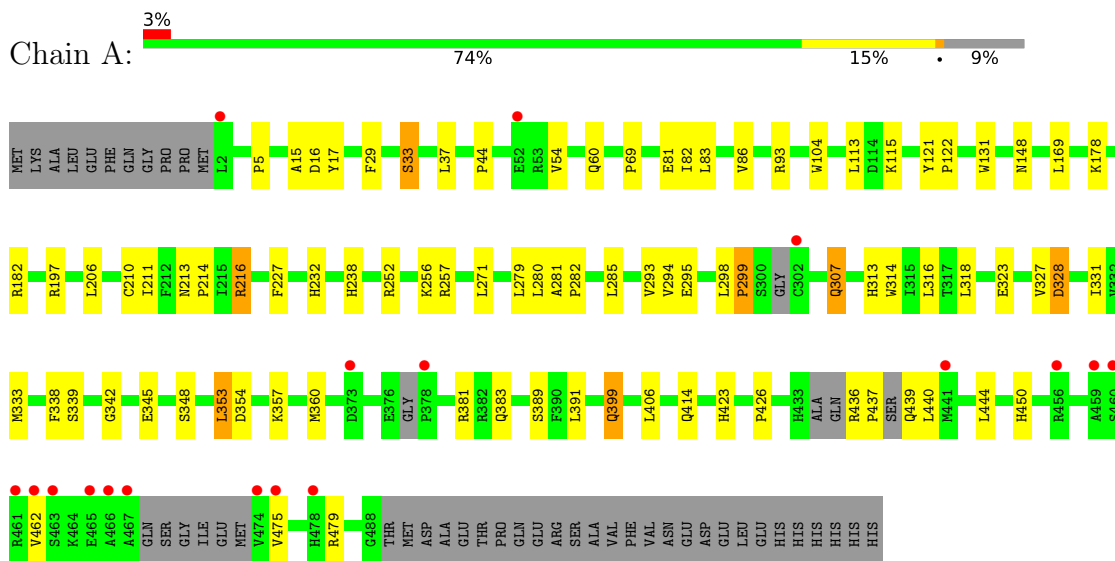
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	195	Total	O	0	0
			195	195		
4	B	182	Total	O	0	0
			182	182		
4	C	248	Total	O	0	0
			248	248		

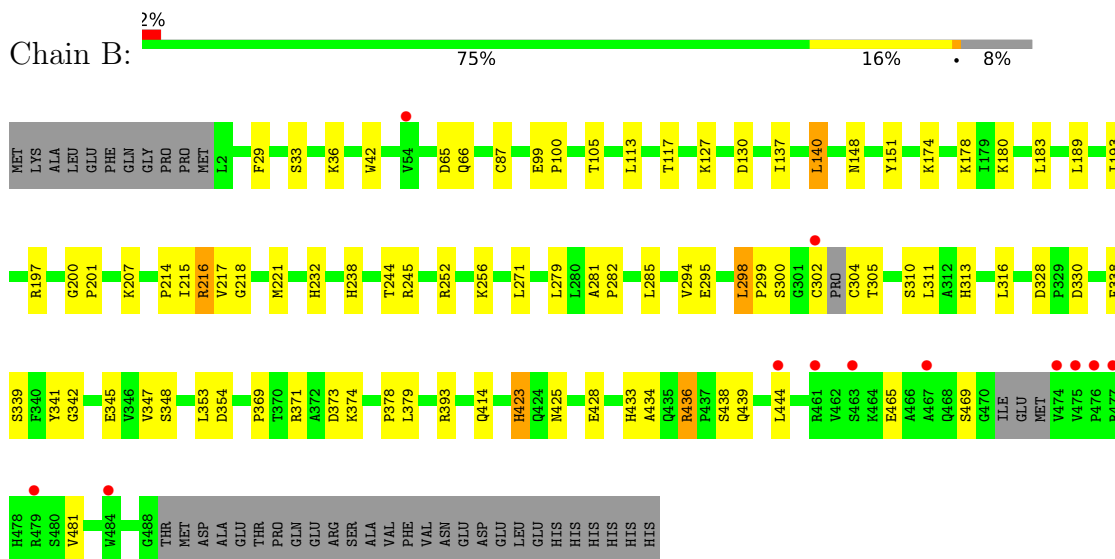
3 Residue-property plots i

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.

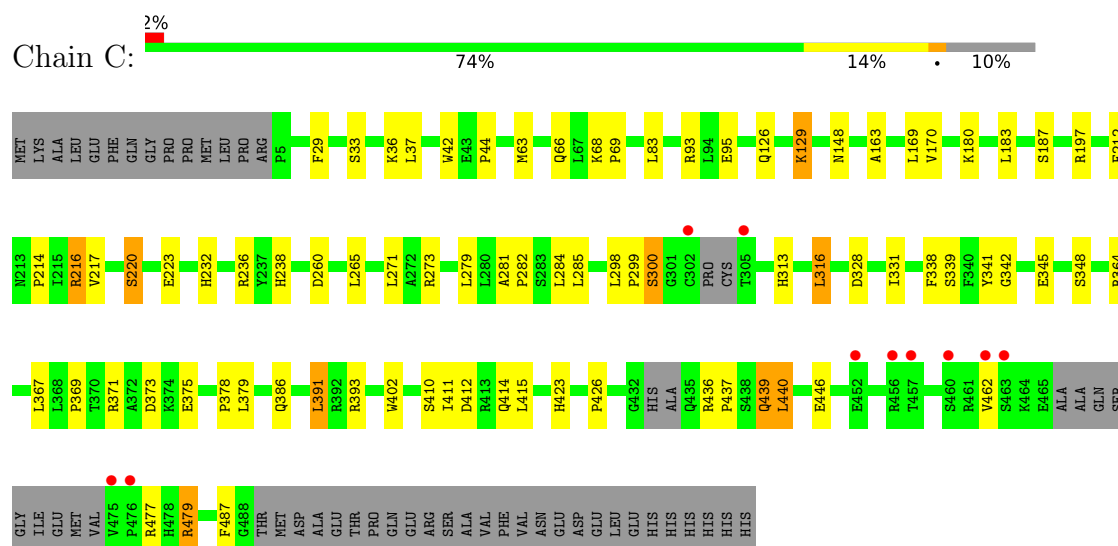
- Molecule 1: RNA-dependent RNA polymerase



