



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 02:07 PM UTC

PDB ID : 6TI8 / pdb_00006ti8
Title : IRAK4 IN COMPLEX WITH inhibitor
Authors : Xue, Y.; Aagaard, A.; Degorce, S.L.
Deposited on : 2019-11-22
Resolution : 2.32 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

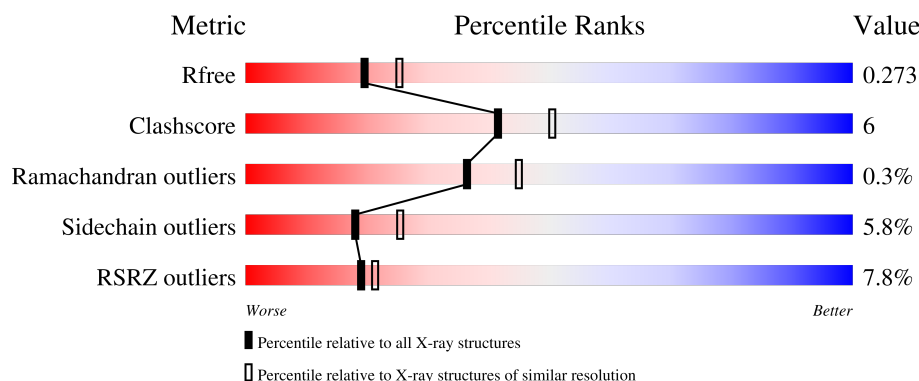
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	308	7% 78% 13% • 8%
1	B	308	8% 70% 20% • 8%
1	C	308	5% 75% 15% • 7%
1	D	308	8% 74% 15% • 8%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9494 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.

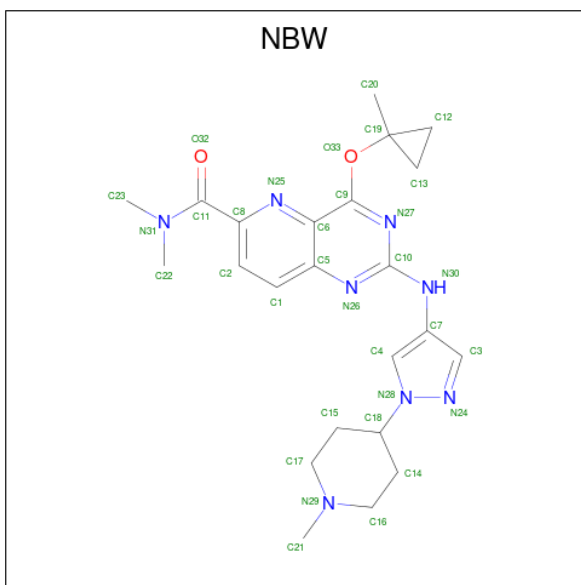
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	P	S	0	0	0
			2240	1407	375	442	2	14			
1	B	282	Total	C	N	O	P	S	0	0	0
			2226	1398	373	439	2	14			
1	C	285	Total	C	N	O	P	S	0	1	0
			2255	1416	380	443	2	14			
1	D	284	Total	C	N	O	P	S	0	0	0
			2245	1410	378	441	2	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3
C	153	GLY	-	expression tag	UNP Q9NWZ3
D	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is {N}, {N}-dimethyl-4-(1-methylcyclopropyl)oxy-2-[[1-(1-methylpiperidin-4-yl)pyrazol-4-yl]amino]pyrido[3,2-d]pyrimidine-6-carboxamide (CCD ID: NBW) (formula: C₂₃H₃₀N₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			33	23	8	2		
2	B	1	Total	C	N	O	0	0
			33	23	8	2		
2	C	1	Total	C	N	O	0	0
			33	23	8	2		
2	D	1	Total	C	N	O	0	0
			33	23	8	2		

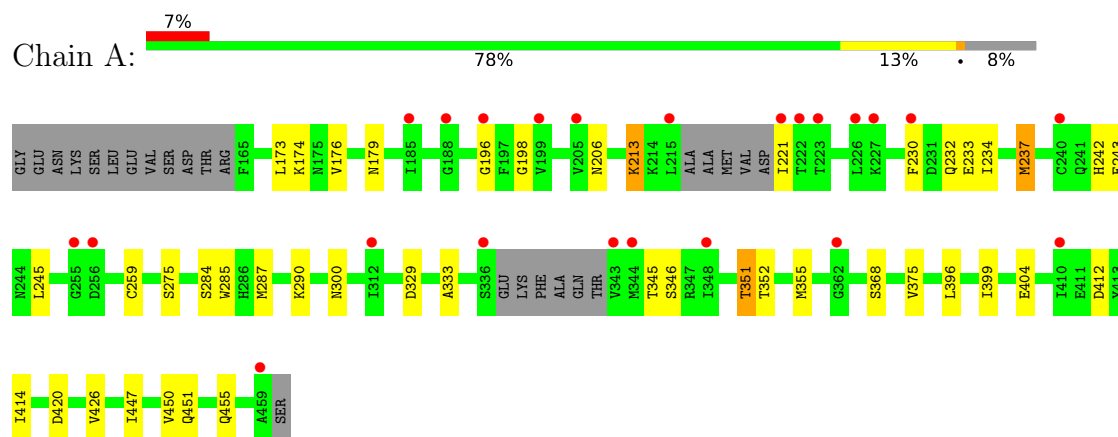
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	107	Total	O	0	0
			107	107		
3	B	82	Total	O	0	0
			82	82		
3	C	101	Total	O	0	0
			101	101		
3	D	106	Total	O	0	0
			106	106		

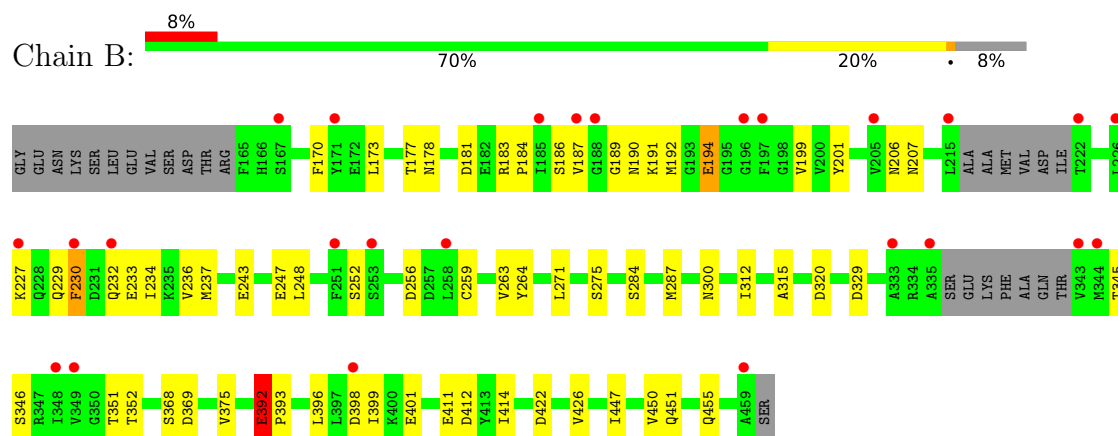
3 Residue-property plots [i](#)

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.

