Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 02:38 am GMT

PDB ID	:	6Q5B
Title	:	OXA-48_P68A-AVI. Evolutionary trade-offs of OXA-48 mediated ceftazidime-avibactam resistance
Authors	:	Frohlich, C.; Sorum, V.; Thomassen, A.M.; Johnsen, P.J.; Leiros, H.K.S.; Samuelsen, O.
Deposited on	:	2018-12-07
Resolution	:	2.22 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:

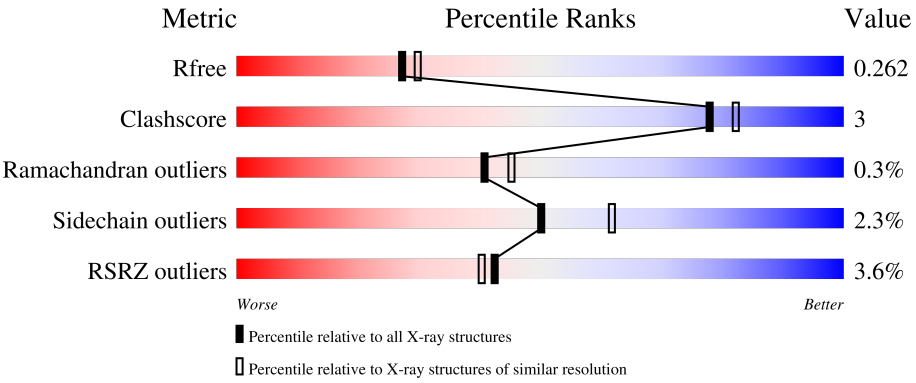
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	265	5% 78% 8% • 12%
1	C	265	3% 83% 5% 13%
2	B	265	3% 84% 7% 9%
2	D	265	2% 82% 8% • 9%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 16144 atoms, of which 7607 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 Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	233	Total	C	H	N	O	S	0	0	0
			3748	1208	1852	335	346	7			
1	C	231	Total	C	H	N	O	S	1	4	0
			3749	1206	1852	339	345	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ALA	PRO	engineered mutation	UNP Q6XEC0
C	68	ALA	PRO	engineered mutation	UNP Q6XEC0

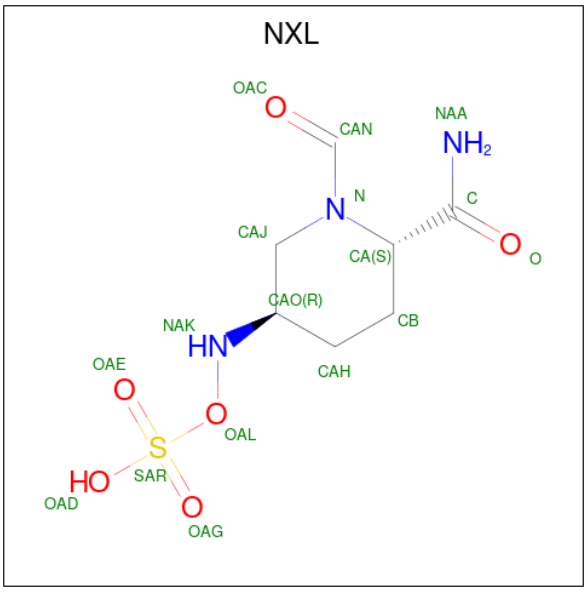
- Molecule 2 is a protein called Beta-lactamase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	242	Total	C	H	N	O	S	0	0	0
			3910	1260	1929	349	365	7			
2	D	242	Total	C	H	N	O	S	3	2	0
			3903	1261	1922	346	367	7			

There are 2 discrepancies between the modelled and reference sequences:

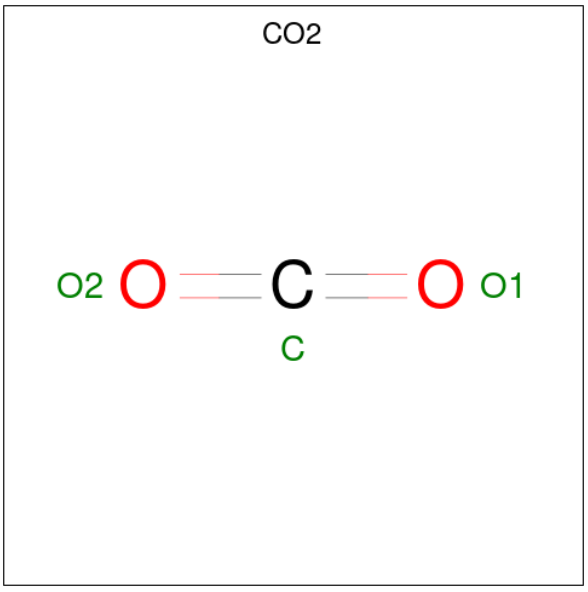
Chain	Residue	Modelled	Actual	Comment	Reference
B	68	ALA	PRO	conflict	UNP Q6XEC0
D	68	ALA	PRO	conflict	UNP Q6XEC0

- Molecule 3 is (2S,5R)-1-formyl-5-[(sulfooxy)amino]piperidine-2-carboxamide (three-letter code: NXL) (formula: $C_7H_{13}N_3O_6S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	0	0
			30	7	13	3	6	1		
3	B	1	Total	C	H	N	O	S	0	0
			30	7	13	3	6	1		
3	C	1	Total	C	H	N	O	S	0	0
			30	7	13	3	6	1		
3	D	1	Total	C	H	N	O	S	0	0
			30	7	13	3	6	1		

- Molecule 4 is CARBON DIOXIDE (three-letter code: CO2) (formula: CO_2).

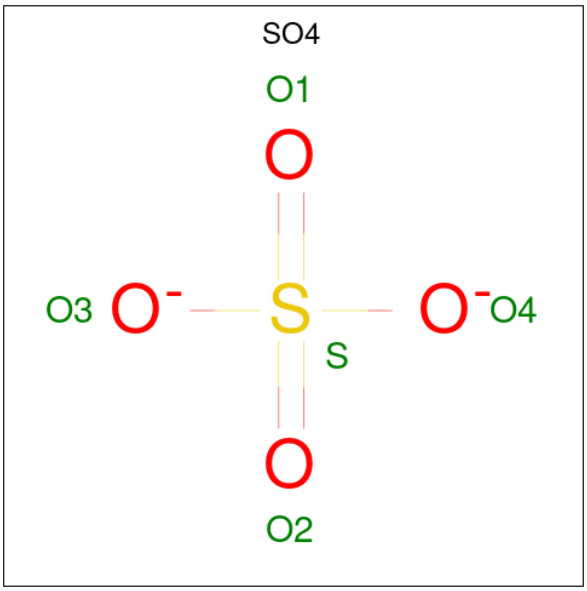


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 3 1 2	0	0
4	C	1	Total C O 3 1 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Cl 2 2	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	176	Total O 176 176	0	0

Continued on next page...

Continued from previous page...

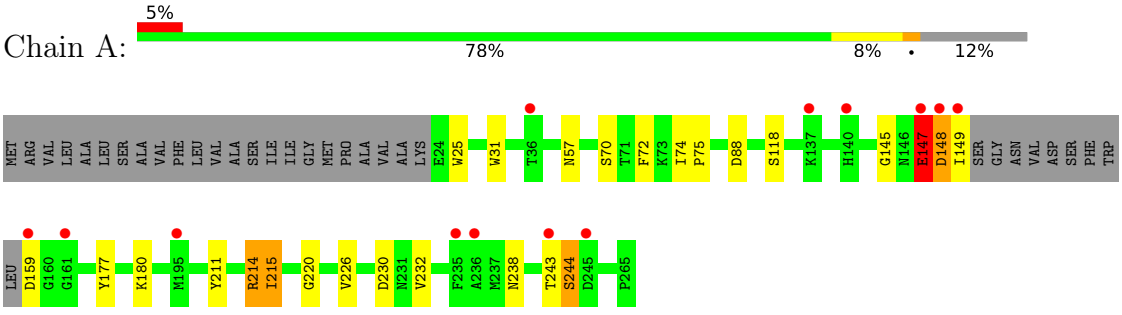
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	171	Total O 171 171	0	0
7	C	162	Total O 162 162	0	0
7	D	190	Total O 190 190	0	0