- Molecule 1: RNA-dependent RNA polymerase



- Molecule 1: RNA-dependent RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	120.86Å 195.95Å 109.24Å 90.00° 114.38° 90.00°	Depositor
Resolution (Å)	45.00 – 2.60 45.02 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.00-2.60) 100.0 (45.02-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.199 , 0.261 0.197 , 0.255	Depositor DCC
R_{free} test set	3578 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtrriage
Anisotropy	0.108	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12242	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, OBU

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	0.48	0/3895	0.62	0/5271
1	B	0.49	0/3926	0.63	0/5317
1	C	0.51	0/3840	0.64	0/5197
All	All	0.49	0/11661	0.63	0/15785

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3801	0	3767	51	0
1	B	3833	0	3789	49	0
1	C	3750	0	3706	51	0
2	A	66	0	26	15	0
2	B	66	0	26	15	0
2	C	66	0	26	9	0
3	A	5	0	0	0	0
3	B	10	0	0	1	0
3	C	20	0	0	0	0
4	A	195	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	182	0	0	2	0
4	C	248	0	0	4	0
All	All	12242	0	11340	180	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 (180) 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:600:0BU:OAN	2:A:600:0BU:CBR	1.68	1.40
2:A:600:0BU:OAN	2:A:600:0BU:CBV	2.02	1.07
2:A:600:0BU:OAN	2:A:600:0BU:NBO	1.88	1.06
1:B:238:HIS:HD2	1:B:348:SER:OG	1.54	0.90
1:A:81:GLU:HB2	4:A:599:HOH:O	1.71	0.89
1:C:148:ASN:HD21	1:C:197:ARG:HH11	1.23	0.86
2:B:600:0BU:CBR	2:B:600:0BU:OAN	2.24	0.85
2:B:600:0BU:NBO	2:B:600:0BU:SCN	2.48	0.85
1:B:148:ASN:HD21	1:B:197:ARG:HH11	1.24	0.85
2:A:600:0BU:OAI	2:A:600:0BU:HBJ	1.77	0.82
2:A:600:0BU:NBO	2:A:600:0BU:SCN	2.55	0.80
1:C:479:ARG:H	1:C:479:ARG:CD	1.96	0.78
1:A:314:TRP:HZ2	1:A:333:MET:HE1	1.51	0.75
1:C:313:HIS:HD2	1:C:342:GLY:O	1.71	0.74
2:A:600:0BU:NBN	2:A:600:0BU:SCM	2.62	0.72
1:B:87:CYS:HB3	4:B:587:HOH:O	1.90	0.70
1:A:437:PRO:HB3	1:A:439:GLN:N	2.07	0.70
1:A:93:ARG:HE	1:A:213:ASN:HD22	1.39	0.69
1:B:433:HIS:ND1	1:B:469:SER:HA	2.09	0.68
1:A:211:ILE:HA	1:A:216[A]:ARG:HH21	1.60	0.67
1:A:232:HIS:HD2	1:A:348:SER:OG	1.77	0.67
1:A:210:CYS:SG	4:A:700:HOH:O	2.53	0.67
1:A:437:PRO:HG3	1:A:440:LEU:HB3	1.76	0.66
2:B:600:0BU:NBO	2:B:600:0BU:OAO	2.27	0.66
1:A:206:LEU:HD23	1:A:307:GLN:HG2	1.79	0.65
1:C:180:LYS:HD3	2:C:600:0BU:HBF	1.79	0.65
1:C:238:HIS:HD2	1:C:348:SER:OG	1.80	0.65
1:A:29:PHE:O	1:A:423:HIS:HE1	1.80	0.64
1:A:232:HIS:HE1	1:A:339:SER:OG	1.80	0.64
1:C:148:ASN:ND2	1:C:197:ARG:HH11	1.93	0.62
1:B:313:HIS:HD2	1:B:342:GLY:O	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:600:0BU:OAA	2:A:600:0BU:HAY	1.98	0.62
1:C:440:LEU:HG	1:C:462:VAL:HG13	1.82	0.62
1:B:244:THR:HG22	1:B:245:ARG:HG3	1.82	0.61
2:B:600:0BU:OAN	2:B:600:0BU:NBO	2.32	0.61
1:A:15:ALA:HB2	1:A:293:VAL:HG23	1.83	0.61
1:A:33:SER:HB3	4:A:553:HOH:O	2.00	0.61
1:C:313:HIS:HE1	1:C:345:GLU:OE2	1.84	0.61
1:B:221:MET:HG2	1:B:393:ARG:HG3	1.83	0.60
1:B:65:ASP:HB3	2:B:600:0BU:HBB	1.84	0.60
1:B:238:HIS:CD2	1:B:348:SER:OG	2.46	0.60
1:C:29:PHE:O	1:C:423:HIS:HE1	1.84	0.60
1:C:148:ASN:HD21	1:C:197:ARG:NH1	1.97	0.59
1:B:313:HIS:HE1	1:B:345:GLU:OE2	1.86	0.59
2:B:600:0BU:OAN	2:B:600:0BU:CBV	2.50	0.59
1:C:386:GLN:HG2	1:C:402:TRP:HZ3	1.68	0.58
1:B:216:ARG:HD3	1:B:339:SER:OG	2.03	0.57
2:A:600:0BU:OAB	2:A:600:0BU:CBB	2.50	0.57
1:C:300:SER:HB2	4:C:681:HOH:O	2.05	0.57
1:C:216:ARG:HD3	1:C:339:SER:OG	2.04	0.57
1:B:338:PHE:CE1	1:B:347:VAL:HG13	2.41	0.56
1:A:444:LEU:HD21	1:A:475:VAL:HG23	1.88	0.56
1:B:29:PHE:O	1:B:423:HIS:HE1	1.87	0.56
1:C:95:GLU:HG3	1:C:265:LEU:HD21	1.87	0.56
1:C:479:ARG:H	1:C:479:ARG:HD3	1.68	0.56
1:A:436:ARG:N	1:A:437:PRO:CD	2.69	0.55
1:A:256:LYS:HG3	1:A:280:LEU:HD13	1.88	0.55
1:C:479:ARG:H	1:C:479:ARG:HD2	1.72	0.55
1:B:252:ARG:HG3	1:B:295:GLU:O	2.07	0.54
2:B:600:0BU:OAT	2:B:600:0BU:HAZ	2.09	0.53
2:A:600:0BU:OAN	2:A:600:0BU:CBG	2.56	0.53
1:A:414:GLN:O	1:A:436:ARG:NH2	2.43	0.52
1:B:65:ASP:HB3	2:B:600:0BU:CBB	2.38	0.52
1:B:178:LYS:HG2	1:B:180:LYS:HE3	1.90	0.52
1:A:313:HIS:HD2	1:A:342:GLY:O	1.92	0.52
2:B:600:0BU:CBB	2:B:600:0BU:OAB	2.57	0.52
1:A:44:PRO:HG2	1:A:426:PRO:HB3	1.92	0.52
1:A:399:GLN:NE2	1:A:399:GLN:H	2.08	0.52
1:A:93:ARG:HE	1:A:213:ASN:ND2	2.05	0.52
1:A:5:PRO:HD2	1:A:16:ASP:HA	1.93	0.51
2:A:600:0BU:OAA	2:A:600:0BU:CAY	2.58	0.51
2:A:600:0BU:OAB	2:A:600:0BU:HBB	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:214:PRO:HB3	1:C:338:PHE:HB2	1.92	0.51
1:C:313:HIS:CD2	1:C:342:GLY:O	2.58	0.51
1:C:328:ASP:HB3	1:C:331:ILE:HG12	1.92	0.51
1:A:436:ARG:N	1:A:437:PRO:HD3	2.26	0.51
2:B:600:0BU:OAN	2:B:600:0BU:CBG	2.58	0.51
1:B:214:PRO:HB3	1:B:338:PHE:HB2	1.92	0.51