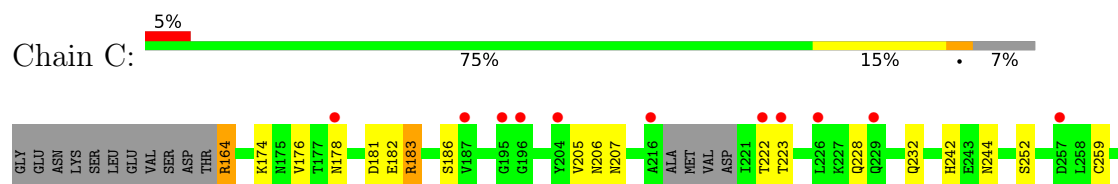
- Molecule 1: Interleukin-1 receptor-associated kinase 4

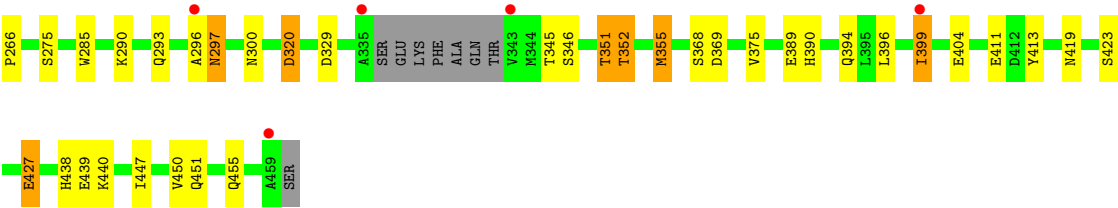


- Molecule 1: Interleukin-1 receptor-associated kinase 4

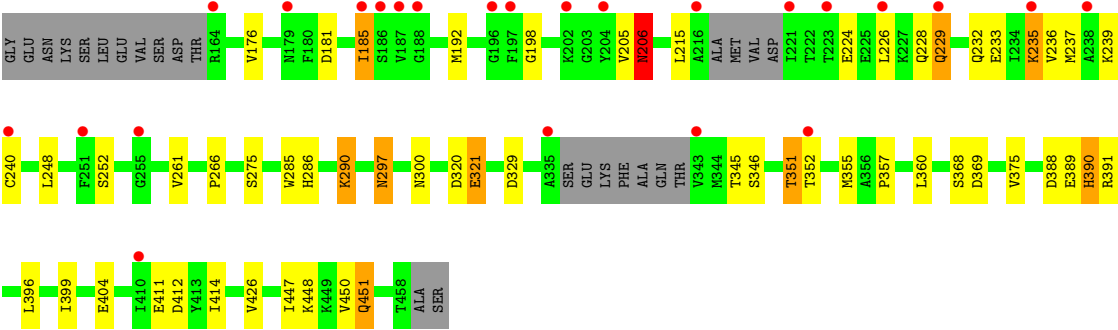


- Molecule 1: Interleukin-1 receptor-associated kinase 4





● Molecule 1: Interleukin-1 receptor-associated kinase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	89.15Å 110.53Å 142.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.66 – 2.32 49.66 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.66-2.32) 99.6 (49.66-2.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.249 , 0.281 0.234 , 0.273	Depositor DCC
R_{free} test set	3070 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9494	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.57 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.7340e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NBW, SEP, TPO

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	0.82	0/2255	1.36	18/3038 (0.6%)
1	B	0.82	1/2241 (0.0%)	1.36	19/3019 (0.6%)
1	C	0.95	3/2273 (0.1%)	1.41	20/3062 (0.7%)
1	D	0.85	0/2260	1.37	25/3044 (0.8%)
All	All	0.86	4/9029 (0.0%)	1.37	82/12163 (0.7%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	297[A]	ASN	CA-C	12.94	1.70	1.52
1	C	297[B]	ASN	CA-C	12.94	1.70	1.52
1	C	355	MET	SD-CE	-6.92	1.62	1.79
1	B	312	ILE	CG1-CD1	-5.65	1.29	1.51

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	296	ALA	CA-C-N	15.61	151.35	121.54
1	C	296	ALA	C-N-CA	15.61	151.35	121.54
1	A	196	GLY	N-CA-C	-8.36	100.17	111.54
1	D	198	GLY	N-CA-C	7.44	119.81	110.96
1	A	198	GLY	N-CA-C	7.41	121.96	111.00
1	B	392	GLU	C-N-CD	6.98	135.95	120.60
1	D	351	THR	CA-C-N	6.71	129.58	120.38
1	D	351	THR	C-N-CA	6.71	129.58	120.38
1	B	170	PHE	CA-C-N	6.68	129.13	120.44
1	B	170	PHE	C-N-CA	6.68	129.13	120.44
1	C	351	THR	CA-C-N	6.64	129.48	120.38
1	C	351	THR	C-N-CA	6.64	129.48	120.38
1	B	351	THR	CA-C-N	6.47	129.25	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	THR	C-N-CA	6.47	129.25	120.38
1	D	320	ASP	CA-C-N	6.22	128.90	120.38
1	D	320	ASP	C-N-CA	6.22	128.90	120.38
1	A	351	THR	CA-C-N	6.19	128.87	120.38
1	A	351	THR	C-N-CA	6.19	128.87	120.38
1	B	275	SER	CA-C-N	5.97	130.60	122.19
1	B	275	SER	C-N-CA	5.97	130.60	122.19
1	B	320	ASP	CA-CB-CG	5.96	118.56	112.60
1	B	263	VAL	N-CA-C	-5.82	101.52	109.37
1	C	275	SER	CA-C-N	5.77	130.33	122.19
1	C	275	SER	C-N-CA	5.77	130.33	122.19
1	C	450	VAL	CA-C-N	5.74	127.90	120.44
1	C	450	VAL	C-N-CA	5.74	127.90	120.44
1	A	285	TRP	CA-C-N	5.73	127.89	120.44
1	A	285	TRP	C-N-CA	5.73	127.89	120.44
1	C	368	SER	CA-C-N	5.71	128.40	120.29
1	C	368	SER	C-N-CA	5.71	128.40	120.29
1	C	369	ASP	CA-CB-CG	5.67	118.27	112.60
1	D	285	TRP	CA-C-N	5.67	127.81	120.44
1	D	285	TRP	C-N-CA	5.67	127.81	120.44
1	D	275	SER	CA-C-N	5.66	130.16	122.19
1	D	275	SER	C-N-CA	5.66	130.16	122.19
1	A	275	SER	CA-C-N	5.62	130.11	122.19
1	A	275	SER	C-N-CA	5.62	130.11	122.19
1	B	450	VAL	CA-C-N	5.61	127.73	120.44
1	B	450	VAL	C-N-CA	5.61	127.73	120.44
1	D	206	ASN	CA-CB-CG	5.60	118.20	112.60
1	B	368	SER	CA-C-N	5.58	128.22	120.29
1	B	368	SER	C-N-CA	5.58	128.22	120.29
1	D	450	VAL	CA-C-N	5.58	127.70	120.44
1	D	450	VAL	C-N-CA	5.58	127.70	120.44
1	C	285	TRP	CA-C-N	5.58	127.69	120.44
1	C	285	TRP	C-N-CA	5.58	127.69	120.44
1	B	369	ASP	CA-CB-CG	5.57	118.17	112.60
1	A	450	VAL	CA-C-N	5.55	127.66	120.44
1	A	450	VAL	C-N-CA	5.55	127.66	120.44
1	D	368	SER	CA-C-N	5.51	128.12	120.29
1	D	368	SER	C-N-CA	5.51	128.12	120.29
1	D	229	GLN	CA-C-N	5.48	127.94	120.54
1	D	229	GLN	C-N-CA	5.48	127.94	120.54
1	A	368	SER	CA-C-N	5.45	128.02	120.29
1	A	368	SER	C-N-CA	5.45	128.02	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	228	GLN	CA-C-N	5.36	127.73	120.44
1	D	228	GLN	C-N-CA	5.36	127.73	120.44
1	A	206	ASN	CA-CB-CG	5.30	117.90	112.60
1	D	412	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	375	VAL	CA-C-N	5.28	127.69	120.46
1	D	375	VAL	C-N-CA	5.28	127.69	120.46
1	A	451	GLN	CA-C-N	5.27	127.29	120.44
1	A	451	GLN	C-N-CA	5.27	127.29	120.44
1	B	451	GLN	CA-C-N	5.23	127.23	120.44
1	B	451	GLN	C-N-CA	5.23	127.23	120.44
1	C	186	SER	CA-C-N	5.21	128.89	121.02
1	C	186	SER	C-N-CA	5.21	128.89	121.02
1	D	451	GLN	CA-C-N	5.19	127.19	120.44
1	D	451	GLN	C-N-CA	5.19	127.19	120.44
1	C	320	ASP	CA-CB-CG	5.16	117.76	112.60
1	C	451	GLN	CA-C-N	5.15	127.13	120.44
1	C	451	GLN	C-N-CA	5.15	127.13	120.44
1	B	412	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	375	VAL	CA-C-N	5.09	127.43	120.46
1	C	375	VAL	C-N-CA	5.09	127.43	120.46
1	A	375	VAL	CA-C-N	5.07	127.41	120.46
1	A	375	VAL	C-N-CA	5.07	127.41	120.46
1	B	375	VAL	CA-C-N	5.07	127.40	120.46
1	B	375	VAL	C-N-CA	5.07	127.40	120.46
1	D	240	CYS	N-CA-C	5.05	116.86	108.02
1	D	369	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	412	ASP	CA-CB-CG	5.01	117.61	112.60