3 Residue-property plots

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

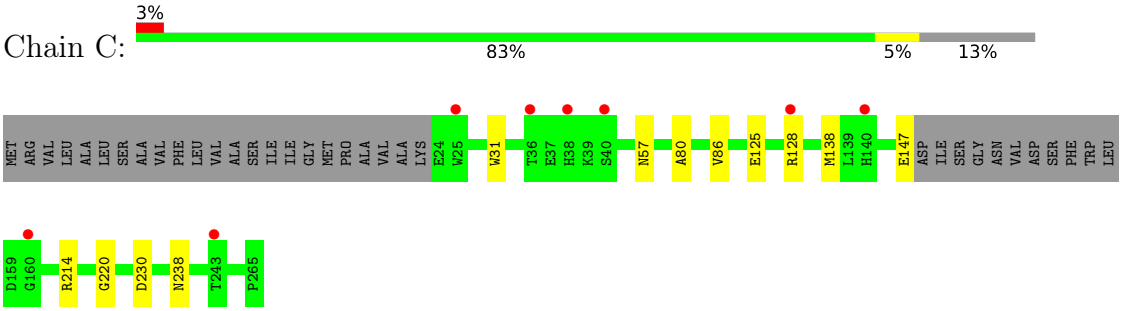
• Molecule 1: Beta-lactamase

Chain A:



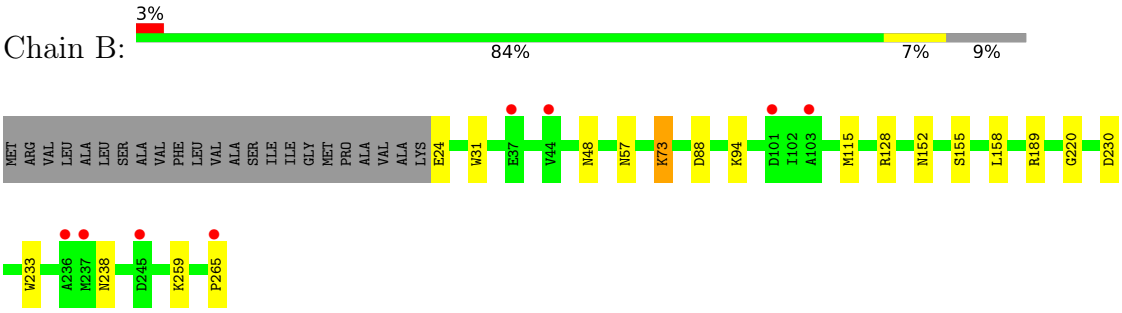
• Molecule 1: Beta-lactamase

Chain C:



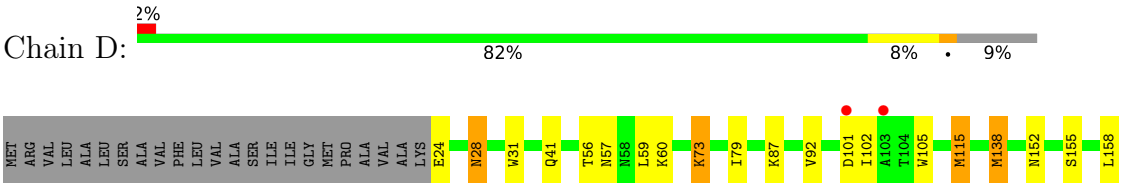
• Molecule 2: Beta-lactamase

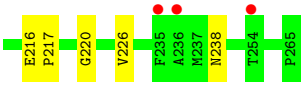
Chain B:



• Molecule 2: Beta-lactamase

Chain D:




E216
P217
G220
V226
F235
A236
M237
N238
T264
P265

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	88.11Å 105.80Å 125.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.83 – 2.22 24.83 – 2.22	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.83-2.22) 99.6 (24.83-2.22)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 2.22Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.204 , 0.262 0.204 , 0.262	Depositor DCC
R_{free} test set	2188 reflections (3.76%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16144	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 53.09 % 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 4.4336e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: KCX, NXL, CO2, CL, SO4

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	0.65	1/1940 (0.1%)	0.71	0/2621
1	C	0.58	0/1958	0.70	0/2645
2	B	0.56	0/2016	0.68	3/2725 (0.1%)
2	D	0.57	0/2019	0.66	1/2730 (0.0%)
All	All	0.59	1/7933 (0.0%)	0.69	4/10721 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ASP	CB-CG	5.30	1.62	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	128	ARG	NE-CZ-NH1	-6.02	117.29	120.30
2	B	115	MET	CG-SD-CE	-5.79	90.94	100.20
2	D	115	MET	CG-SD-CE	-5.59	91.25	100.20
2	B	189	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1896	1852	1848	15	0
1	C	1897	1852	1822	4	0
2	B	1981	1929	1929	11	0
2	D	1981	1922	1912	14	0
3	A	17	13	12	1	0
3	B	17	13	12	1	0
3	C	17	13	12	0	0
3	D	17	13	12	0	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	2	0	0	1	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
6	C	5	0	0	0	0
7	A	176	0	0	2	0
7	B	171	0	0	4	0
7	C	162	0	0	0	1
7	D	190	0	0	7	1
All	All	8537	7607	7559	45	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 3.

All (45) 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:A:145:GLY:O	7:A:401:HOH:O	2.00	0.79
2:D:24:GLU:OE1	7:D:401:HOH:O	2.07	0.73
2:D:73:KCX:OQ1	7:D:402:HOH:O	2.09	0.70
2:B:73:KCX:OQ1	7:B:401:HOH:O	2.10	0.69
1:A:211:TYR:OH	1:A:243:THR:O	2.08	0.68
2:B:158:LEU:HD21	7:B:401:HOH:O	1.93	0.67
1:A:149:ILE:HD13	1:A:149:ILE:H	1.65	0.61
1:A:72:PHE:CG	1:A:159:ASP:N	2.71	0.58
1:A:72:PHE:CB	1:A:159:ASP:N	2.68	0.57
1:A:25:TRP:O	7:A:402:HOH:O	2.18	0.54
2:B:230:ASP:OD1	2:B:230:ASP:N	2.40	0.54
1:A:243:THR:OG1	1:A:244:SER:N	2.41	0.53
1:C:125:GLU:OE2	1:C:128:ARG:NH1	2.41	0.53
1:A:145:GLY:C	1:A:147:GLU:OE2	2.48	0.52
2:B:220:GLY:O	2:B:238:ASN:HA	2.09	0.52
1:A:88:ASP:O	5:A:304:CL:CL	2.65	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:LEU:HD21	7:D:402:HOH:O	2.11	0.50
1:A:220:GLY:O	1:A:238:ASN:HA	2.13	0.49
1:A:177:TYR:CZ	1:A:232:VAL:HG21	2.49	0.47
2:D:216:GLU:OE2	2:D:217:PRO:HA	2.15	0.47
1:A:214:ARG:O	1:A:215:ILE:HD12	2.15	0.47
2:B:88:ASP:OD1	2:B:88:ASP:C	2.54	0.46
1:C:220:GLY:O	1:C:238:ASN:HA	2.15	0.46
2:D:60:LYS:HG2	7:D:504:HOH:O	2.16	0.46
1:A:74:ILE:HB	1:A:75:PRO:CD	2.47	0.45
2:D:87:LYS:NZ	7:D:408:HOH:O	2.48	0.45
2:D:152:ASN:HB2	2:D:155:SER:OG	2.17	0.45
2:D:102:ILE:HD12	2:D:105:TRP:CZ2	2.51	0.45
2:B:31:TRP:HB2	2:B:57:ASN:HB3	1.98	0.45
2:B:24:GLU:OE2	7:B:402:HOH:O	2.21	0.44
1:A:31:TRP:HB2	1:A:57:ASN:HB3	2.00	0.44
2:B:152:ASN:HB2	2:B:155:SER:OG	2.18	0.43
2:D:31:TRP:HB2	2:D:57:ASN:HB3	2.00	0.42
2:D:158:LEU:CD2	7:D:402:HOH:O	2.66	0.42
1:A:70:SER:N	3:A:301:NXL:OAC	2.53	0.42
1:C:31:TRP:HB2	1:C:57:ASN:HB3	2.02	0.42
2:B:48:ASN:HB2	2:B:233:TRP:CH2	2.55	0.42
2:B:24:GLU:N	7:B:411:HOH:O	2.52	0.42
2:D:79:ILE:HG12	2:D:138:MET:HG2	2.02	0.42
2:D:56:THR:CG2	2:D:59:LEU:HD23	2.49	0.41
2:D:28:ASN:CG	7:D:403:HOH:O	2.57	0.41
2:B:259:LYS:HE2	2:B:265:PRO:O	2.21	0.40
1:C:80:ALA:HB1	1:C:86:VAL:HG23	2.02	0.40
2:D:220:GLY:O	2:D:238:ASN:HA	2.21	0.40
3:B:301:NXL:OAL	3:B:301:NXL:H7	2.21	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)
7:C:541:HOH:O	7:D:577:HOH:O[3_654]	2.10	0.10