1:A:328:ASP:HB2	1:A:331:ILE:HG12	1.92	0.51
1:B:232:HIS:HE1	1:B:339:SER:OG	1.93	0.51
1:A:115:LYS:HE2	1:A:131:TRP:CD2	2.46	0.51
1:B:66:GLN:HE21	1:B:183:LEU:H	1.58	0.51
1:A:354:ASP:OD2	1:A:357:LYS:HD2	2.10	0.51
1:B:244:THR:HA	3:B:517:SO4:O3	2.11	0.51
1:A:339:SER:O	1:A:345:GLU:HA	2.11	0.50
1:C:232:HIS:HE1	1:C:339:SER:OG	1.93	0.50
1:A:327:VAL:HG12	1:A:331:ILE:HB	1.93	0.50
1:A:238:HIS:HD2	1:A:348:SER:OG	1.94	0.50
1:C:170:VAL:HG12	2:C:600:0BU:HBA	1.94	0.50
2:C:600:0BU:NBO	2:C:600:0BU:SCN	2.84	0.50
1:B:302:CYS:HB2	1:B:305:THR:H	1.76	0.50
1:C:63:MET:CE	1:C:163:ALA:HB1	2.42	0.50
1:A:182:ARG:NH1	2:A:600:0BU:CBR	2.75	0.50
1:A:281:ALA:O	1:A:282:PRO:C	2.49	0.50
1:A:298:LEU:HD22	1:A:299:PRO:HD2	1.93	0.50
2:C:600:0BU:NBO	2:C:600:0BU:OAO	2.45	0.50
1:A:182:ARG:NH1	2:A:600:0BU:OAC	2.45	0.49
1:C:93:ARG:NH2	1:C:212:PHE:O	2.31	0.49
1:C:414:GLN:OE1	1:C:439:GLN:NE2	2.46	0.49
1:B:302:CYS:C	1:B:304:CYS:SG	2.91	0.49
1:C:214:PRO:O	1:C:216:ARG:HD2	2.13	0.49
1:B:369:PRO:HB2	1:B:379:LEU:HD21	1.94	0.49
1:C:386:GLN:HG2	1:C:402:TRP:CZ3	2.47	0.49
1:C:479:ARG:CD	1:C:479:ARG:N	2.71	0.49
1:C:217:VAL:HB	4:C:584:HOH:O	2.12	0.49
1:C:220:SER:OG	1:C:223:GLU:HG2	2.13	0.48
1:B:414:GLN:O	1:B:436:ARG:NH2	2.39	0.48
2:B:600:0BU:OAI	2:B:600:0BU:HBJ	2.12	0.48
1:C:44:PRO:HG2	1:C:426:PRO:HB3	1.96	0.48
1:A:257:ARG:HD3	4:A:630:HOH:O	2.14	0.48
1:C:411:ILE:HD11	1:C:446:GLU:HB3	1.96	0.48
1:A:314:TRP:CZ2	1:A:333:MET:HE1	2.39	0.47
1:A:86:VAL:HG13	1:A:318:LEU:HD23	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:HD21	1:A:197:ARG:HH11	1.60	0.47
1:C:373:ASP:OD2	1:C:375:GLU:HB2	2.14	0.47
1:A:313:HIS:HE1	1:A:345:GLU:OE2	1.98	0.47
1:C:29:PHE:HB2	1:C:44:PRO:HG3	1.97	0.47
1:B:117:THR:OG1	1:B:127:LYS:NZ	2.48	0.47
1:C:281:ALA:O	1:C:282:PRO:C	2.54	0.46
1:B:425:ASN:ND2	1:B:428:GLU:HG3	2.30	0.46
2:B:600:0BU:OAT	2:B:600:0BU:CAZ	2.62	0.46
1:C:364:ARG:HD2	4:C:639:HOH:O	2.15	0.46
1:B:338:PHE:HE1	1:B:347:VAL:HG13	1.78	0.46
1:B:252:ARG:NH2	1:B:299:PRO:HG3	2.31	0.46
1:B:371:ARG:NH1	1:B:378:PRO:O	2.40	0.46
2:C:600:0BU:OAK	2:C:600:0BU:HBK	2.16	0.46
1:A:406:LEU:O	1:A:450:HIS:HE1	1.99	0.46
1:C:236:ARG:HD3	4:C:636:HOH:O	2.15	0.46
1:B:339:SER:O	1:B:345:GLU:HA	2.16	0.45
1:C:313:HIS:CE1	1:C:345:GLU:OE2	2.66	0.45
1:A:82:ILE:HD13	1:A:323:GLU:HG3	1.98	0.45
1:B:373:ASP:O	1:B:374:LYS:HB2	2.17	0.45
1:A:353:LEU:O	1:A:381:ARG:NH1	2.50	0.45
1:C:341:TYR:CD1	1:C:391:LEU:HD11	2.52	0.45
1:B:130:ASP:HB3	1:B:137:ILE:O	2.18	0.44
1:B:151:TYR:CE2	1:B:271:LEU:HD23	2.52	0.44
1:B:207:LYS:HG3	1:B:218:GLY:HA3	1.98	0.44
1:B:189:LEU:O	1:B:193:ILE:HG12	2.17	0.44
1:C:68:LYS:N	1:C:69:PRO:HD2	2.33	0.44
2:A:600:0BU:NBN	2:A:600:0BU:OAT	2.29	0.43
1:C:298:LEU:HA	1:C:299:PRO:HD2	1.87	0.43
1:C:126:GLN:O	1:C:129:LYS:HB2	2.18	0.43
1:C:339:SER:O	1:C:345:GLU:HA	2.19	0.43
1:A:60:GLN:NE2	1:A:60:GLN:H	2.17	0.43
1:B:215:ILE:HG12	1:B:310:SER:HB3	2.00	0.43
1:B:130:ASP:HB2	1:B:140:LEU:HD22	2.01	0.42
1:B:99:GLU:HA	1:B:100:PRO:HD3	1.89	0.42
1:C:238:HIS:CD2	1:C:348:SER:OG	2.65	0.42
2:C:600:0BU:OAB	2:C:600:0BU:CBB	2.66	0.42
2:C:600:0BU:NBN	2:C:600:0BU:SCM	2.92	0.42
1:B:298:LEU:HD22	1:B:299:PRO:HD2	2.00	0.42
1:A:121:TYR:HA	1:A:122:PRO:HA	1.70	0.42
1:C:369:PRO:HB2	1:C:379:LEU:HD11	2.00	0.42
1:B:215:ILE:HD11	1:B:311:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:PRO:HB3	1:A:338:PHE:HB2	2.02	0.42
1:B:140:LEU:HG	1:B:189:LEU:HD22	2.00	0.42
2:B:600:0BU:HBB	2:B:600:0BU:OAB	2.20	0.42
1:A:29:PHE:HB2	1:A:44:PRO:HG3	2.02	0.42
1:A:115:LYS:HE2	1:A:131:TRP:CE2	2.55	0.42
1:C:412:ASP:O	1:C:415:LEU:HB2	2.19	0.41
1:B:42:TRP:HH2	2:B:600:0BU:CBK	2.33	0.41
1:C:371:ARG:NH1	1:C:378:PRO:O	2.46	0.41
2:C:600:0BU:OAA	2:C:600:0BU:HAY	2.20	0.41
1:C:260:ASP:HA	1:C:273:ARG:HH22	1.86	0.41
1:A:16:ASP:OD1	1:A:17:TYR:N	2.50	0.41
1:A:69:PRO:HD3	2:A:600:0BU:OAT	2.21	0.41
1:C:66:GLN:HE21	1:C:183:LEU:H	1.67	0.41
1:B:105:THR:HB	4:B:742:HOH:O	2.21	0.41
1:A:252:ARG:NH2	4:A:701:HOH:O	2.41	0.41
1:B:354:ASP:C	1:B:354:ASP:OD1	2.59	0.41
1:C:42:TRP:HH2	2:C:600:0BU:CBK	2.34	0.41
1:B:217:VAL:HA	1:B:341:TYR:CE1	2.56	0.40
1:C:232:HIS:HD2	1:C:348:SER:OG	2.04	0.40
1:A:444:LEU:HD13	1:A:462:VAL:HG21	2.03	0.40
1:B:281:ALA:O	1:B:282:PRO:C	2.60	0.40
1:B:174:LYS:NZ	2:B:600:0BU:OAN	2.54	0.40
1:B:200:GLY:N	1:B:201:PRO:CD	2.83	0.40
1:B:214:PRO:CB	1:B:338:PHE:HB2	2.51	0.40
1:C:316:LEU:HG	1:C:367:LEU:HD11	2.02	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	465/525 (89%)	450 (97%)	14 (3%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	477/525 (91%)	456 (96%)	19 (4%)	2 (0%)	34	57
1	C	463/525 (88%)	451 (97%)	10 (2%)	2 (0%)	34	57
All	All	1405/1575 (89%)	1357 (97%)	43 (3%)	5 (0%)	34	57