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	2240	0	2205	14	0
1	B	2226	0	2189	43	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2255	0	2224	28	1
1	D	2245	0	2213	29	0
2	A	33	0	0	1	0
2	B	33	0	0	1	0
2	C	33	0	0	1	0
2	D	33	0	0	0	0
3	A	107	0	0	0	0
3	B	82	0	0	0	0
3	C	101	0	0	1	0
3	D	106	0	0	0	0
All	All	9494	0	8831	114	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 6.

All (114) 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:D:235:LYS:HE2	1:D:239:LYS:HD2	1.40	1.03
1:B:184:PRO:HD2	1:B:187:VAL:CG2	1.88	1.03
1:C:389:GLU:N	1:C:389:GLU:OE1	1.92	1.03
1:B:191:LYS:NZ	1:B:194:GLU:OE1	1.96	0.98
1:C:164:ARG:HH11	1:C:164:ARG:HG3	1.30	0.95
1:B:398:ASP:O	1:B:401:GLU:HB2	1.66	0.94
1:A:232:GLN:NE2	1:A:333:ALA:O	2.01	0.94
1:B:184:PRO:HD2	1:B:187:VAL:HG21	1.46	0.94
1:A:284:SER:H	1:A:287:MET:HE3	1.34	0.93
1:D:235:LYS:CE	1:D:239:LYS:HD2	2.01	0.91
1:B:183:ARG:HH11	1:B:187:VAL:HG12	1.38	0.88
1:B:233:GLU:O	1:B:237:MET:HG2	1.73	0.88
1:D:389:GLU:HG3	1:D:390:HIS:ND1	1.90	0.86
1:D:388:ASP:OD2	1:D:391:ARG:HB2	1.77	0.84
1:C:438:HIS:HD2	1:C:440:LYS:H	1.28	0.82
1:D:389:GLU:HG3	1:D:390:HIS:CE1	2.15	0.81
1:B:237:MET:HE3	1:B:248:LEU:HB2	1.63	0.80
1:B:191:LYS:NZ	1:B:194:GLU:CD	2.40	0.79
1:B:184:PRO:HG2	1:B:187:VAL:HG23	1.67	0.77
1:D:232:GLN:O	1:D:236:VAL:HG23	1.84	0.77
1:B:284:SER:H	1:B:287:MET:HE3	1.48	0.76
1:D:185:ILE:HD12	1:D:192:MET:HA	1.67	0.76
1:B:183:ARG:NH1	1:B:187:VAL:HG12	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PRO:HG3	1:D:321:GLU:HG3	1.71	0.73
1:D:205:VAL:O	1:D:206:ASN:HB3	1.88	0.72
1:B:191:LYS:HZ1	1:B:194:GLU:CD	1.98	0.70
1:C:389:GLU:HA	1:C:394:GLN:HE21	1.58	0.69
1:A:230:PHE:O	1:A:234:ILE:HD12	1.92	0.69
1:B:184:PRO:CD	1:B:187:VAL:CG2	2.73	0.65
1:B:233:GLU:O	1:B:237:MET:CG	2.44	0.64
1:C:352:THR:HA	1:C:355:MET:HE3	1.79	0.64
1:A:233:GLU:O	1:A:237:MET:HB2	1.99	0.61
1:C:438:HIS:CD2	1:C:440:LYS:H	2.16	0.61
1:D:297:ASN:OD1	1:D:451:GLN:NE2	2.33	0.61
1:C:206:ASN:O	1:C:207:ASN:HB2	2.02	0.60
1:C:252:SER:HB3	1:C:259:CYS:HB2	1.84	0.60
1:B:422:ASP:CG	1:D:206:ASN:HD21	2.09	0.59
1:B:207:ASN:HB3	1:D:448:LYS:HE2	1.84	0.59
1:D:389:GLU:CG	1:D:390:HIS:CE1	2.86	0.59
1:D:286:HIS:O	1:D:290:LYS:HD2	2.03	0.59
1:B:191:LYS:HZ3	1:B:194:GLU:CD	2.09	0.58
1:C:293:GLN:O	1:C:297[A]:ASN:HB2	2.04	0.58
1:C:164:ARG:HG3	1:C:164:ARG:NH1	2.07	0.57
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.85	0.57
1:B:191:LYS:CE	1:B:194:GLU:OE1	2.53	0.56
1:D:396:LEU:O	1:D:399:ILE:HG12	2.06	0.56
1:B:396:LEU:O	1:B:399:ILE:HG12	2.06	0.56
1:C:390:HIS:N	1:C:390:HIS:CD2	2.73	0.56
1:A:396:LEU:O	1:A:399:ILE:HG12	2.07	0.54
1:B:184:PRO:CG	1:B:187:VAL:HG23	2.37	0.54
1:B:184:PRO:HD2	1:B:187:VAL:HG23	1.86	0.54
1:A:420:ASP:HA	1:C:207:ASN:O	2.08	0.53
1:D:235:LYS:HE3	1:D:239:LYS:HE3	1.90	0.53
1:B:184:PRO:CD	1:B:187:VAL:HG21	2.29	0.52
1:C:244:ASN:OD1	1:C:297[B]:ASN:ND2	2.42	0.52
1:B:230:PHE:C	1:B:230:PHE:CD2	2.88	0.52
1:B:191:LYS:NZ	1:B:194:GLU:OE2	2.43	0.51
1:B:192:MET:SD	1:B:264:TYR:HE1	2.33	0.51
1:C:164:ARG:NH1	1:C:164:ARG:CG	2.73	0.51
1:C:389:GLU:CA	1:C:394:GLN:HE21	2.23	0.51
1:C:399:ILE:HG12	1:C:413:TYR:CZ	2.45	0.51
1:B:230:PHE:CZ	1:B:234:ILE:HD11	2.45	0.50
1:B:177:THR:O	1:B:190:ASN:OD1	2.30	0.50
1:C:266:PRO:HD2	1:C:320:ASP:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:NBW:C3	2:C:501:NBW:N27	2.75	0.48
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.10	0.47
1:B:184:PRO:HD2	1:B:187:VAL:CB	2.42	0.47
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.96	0.47
1:D:390:HIS:ND1	1:D:390:HIS:N	2.60	0.47
1:B:392:GLU:HA	1:B:393:PRO:HA	1.80	0.46
1:D:266:PRO:CG	1:D:321:GLU:HG3	2.43	0.46