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	229/265 (86%)	219 (96%)	7 (3%)	3 (1%)	12 9
1	C	231/265 (87%)	223 (96%)	8 (4%)	0	100 100
2	B	239/265 (90%)	234 (98%)	5 (2%)	0	100 100
2	D	241/265 (91%)	237 (98%)	4 (2%)	0	100 100
All	All	940/1060 (89%)	913 (97%)	24 (3%)	3 (0%)	41 45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	ASP
1	A	244	SER
1	A	147	GLU

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	198/227 (87%)	191 (96%)	7 (4%)	36 44
1	C	201/227 (88%)	197 (98%)	4 (2%)	55 67
2	B	209/226 (92%)	208 (100%)	1 (0%)	88 94
2	D	206/226 (91%)	198 (96%)	8 (4%)	32 40
All	All	814/906 (90%)	794 (98%)	20 (2%)	50 58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	SER
1	A	147	GLU
1	A	180	LYS
1	A	214	ARG
1	A	215	ILE
1	A	226	VAL
1	A	230	ASP
2	B	94	LYS
1	C	138	MET
1	C	147	GLU
1	C	214	ARG
1	C	230	ASP
2	D	28	ASN
2	D	41[A]	GLN
2	D	41[B]	GLN
2	D	92	VAL
2	D	101	ASP
2	D	115	MET
2	D	138	MET
2	D	226	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 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	$\#\|Z\| > 2$
2	KCX	B	73	2	9,11,12	1.18	1 (11%)	5,12,14	1.18	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	KCX	D	73	2	9,11,12	1.18	1 (11%)	5,12,14	1.90	1 (20%)

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	KCX	B	73	2	-	0/9/10/12	-
2	KCX	D	73	2	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	73	KCX	CE-NZ	2.34	1.51	1.46
2	B	73	KCX	CE-NZ	2.19	1.51	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	73	KCX	OQ1-CX-NZ	-4.16	118.52	124.96
2	B	73	KCX	OQ1-CX-NZ	-2.40	121.23	124.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	73	KCX	1	0
2	D	73	KCX	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	CO2	C	302	-	2,2,2	1.14	0	1,1,1	0.47	0
3	NXL	A	301	1	14,17,17	1.92	3 (21%)	17,24,24	2.12	5 (29%)
4	CO2	A	302	-	2,2,2	1.12	0	1,1,1	0.53	0
6	SO4	C	304	-	4,4,4	0.23	0	6,6,6	0.44	0
3	NXL	D	301	2	14,17,17	2.39	4 (28%)	17,24,24	2.62	10 (58%)
3	NXL	C	301	1	14,17,17	2.45	3 (21%)	17,24,24	2.31	7 (41%)
3	NXL	B	301	2	14,17,17	2.18	2 (14%)	17,24,24	1.75	5 (29%)