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	434	ALA
1	C	300	SER
1	B	300	SER
1	C	437	PRO
1	A	299	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	409/449 (91%)	383 (94%)	26 (6%)	17	35
1	B	411/449 (92%)	390 (95%)	21 (5%)	24	46
1	C	403/449 (90%)	380 (94%)	23 (6%)	20	41
All	All	1223/1347 (91%)	1153 (94%)	70 (6%)	21	41

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

Mol	Chain	Res	Type
1	A	33	SER
1	A	37	LEU
1	A	54	VAL
1	A	83	LEU
1	A	104	TRP
1	A	113	LEU
1	A	169	LEU
1	A	178	LYS
1	A	216[A]	ARG

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Mol	Chain	Res	Type
1	A	216[B]	ARG
1	A	227	PHE
1	A	271	LEU
1	A	279	LEU
1	A	285	LEU
1	A	294	VAL
1	A	295	GLU
1	A	307	GLN
1	A	316	LEU
1	A	328	ASP
1	A	353	LEU
1	A	360	MET
1	A	383	GLN
1	A	389	SER
1	A	391	LEU
1	A	399	GLN
1	A	479	ARG
1	B	33	SER
1	B	36	LYS
1	B	113	LEU
1	B	140	LEU
1	B	216	ARG
1	B	256	LYS
1	B	279	LEU
1	B	285	LEU
1	B	294	VAL
1	B	298	LEU
1	B	316	LEU
1	B	328	ASP
1	B	330	ASP
1	B	353	LEU
1	B	423	HIS
1	B	436	ARG
1	B	438	SER
1	B	439	GLN
1	B	444	LEU
1	B	465	GLU
1	B	481	VAL
1	C	33	SER
1	C	36	LYS
1	C	37	LEU
1	C	83	LEU

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Mol	Chain	Res	Type
1	C	129	LYS
1	C	169	LEU
1	C	187	SER
1	C	216	ARG
1	C	220	SER
1	C	271	LEU
1	C	279	LEU
1	C	284	LEU
1	C	285	LEU
1	C	316	LEU
1	C	391	LEU
1	C	393	ARG
1	C	410	SER
1	C	436	ARG
1	C	439	GLN
1	C	440	LEU
1	C	477	ARG
1	C	479	ARG
1	C	487	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	GLN
1	A	61	GLN
1	A	148	ASN
1	A	213	ASN
1	A	232	HIS
1	A	238	HIS
1	A	250	GLN
1	A	251	GLN
1	A	313	HIS
1	A	399	GLN
1	A	423	HIS
1	A	450	HIS
1	A	478	HIS
1	B	66	GLN
1	B	124	HIS
1	B	143	GLN
1	B	148	ASN
1	B	213	ASN
1	B	232	HIS