1:C:242:HIS:HE1	1:C:297[B]:ASN:ND2	2.12	0.46
1:B:232:GLN:O	1:B:236:VAL:HG23	2.16	0.46
1:C:389:GLU:HA	1:C:394:GLN:NE2	2.29	0.46
2:A:501:NBW:N27	2:A:501:NBW:C3	2.77	0.45
1:C:423:SER:O	1:C:427:GLU:HB2	2.17	0.45
1:B:183:ARG:HH11	1:B:187:VAL:CG1	2.20	0.45
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.45
1:D:235:LYS:CE	1:D:239:LYS:CD	2.86	0.45
1:B:192:MET:HE2	1:B:201:TYR:C	2.42	0.44
1:C:396:LEU:HD12	1:C:399:ILE:HD13	2.00	0.44
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.98	0.44
1:B:271:LEU:HD22	1:B:315:ALA:HB2	2.00	0.44
1:A:242:HIS:HB3	1:A:245:LEU:HG	2.00	0.44
1:B:184:PRO:CD	1:B:187:VAL:HG23	2.45	0.44
1:C:352:THR:HA	1:C:355:MET:CE	2.47	0.44
1:D:351:THR:O	1:D:355:MET:HG3	2.18	0.43
1:D:215:LEU:HB3	1:D:226:LEU:HD21	1.99	0.43
1:B:229:GLN:NE2	1:B:229:GLN:C	2.76	0.43
1:B:284:SER:N	1:B:287:MET:HE3	2.25	0.43
1:D:235:LYS:HE3	1:D:239:LYS:CE	2.48	0.43
1:B:181:ASP:OD1	1:B:189:GLY:HA2	2.19	0.43
1:D:414:ILE:HG12	1:D:426:VAL:HG11	2.00	0.42
1:D:321:GLU:H	1:D:321:GLU:CD	2.27	0.42
1:C:181:ASP:OD1	1:C:183:ARG:HD3	2.19	0.42
1:C:351:THR:O	1:C:355:MET:HG3	2.19	0.42
1:C:439:GLU:HG2	3:C:683:HOH:O	2.20	0.42
1:D:357:PRO:HA	1:D:360:LEU:HD12	2.01	0.42
1:A:351:THR:O	1:A:355:MET:HG3	2.20	0.42
2:B:501:NBW:C3	2:B:501:NBW:N27	2.82	0.42
1:A:414:ILE:HG12	1:A:426:VAL:HG11	2.02	0.41
1:D:248:LEU:HD12	1:D:261:VAL:O	2.20	0.41
1:A:284:SER:N	1:A:287:MET:HE3	2.16	0.41
1:A:213:LYS:O	1:A:259:CYS:HA	2.21	0.41
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:HB3	1:B:190:ASN:OD1	2.21	0.41
1:B:229:GLN:C	1:B:229:GLN:CD	2.89	0.41
1:D:290:LYS:HD2	1:D:290:LYS:N	2.36	0.41
1:C:300:ASN:HA	1:C:447:ILE:HG21	2.03	0.41
1:B:173:LEU:HD23	1:B:173:LEU:HA	1.93	0.41
1:C:389:GLU:N	1:C:389:GLU:CD	2.72	0.41
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.03	0.41
1:D:389:GLU:CD	1:D:390:HIS:HE1	2.29	0.40
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.02	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:178:ASN:O	1:C:183:ARG:NH1[2_365]	2.18	0.02

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	276/308 (90%)	268 (97%)	8 (3%)	0	100	100
1	B	274/308 (89%)	268 (98%)	5 (2%)	1 (0%)	30	37
1	C	278/308 (90%)	273 (98%)	5 (2%)	0	100	100
1	D	276/308 (90%)	270 (98%)	4 (1%)	2 (1%)	18	22
All	All	1104/1232 (90%)	1079 (98%)	22 (2%)	3 (0%)	36	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	181	ASP

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Mol	Chain	Res	Type
1	B	206	ASN
1	D	206	ASN

5.3.2 Protein sidechains ⓘ

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	246/266 (92%)	237 (96%)	9 (4%)	30	44
1	B	244/266 (92%)	231 (95%)	13 (5%)	20	29
1	C	247/266 (93%)	228 (92%)	19 (8%)	12	15
1	D	246/266 (92%)	230 (94%)	16 (6%)	15	21
All	All	983/1064 (92%)	926 (94%)	57 (6%)	18	25

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	213	LYS
1	A	221	ILE
1	A	237	MET
1	A	243	GLU
1	A	290	LYS
1	A	329	ASP
1	A	352	THR
1	A	404	GLU
1	A	455	GLN
1	B	186	SER
1	B	194	GLU
1	B	199	VAL
1	B	227	LYS
1	B	230	PHE
1	B	243	GLU
1	B	247	GLU
1	B	256	ASP
1	B	329	ASP
1	B	352	THR

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Mol	Chain	Res	Type
1	B	392	GLU
1	B	411	GLU
1	B	455	GLN
1	C	164	ARG
1	C	174	LYS
1	C	176	VAL
1	C	182	GLU
1	C	183	ARG
1	C	205	VAL
1	C	222	THR
1	C	223	THR
1	C	228	GLN
1	C	232	GLN
1	C	290	LYS
1	C	329	ASP
1	C	352	THR
1	C	399	ILE
1	C	404	GLU
1	C	411	GLU
1	C	419	ASN
1	C	427	GLU
1	C	455	GLN
1	D	176	VAL
1	D	185	ILE
1	D	224	GLU
1	D	229	GLN
1	D	233	GLU
1	D	235	LYS
1	D	237	MET
1	D	252	SER
1	D	290	LYS
1	D	297	ASN
1	D	321	GLU
1	D	329	ASP
1	D	352	THR
1	D	390	HIS
1	D	404	GLU
1	D	411	GLU

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

Mol	Chain	Res	Type
1	A	206	ASN
1	A	293	GLN
1	A	297	ASN
1	A	390	HIS
1	A	451	GLN
1	A	452	GLN
1	B	175	ASN
1	B	228	GLN
1	B	267	ASN
1	B	293	GLN
1	B	297	ASN
1	B	451	GLN
1	B	452	GLN
1	C	179	ASN
1	C	232	GLN
1	C	241	GLN
1	C	242	HIS
1	C	390	HIS
1	C	394	GLN
1	C	419	ASN
1	C	438	HIS
1	C	451	GLN
1	C	452	GLN
1	D	179	ASN
1	D	207	ASN
1	D	229	GLN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	TPO	A	345	1	8,10,11	1.17	0	10,14,16	1.25	1 (10%)
1	TPO	B	345	1	8,10,11	1.23	0	10,14,16	1.19	1 (10%)
1	TPO	D	345	1	8,10,11	1.27	1 (12%)	10,14,16	1.06	0
1	TPO	C	345	1	8,10,11	1.18	0	10,14,16	1.15	1 (10%)
1	SEP	B	346	1	8,9,10	0.89	0	7,12,14	2.01	1 (14%)
1	SEP	A	346	1	8,9,10	0.84	0	7,12,14	1.99	2 (28%)
1	SEP	D	346	1	8,9,10	0.82	0	7,12,14	2.20	2 (28%)
1	SEP	C	346	1	8,9,10	0.90	0	7,12,14	1.99	1 (14%)

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
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	5/9/11/13	-
1	TPO	D	345	1	-	3/9/11/13	-
1	TPO	C	345	1	-	5/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	SEP	D	346	1	-	0/6/8/10	-
1	SEP	C	346	1	-	0/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	345	TPO	CB-CA	2.15	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	346	SEP	OG-CB-CA	4.92	112.93	108.14
1	B	346	SEP	OG-CB-CA	4.57	112.59	108.14
1	C	346	SEP	OG-CB-CA	4.45	112.47	108.14
1	A	346	SEP	OG-CB-CA	4.33	112.35	108.14
1	A	345	TPO	O3P-P-OG1	2.56	115.81	105.85
1	B	345	TPO	O3P-P-OG1	2.50	115.59	105.85
1	C	345	TPO	O3P-P-OG1	2.28	114.72	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	O2P-P-OG	2.18	112.34	106.67
1	D	346	SEP	O3P-P-OG	2.12	112.19	106.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	C	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O2P
1	B	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O2P
1	C	345	TPO	CB-OG1-P-O3P
1	D	345	TPO	CB-OG1-P-O2P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NBW	C	501	-	31,37,37	1.06	1 (3%)	41,55,55	1.65	9 (21%)
2	NBW	B	501	-	31,37,37	1.19	1 (3%)	41,55,55	2.11	13 (31%)
2	NBW	A	501	-	31,37,37	1.39	5 (16%)	41,55,55	2.29	14 (34%)
2	NBW	D	501	-	31,37,37	1.16	1 (3%)	41,55,55	1.69	11 (26%)

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	NBW	C	501	-	-	2/19/35/35	0/5/5/5
2	NBW	B	501	-	-	1/19/35/35	0/5/5/5
2	NBW	A	501	-	-	1/19/35/35	0/5/5/5
2	NBW	D	501	-	-	5/19/35/35	0/5/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	NBW	C11-N31	4.48	1.40	1.34
2	B	501	NBW	C11-N31	4.07	1.40	1.34
2	D	501	NBW	C11-N31	3.12	1.38	1.34
2	C	501	NBW	C11-N31	2.48	1.37	1.34
2	A	501	NBW	C6-C5	-2.48	1.38	1.42
2	A	501	NBW	C1-C5	-2.40	1.37	1.41
2	A	501	NBW	O33-C9	2.16	1.39	1.36
2	A	501	NBW	C8-C11	-2.14	1.47	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NBW	C19-O33-C9	-7.35	115.57	123.24
2	B	501	NBW	C14-C18-N28	5.76	118.83	110.95
2	B	501	NBW	C15-C18-N28	5.47	118.44	110.95
2	A	501	NBW	C14-C18-N28	5.29	118.20	110.95
2	B	501	NBW	C19-O33-C9	-4.70	118.33	123.24
2	C	501	NBW	C19-O33-C9	-3.84	119.23	123.24
2	A	501	NBW	C5-C6-N25	3.81	125.48	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NBW	C19-O33-C9	-3.80	119.28	123.24
2	D	501	NBW	C14-C18-N28	3.68	116.00	110.95
2	C	501	NBW	C1-C5-C6	-3.68	114.94	119.55
2	A	501	NBW	C4-N28-N24	3.66	114.92	112.45
2	D	501	NBW	C21-N29-C17	-3.45	104.06	110.63
2	B	501	NBW	C1-C5-C6	-3.30	115.41	119.55
2	A	501	NBW	C16-C14-C18	-3.29	104.75	110.78
2	B	501	NBW	C5-C6-N25	3.15	124.77	121.41
2	A	501	NBW	C17-N29-C16	3.14	114.53	109.54
2	A	501	NBW	C18-N28-N24	-3.10	116.17	120.41
2	A	501	NBW	C21-N29-C17	-2.94	105.03	110.63
2	C	501	NBW	C1-C5-N26	2.84	122.83	118.69
2	C	501	NBW	C5-C6-N25	2.82	124.43	121.41
2	D	501	NBW	C5-C6-N25	2.82	124.42	121.41
2	A	501	NBW	C15-C18-N28	2.79	114.77	110.95
2	B	501	NBW	C1-C5-N26	2.76	122.72	118.69
2	D	501	NBW	C1-C5-C6	-2.64	116.24	119.55
2	A	501	NBW	O32-C11-C8	-2.59	114.23	118.90
2	C	501	NBW	C21-N29-C17	-2.59	105.70	110.63
2	C	501	NBW	C13-C19-C12	-2.52	59.12	61.19
2	D	501	NBW	C15-C18-N28	2.52	114.40	110.95
2	A	501	NBW	C1-C5-C6	-2.50	116.42	119.55
2	C	501	NBW	C12-C13-C19	2.49	60.69	59.41
2	D	501	NBW	C17-N29-C16	2.45	113.44	109.54
2	A	501	NBW	C21-N29-C16	-2.45	105.97	110.63
2	B	501	NBW	C18-N28-N24	-2.43	117.08	120.41
2	A	501	NBW	C15-C17-N29	2.34	114.22	111.20
2	B	501	NBW	C17-N29-C16	2.32	113.23	109.54
2	C	501	NBW	C15-C18-N28	2.32	114.13	110.95
2	D	501	NBW	C4-N28-N24	2.31	114.01	112.45
2	B	501	NBW	C12-C13-C19	2.30	60.59	59.41
2	B	501	NBW	C15-C17-N29	2.25	114.09	111.20
2	B	501	NBW	N26-C10-N27	-2.22	122.61	126.25
2	A	501	NBW	N26-C10-N27	-2.18	122.68	126.25
2	C	501	NBW	C14-C18-N28	2.13	113.86	110.95
2	D	501	NBW	C13-C19-C12	-2.12	59.45	61.19
2	D	501	NBW	C18-N28-N24	-2.11	117.52	120.41
2	B	501	NBW	C21-N29-C17	-2.09	106.66	110.63
2	B	501	NBW	C13-C19-C12	-2.07	59.50	61.19
2	D	501	NBW	C17-C15-C18	-2.00	107.11	110.78

There are no chirality outliers.