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Mol	Chain	Res	Type
1	B	234	ASN
1	B	238	HIS
1	B	313	HIS
1	B	423	HIS
1	B	425	ASN
1	B	435	GLN
1	B	478	HIS
1	C	61	GLN
1	C	66	GLN
1	C	148	ASN
1	C	232	HIS
1	C	238	HIS
1	C	250	GLN
1	C	251	GLN
1	C	313	HIS
1	C	414	GLN
1	C	423	HIS
1	C	439	GLN
1	C	478	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
2	0BU	B	600	-	67,71,71	1.86	14 (20%)	97,113,113	1.24	6 (6%)
3	SO4	A	516	-	4,4,4	0.10	0	6,6,6	0.12	0
2	0BU	C	600	-	67,71,71	1.64	9 (13%)	97,113,113	1.21	8 (8%)
2	0BU	A	600	-	67,71,71	1.81	12 (17%)	97,113,113	1.29	9 (9%)
3	SO4	C	516	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	B	516	-	4,4,4	0.18	0	6,6,6	0.33	0
3	SO4	C	517	-	4,4,4	0.18	0	6,6,6	0.16	0
3	SO4	C	518	-	4,4,4	0.12	0	6,6,6	0.29	0
3	SO4	B	517	-	4,4,4	0.17	0	6,6,6	0.11	0
3	SO4	C	519	-	4,4,4	0.17	0	6,6,6	0.22	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	0BU	A	600	-	-	14/60/60/60	0/6/6/6
2	0BU	B	600	-	-	17/60/60/60	0/6/6/6
2	0BU	C	600	-	-	7/60/60/60	0/6/6/6

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	0BU	CBU-CBQ	-5.57	1.38	1.50
2	B	600	0BU	CBV-CBR	-5.20	1.39	1.50
2	A	600	0BU	CBV-CBR	-5.15	1.39	1.50
2	A	600	0BU	CBU-CBQ	-5.06	1.39	1.50
2	C	600	0BU	CBU-CBQ	-4.81	1.40	1.50
2	C	600	0BU	CBS-NBL	-4.34	1.32	1.41
2	C	600	0BU	CBV-CBR	-4.24	1.41	1.50
2	B	600	0BU	CBT-NBM	-4.20	1.33	1.41
2	B	600	0BU	CBS-NBL	-3.91	1.33	1.41
2	A	600	0BU	CBS-NBL	-3.83	1.33	1.41
2	A	600	0BU	CBT-NBM	-3.65	1.34	1.41
2	C	600	0BU	CBT-NBM	-3.53	1.34	1.41
2	B	600	0BU	CCD-CCH	-3.52	1.39	1.43
2	A	600	0BU	CBX-SCJ	3.33	1.84	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	0BU	CCC-CCG	-3.23	1.39	1.43
2	A	600	0BU	CCD-CCH	-3.03	1.39	1.43
2	B	600	0BU	CBZ-NBO	-3.00	1.33	1.41
2	C	600	0BU	CBZ-NBO	-2.90	1.33	1.41
2	A	600	0BU	CBY-NBN	-2.75	1.34	1.41
2	B	600	0BU	CBY-NBN	-2.66	1.34	1.41
2	C	600	0BU	CBY-NBN	-2.63	1.34	1.41
2	A	600	0BU	CCC-CCG	-2.47	1.40	1.43
2	A	600	0BU	CBZ-NBO	-2.44	1.35	1.41
2	B	600	0BU	CBZ-CCH	-2.29	1.39	1.42
2	C	600	0BU	CBE-CCB	2.29	1.40	1.37
2	B	600	0BU	CCB-CCF	-2.09	1.39	1.43
2	B	600	0BU	OAS-SCL	2.08	1.54	1.43
2	A	600	0BU	OAF-SCJ	2.04	1.54	1.43
2	C	600	0BU	OAF-SCJ	2.04	1.54	1.43
2	B	600	0BU	OAE-SCI	2.02	1.53	1.43
2	B	600	0BU	OAN-SCN	2.01	1.53	1.43
2	A	600	0BU	OAJ-SCL	2.01	1.53	1.43
2	A	600	0BU	OAS-SCL	2.00	1.53	1.43
2	C	600	0BU	OAH-SCK	2.00	1.53	1.43
2	B	600	0BU	CBY-CCG	-2.00	1.40	1.42

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	0BU	CBZ-NBO-CBR	-5.94	111.02	128.64
2	A	600	0BU	CBZ-NBO-CBR	-5.67	111.85	128.64
2	C	600	0BU	CBZ-NBO-CBR	-5.65	111.90	128.64
2	B	600	0BU	CBY-NBN-CBQ	-4.39	115.63	128.64
2	A	600	0BU	CBY-NBN-CBQ	-4.37	115.69	128.64
2	B	600	0BU	CCD-CCH-CCF	3.39	119.53	116.34
2	A	600	0BU	CBS-NBL-CBP	-3.28	119.89	126.61
2	B	600	0BU	CCC-CCG-CCE	3.23	119.38	116.34
2	C	600	0BU	CBS-NBL-CBP	-3.17	120.12	126.61
2	C	600	0BU	CBY-NBN-CBQ	-2.86	120.15	128.64
2	B	600	0BU	CBT-NBM-CBP	-2.79	120.90	126.61
2	A	600	0BU	CCC-CCG-CCE	2.75	118.92	116.34
2	A	600	0BU	CCD-CCH-CCF	2.56	118.75	116.34
2	B	600	0BU	CBS-NBL-CBP	-2.40	121.71	126.61
2	A	600	0BU	CBT-NBM-CBP	-2.31	121.89	126.61
2	C	600	0BU	CBC-CBE-CCB	-2.30	118.89	121.66
2	C	600	0BU	CBB-CBY-NBN	-2.19	117.23	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	0BU	CBV-CBR-NBO	2.19	120.74	115.92
2	C	600	0BU	CBK-CBX-CBI	-2.16	118.63	120.97
2	A	600	0BU	OAC-CBR-CBV	-2.14	117.12	120.94
2	A	600	0BU	CBK-CBX-CBI	-2.12	118.68	120.97
2	C	600	0BU	CCC-CCG-CCE	2.11	118.33	116.34
2	C	600	0BU	CBB-CBD-CCA	-2.04	119.20	121.66