All (9) torsion outliers are listed below:

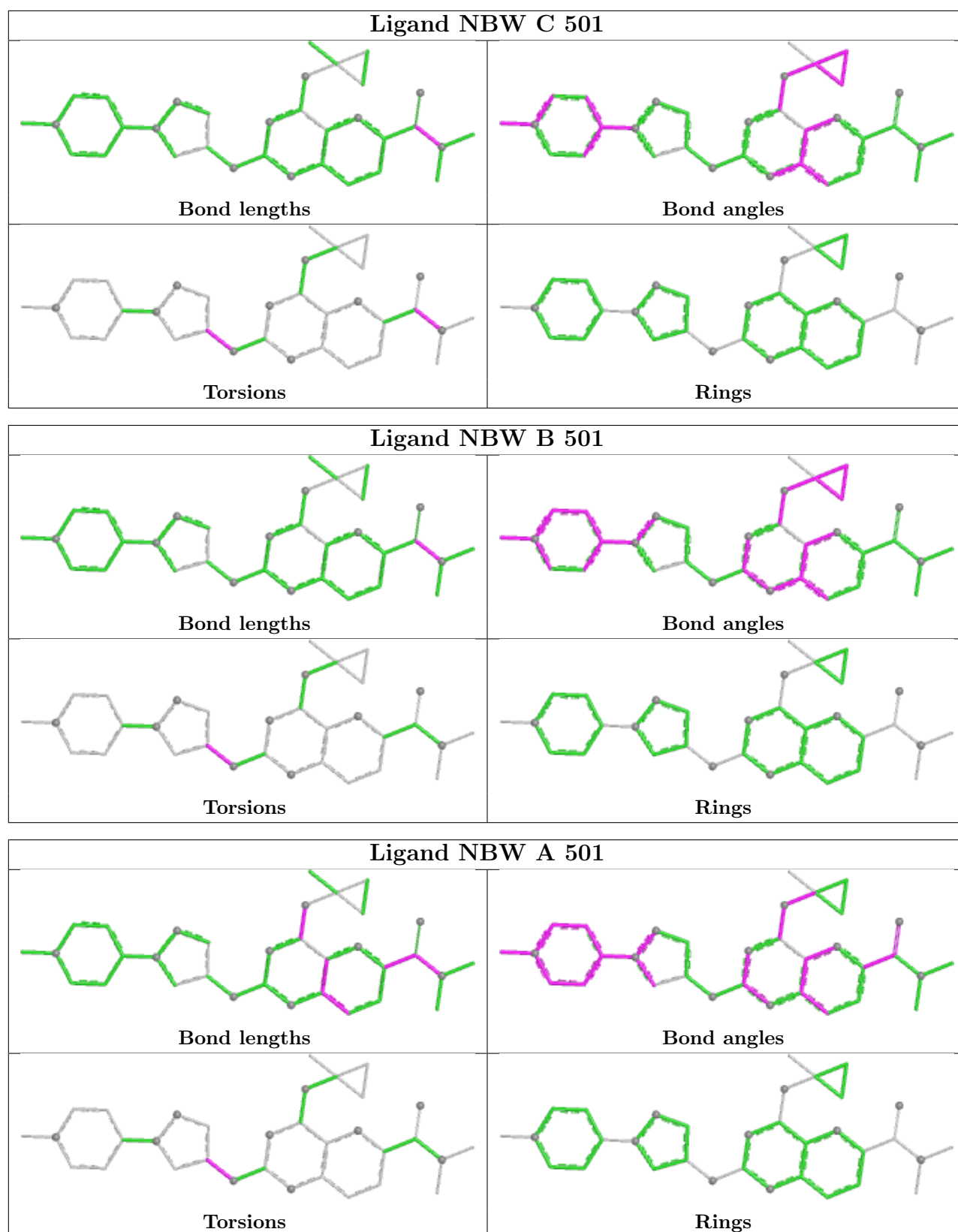
Mol	Chain	Res	Type	Atoms
2	A	501	NBW	C4-C7-N30-C10
2	B	501	NBW	C4-C7-N30-C10
2	C	501	NBW	C4-C7-N30-C10
2	D	501	NBW	C4-C7-N30-C10
2	D	501	NBW	C8-C11-N31-C23
2	D	501	NBW	O32-C11-N31-C23
2	C	501	NBW	C8-C11-N31-C23
2	D	501	NBW	C12-C19-O33-C9
2	D	501	NBW	C13-C19-O33-C9

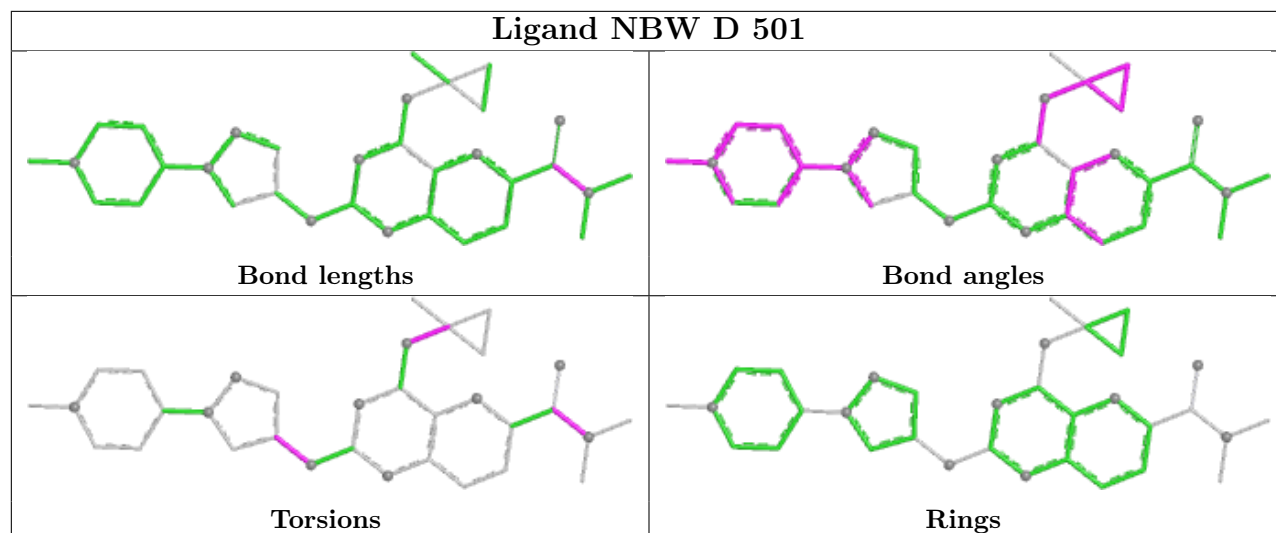
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	NBW	1	0
2	B	501	NBW	1	0
2	A	501	NBW	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 [i](#)