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	0BU	CBD-CCA-SCK-OAH
2	A	600	0BU	CBD-CCA-SCK-OAI
2	A	600	0BU	CCE-CCA-SCK-OAH
2	A	600	0BU	CCE-CCA-SCK-OAR
2	B	600	0BU	CBH-CCC-SCM-OAM
2	B	600	0BU	CBH-CCC-SCM-OAT
2	B	600	0BU	CCG-CCC-SCM-OAL
2	B	600	0BU	CCG-CCC-SCM-OAM
2	B	600	0BU	CCG-CCC-SCM-OAT
2	C	600	0BU	CBF-CBS-NBL-CBP
2	A	600	0BU	CAX-CBS-NBL-CBP
2	C	600	0BU	CAX-CBS-NBL-CBP
2	A	600	0BU	CBF-CBS-NBL-CBP
2	B	600	0BU	CAX-CBS-NBL-CBP
2	B	600	0BU	CBF-CBS-NBL-CBP
2	B	600	0BU	OAC-CBR-CBV-CBA
2	B	600	0BU	NBO-CBR-CBV-CBA
2	A	600	0BU	CBC-CBZ-NBO-CBR
2	C	600	0BU	CBC-CBZ-NBO-CBR
2	B	600	0BU	OAC-CBR-CBV-CBG
2	A	600	0BU	CCE-CCA-SCK-OAI
2	A	600	0BU	CCH-CCD-SCN-OAN
2	B	600	0BU	CCE-CCA-SCK-OAI
2	B	600	0BU	NBO-CBR-CBV-CBG
2	B	600	0BU	CBC-CBZ-NBO-CBR
2	A	600	0BU	CBI-CCD-SCN-OAN
2	B	600	0BU	CBD-CCA-SCK-OAI
2	A	600	0BU	CCH-CCD-SCN-OAU
2	B	600	0BU	CCE-CCA-SCK-OAH
2	A	600	0BU	CBD-CCA-SCK-OAR
2	A	600	0BU	CBI-CCD-SCN-OAO

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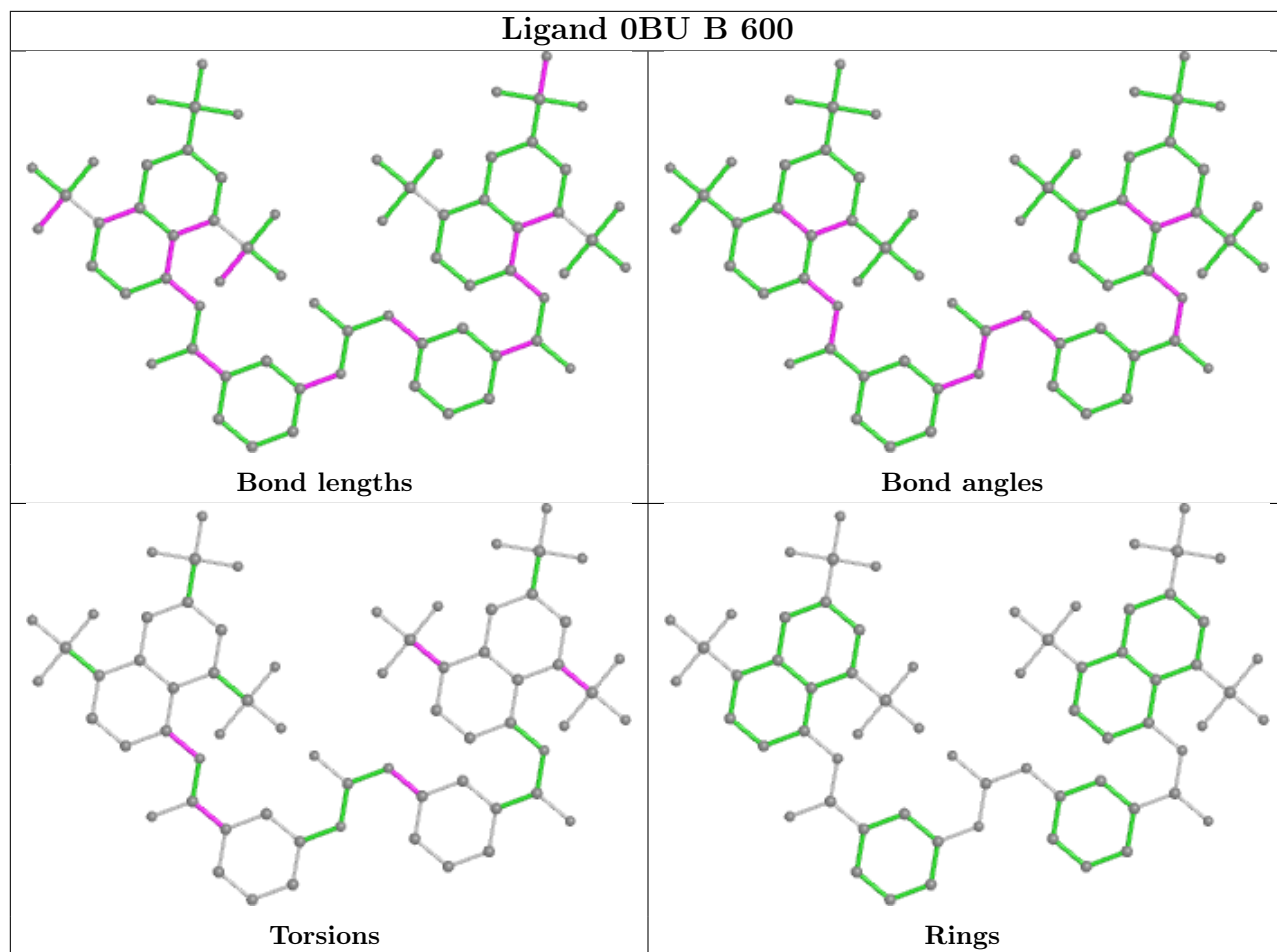
Mol	Chain	Res	Type	Atoms
2	A	600	0BU	CCH-CCD-SCN-OAO
2	B	600	0BU	CBH-CCC-SCM-OAL
2	C	600	0BU	CCF-CCB-SCL-OAJ
2	B	600	0BU	CCH-CBZ-NBO-CBR
2	C	600	0BU	CCF-CCB-SCL-OAS
2	C	600	0BU	CCH-CCD-SCN-OAN
2	C	600	0BU	CCH-CBZ-NBO-CBR