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	282/308 (91%)	0.67	23 (8%)	17 20	39, 62, 115, 193	0
1	B	280/308 (90%)	0.66	25 (8%)	15 17	39, 66, 121, 197	0
1	C	283/308 (91%)	0.55	16 (5%)	29 32	35, 58, 104, 153	2 (0%)
1	D	282/308 (91%)	0.70	24 (8%)	16 18	40, 62, 101, 135	0
All	All	1127/1232 (91%)	0.65	88 (7%)	19 21	35, 62, 114, 197	2 (0%)

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	5.2
1	D	221	ILE	5.0
1	B	226	LEU	4.8
1	A	226	LEU	4.7
1	B	343	VAL	4.5
1	B	344	MET	4.4
1	A	343	VAL	4.2
1	B	335	ALA	4.2
1	C	216	ALA	4.2
1	C	178	ASN	4.1
1	D	335	ALA	3.8
1	B	197	PHE	3.8
1	C	296	ALA	3.6
1	A	348	ILE	3.5
1	C	223	THR	3.5
1	D	179	ASN	3.5
1	C	399	ILE	3.4
1	C	459	ALA	3.4
1	B	348	ILE	3.3
1	A	222	THR	3.3
1	C	226	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	188	GLY	3.2
1	D	255	GLY	3.2
1	B	230	PHE	3.2
1	C	335	ALA	3.1
1	D	216	ALA	3.1
1	D	197	PHE	3.0
1	C	229	GLN	3.0
1	A	336	SER	3.0
1	A	255	GLY	3.0
1	A	223	THR	2.9
1	D	343	VAL	2.9
1	D	196	GLY	2.8
1	D	187	VAL	2.8
1	A	410	ILE	2.8
1	A	459	ALA	2.8
1	B	187	VAL	2.8
1	D	223	THR	2.8
1	B	171	TYR	2.8
1	A	215	LEU	2.7
1	C	204	TYR	2.7
1	A	196	GLY	2.7
1	D	204	TYR	2.7
1	B	251	PHE	2.7
1	A	256	ASP	2.7
1	B	196	GLY	2.6
1	D	186	SER	2.6
1	D	238	ALA	2.6
1	C	187	VAL	2.6
1	A	185	ILE	2.6
1	B	215	LEU	2.6
1	D	164	ARG	2.5
1	A	230	PHE	2.5
1	B	232	GLN	2.5
1	A	205	VAL	2.4
1	B	188	GLY	2.4
1	D	240	CYS	2.4
1	C	195	GLY	2.4
1	D	202	LYS	2.4
1	A	227	LYS	2.4
1	C	343	VAL	2.4
1	B	333	ALA	2.3
1	A	199	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	410	ILE	2.3
1	D	188	GLY	2.3
1	D	226	LEU	2.3
1	C	222	THR	2.3
1	B	227	LYS	2.3
1	D	235	LYS	2.3
1	B	258	LEU	2.2
1	C	196	GLY	2.2
1	B	349	VAL	2.2
1	B	222	THR	2.2
1	D	352	THR	2.2
1	B	185	ILE	2.2
1	B	253	SER	2.2
1	B	205	VAL	2.1
1	D	251	PHE	2.1
1	A	362	GLY	2.1
1	A	240	CYS	2.1
1	A	312	ILE	2.1
1	D	229	GLN	2.1
1	D	185	ILE	2.1
1	C	257	ASP	2.1
1	B	167	SER	2.0
1	A	344	MET	2.0
1	B	459	ALA	2.0
1	B	398	ASP	2.0

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

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
1	SEP	D	346	10/11	0.46	0.13	119,126,135,137	0
1	SEP	A	346	10/11	0.47	0.16	127,134,142,143	0
1	SEP	B	346	10/11	0.52	0.17	129,134,142,143	0
1	SEP	C	346	10/11	0.61	0.12	115,121,129,131	0
1	TPO	D	345	11/12	0.78	0.14	112,118,121,124	0
1	TPO	A	345	11/12	0.80	0.13	118,123,127,128	0
1	TPO	C	345	11/12	0.81	0.14	109,114,117,120	0
1	TPO	B	345	11/12	0.88	0.13	119,122,127,128	0

6.3 Carbohydrates [i](#)

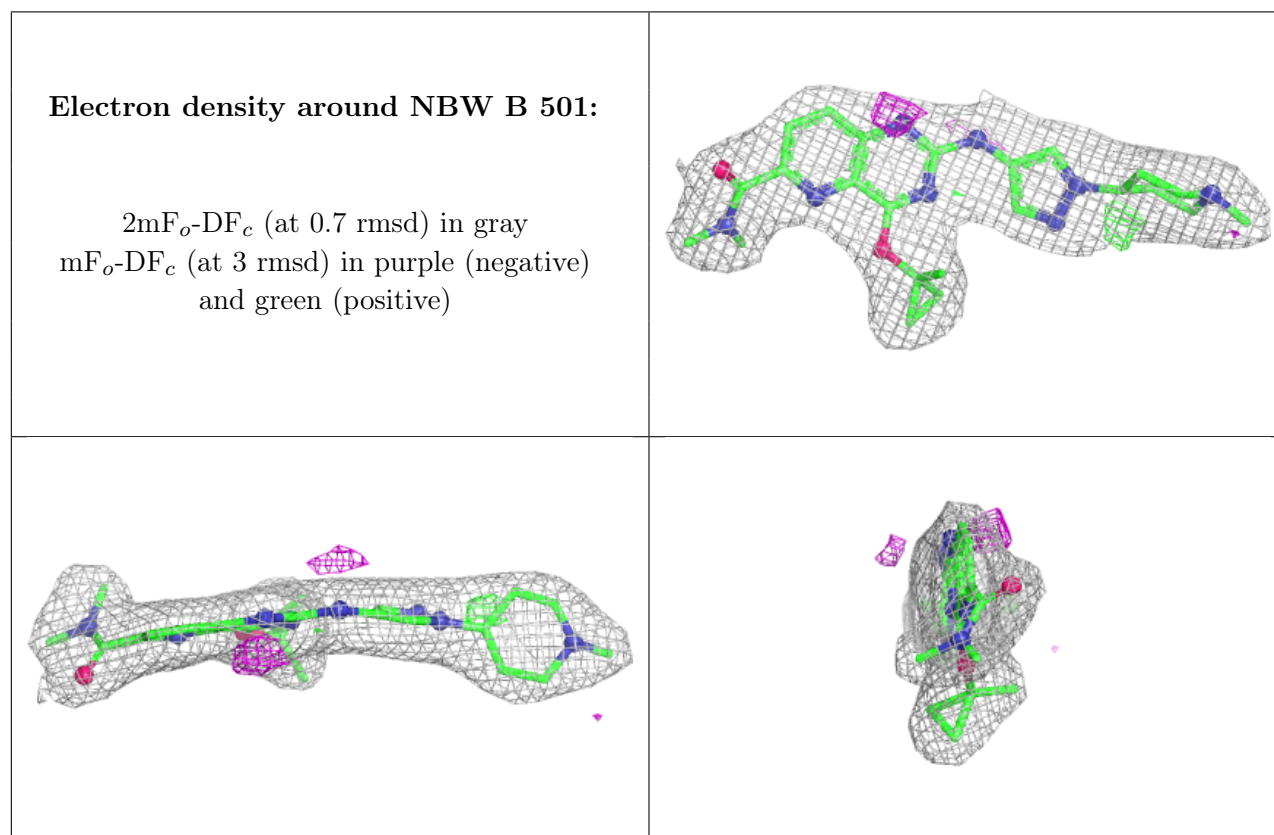
There are no oligosaccharides in this entry.

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.

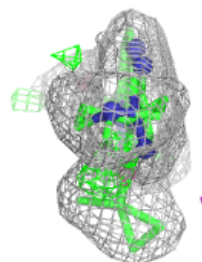
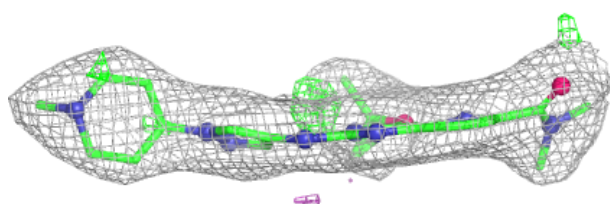
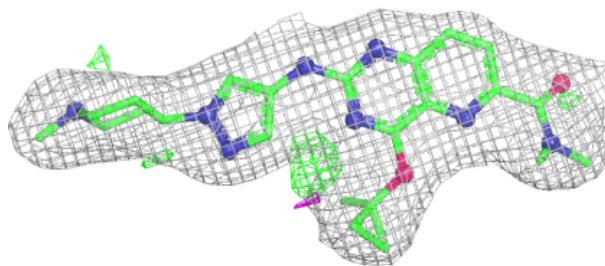
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NBW	B	501	33/33	0.93	0.09	38,45,50,51	0
2	NBW	D	501	33/33	0.93	0.09	37,42,46,47	0
2	NBW	A	501	33/33	0.94	0.09	33,41,53,55	0
2	NBW	C	501	33/33	0.95	0.09	30,43,58,58	0

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.

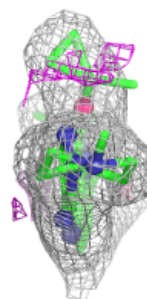
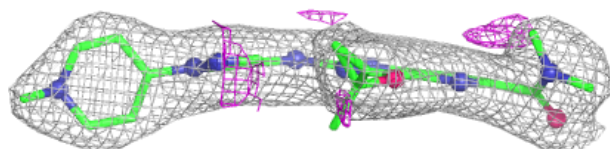
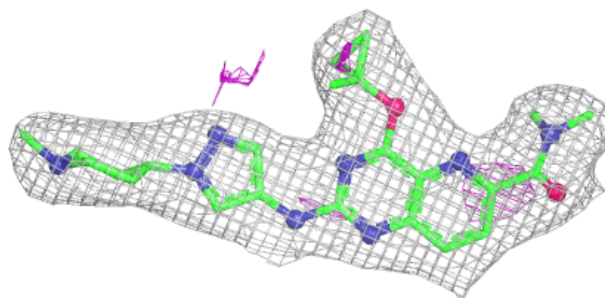


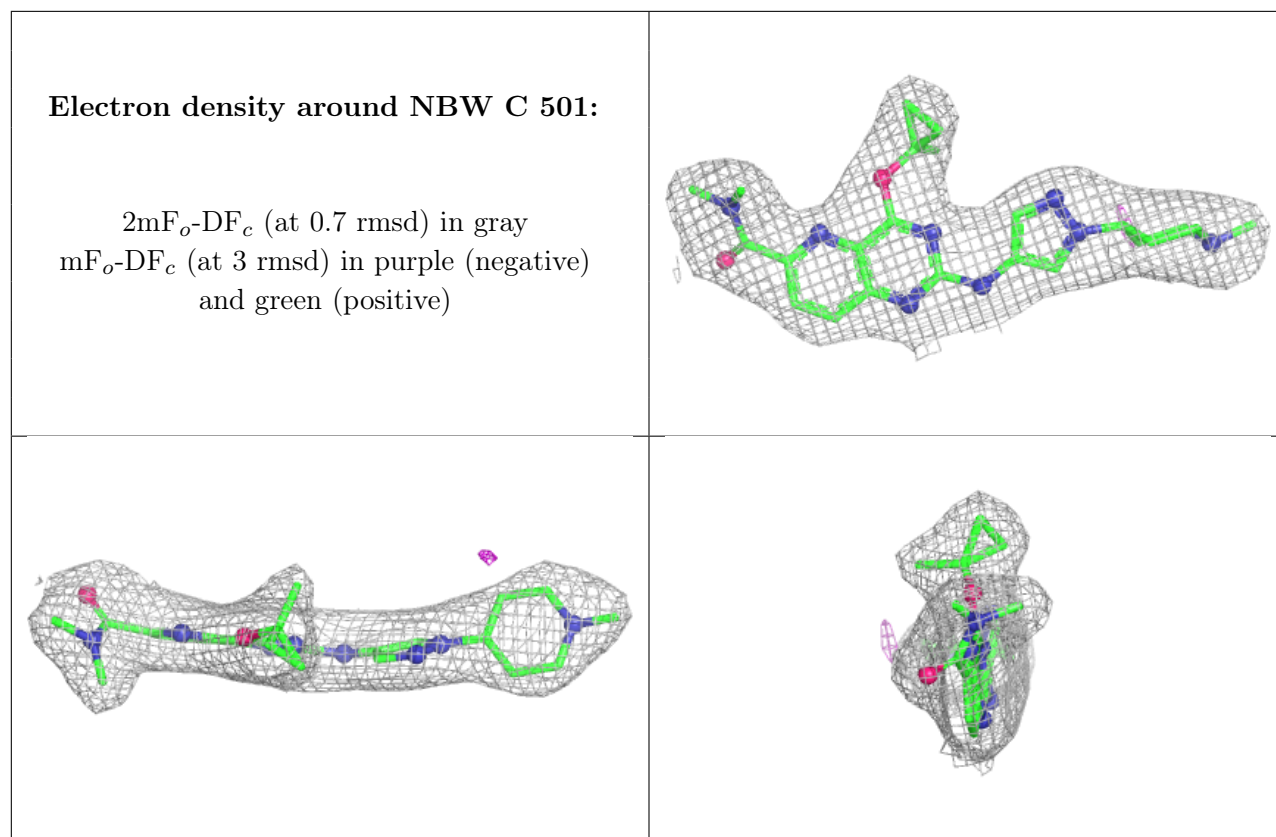
Electron density around NBW D 501:

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

**Electron density around NBW A 501:**

$2mF_o-DF_c$ (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.