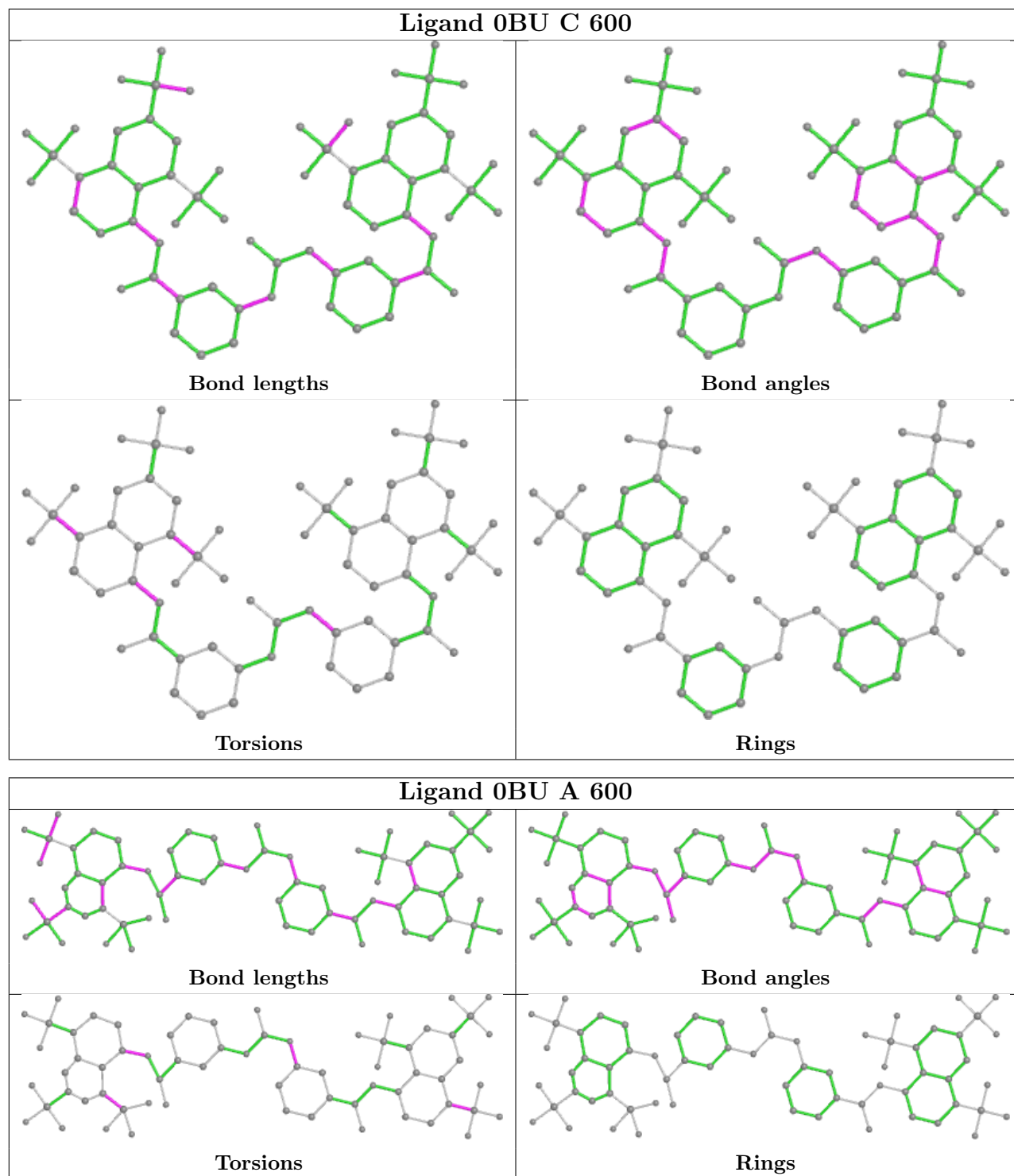
There are no ring outliers.

4 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	0BU	15	0
2	C	600	0BU	9	0
2	A	600	0BU	15	0
3	B	517	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	476/525 (90%)	-0.03	18 (3%) 40 33	26, 45, 78, 98	3 (0%)
1	B	483/525 (92%)	-0.13	12 (2%) 57 51	21, 42, 80, 105	1 (0%)
1	C	471/525 (89%)	-0.18	10 (2%) 63 58	17, 35, 69, 96	2 (0%)
All	All	1430/1575 (90%)	-0.11	40 (2%) 53 46	17, 40, 77, 105	6 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	463	SER	4.5
1	C	475	VAL	4.0
1	C	302	CYS	4.0
1	B	467	ALA	3.9
1	A	302	CYS	3.8
1	A	441	MET	3.7
1	C	456	ARG	3.7
1	C	463	SER	3.6
1	A	465	GLU	3.2
1	A	474	VAL	3.2
1	A	475	VAL	3.1
1	C	305	THR	3.0
1	A	2	LEU	2.9
1	B	475	VAL	2.9
1	B	477	ARG	2.9
1	B	474	VAL	2.8
1	A	478	HIS	2.8
1	A	466	ALA	2.7
1	B	484	TRP	2.7
1	C	452	GLU	2.7
1	B	461	ARG	2.7
1	C	460	SER	2.6
1	A	467	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	476	PRO	2.6
1	B	302	CYS	2.6
1	A	462	VAL	2.5
1	A	459	ALA	2.5
1	A	461	ARG	2.4
1	C	476	PRO	2.3
1	A	456	ARG	2.3
1	C	462	VAL	2.3
1	C	457	THR	2.2
1	B	479	ARG	2.2
1	B	54	VAL	2.2
1	B	444	LEU	2.2
1	A	52	GLU	2.2
1	A	373	ASP	2.2
1	A	378	PRO	2.2
1	A	460	SER	2.1
1	B	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

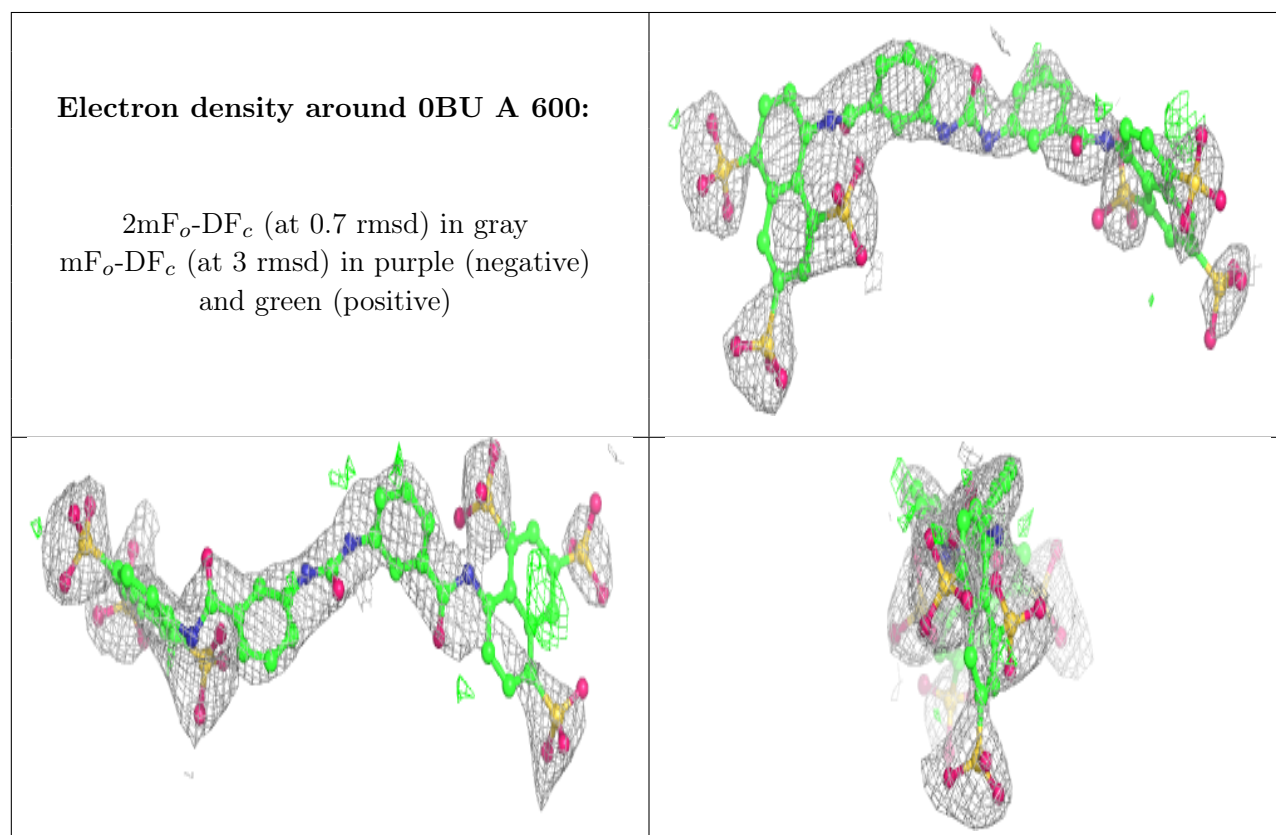
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	0BU	A	600	66/66	0.75	0.33	26,43,67,69	66
2	0BU	B	600	66/66	0.80	0.28	35,45,56,58	66
3	SO4	B	516	5/5	0.83	0.25	88,89,90,91	0
2	0BU	C	600	66/66	0.87	0.20	53,76,92,94	0
3	SO4	C	518	5/5	0.88	0.19	77,80,83,84	0
3	SO4	C	517	5/5	0.92	0.17	91,92,93,93	0

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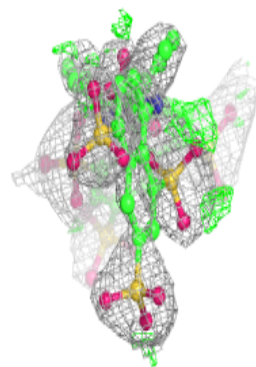
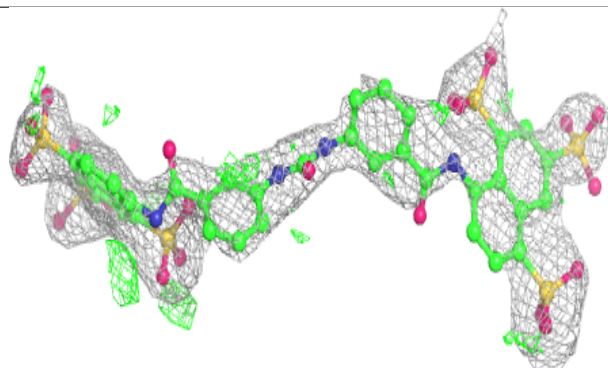
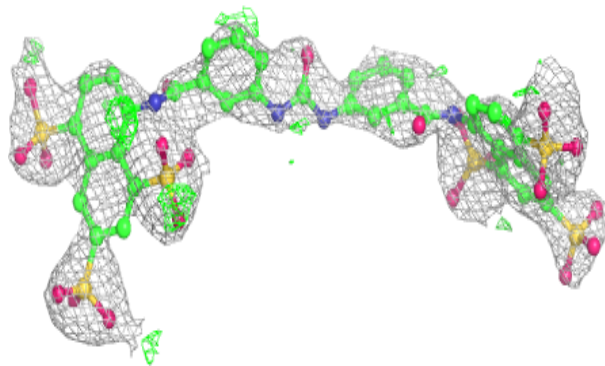
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	A	516	5/5	0.93	0.16	94,95,96,96	0
3	SO4	B	517	5/5	0.95	0.12	77,77,81,83	0
3	SO4	C	519	5/5	0.97	0.18	51,56,61,62	0
3	SO4	C	516	5/5	0.98	0.11	57,59,61,61	0

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.

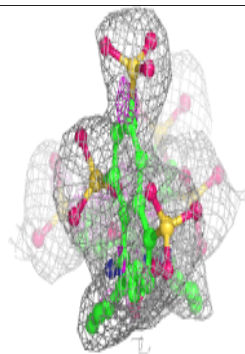
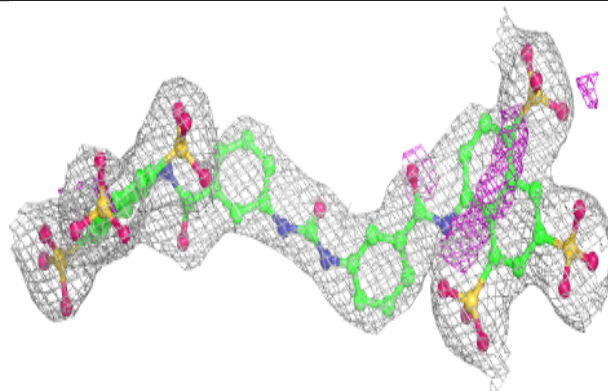
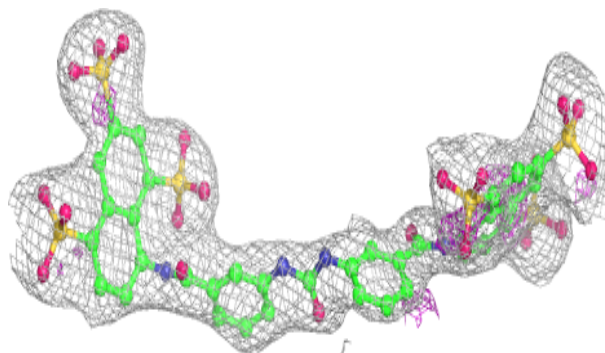


Electron density around 0BU B 600:

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

**Electron density around 0BU C 600:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.