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	NXL	C	301	1	-	2/5/25/25	0/1/1/1
3	NXL	A	301	1	-	3/5/25/25	0/1/1/1
3	NXL	B	301	2	-	2/5/25/25	0/1/1/1
3	NXL	D	301	2	-	2/5/25/25	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	NXL	CAN-N	6.12	1.47	1.34
3	C	301	NXL	CAN-N	5.93	1.47	1.34
3	B	301	NXL	C-NAA	5.36	1.46	1.32
3	C	301	NXL	C-NAA	5.31	1.46	1.32
3	A	301	NXL	C-NAA	5.17	1.45	1.32
3	B	301	NXL	CAN-N	5.06	1.45	1.34
3	D	301	NXL	C-NAA	4.52	1.44	1.32
3	A	301	NXL	CAN-N	3.61	1.42	1.34
3	C	301	NXL	CAJ-N	3.28	1.52	1.47
3	D	301	NXL	CAJ-N	3.01	1.52	1.47
3	A	301	NXL	CAJ-N	2.22	1.51	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	301	NXL	O-C	-2.08	1.19	1.23

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	301	NXL	CB-CAH-CAO	5.59	117.67	111.48
3	A	301	NXL	CB-CAH-CAO	5.48	117.55	111.48
3	C	301	NXL	O-C-NAA	-4.70	114.82	123.00
3	D	301	NXL	CAH-CAO-CAJ	4.65	115.76	109.71
3	B	301	NXL	OAL-SAR-OAG	4.36	117.13	103.29
3	C	301	NXL	OAC-CAN-N	-3.97	114.35	125.59
3	D	301	NXL	OAC-CAN-N	-3.95	114.42	125.59
3	A	301	NXL	O-C-NAA	-3.90	116.22	123.00
3	C	301	NXL	OAL-SAR-OAE	3.60	114.71	103.29
3	C	301	NXL	CB-CAH-CAO	3.38	115.23	111.48
3	C	301	NXL	CA-C-NAA	3.20	124.35	116.55
3	B	301	NXL	CAH-CAO-CAJ	2.82	113.37	109.71
3	D	301	NXL	O-C-NAA	-2.81	118.11	123.00
3	C	301	NXL	OAD-SAR-OAG	-2.80	98.75	108.49
3	D	301	NXL	CB-CA-C	-2.69	107.29	112.12
3	A	301	NXL	O-C-CA	2.68	125.04	120.26
3	D	301	NXL	O-C-CA	2.45	124.64	120.26
3	D	301	NXL	C-CA-N	2.37	116.94	111.27
3	A	301	NXL	CAJ-CAO-NAK	2.30	117.75	109.02
3	D	301	NXL	OAD-SAR-OAG	2.30	116.48	108.49
3	A	301	NXL	OAL-SAR-OAG	2.27	110.48	103.29
3	D	301	NXL	OAL-SAR-OAE	2.24	110.39	103.29
3	B	301	NXL	O-C-CA	2.20	124.19	120.26
3	B	301	NXL	O-C-NAA	-2.16	119.25	123.00
3	C	301	NXL	CAO-CAJ-N	2.13	113.11	110.11
3	B	301	NXL	OAD-SAR-OAE	2.08	115.72	108.49
3	D	301	NXL	OAL-SAR-OAG	2.01	109.68	103.29

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	NXL	O-C-CA-N
3	A	301	NXL	O-C-CA-CB
3	A	301	NXL	NAA-C-CA-CB
3	C	301	NXL	NAA-C-CA-CB
3	C	301	NXL	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	301	NXL	NAA-C-CA-CB
3	D	301	NXL	O-C-CA-CB
3	B	301	NXL	NAA-C-CA-CB
3	B	301	NXL	O-C-CA-CB

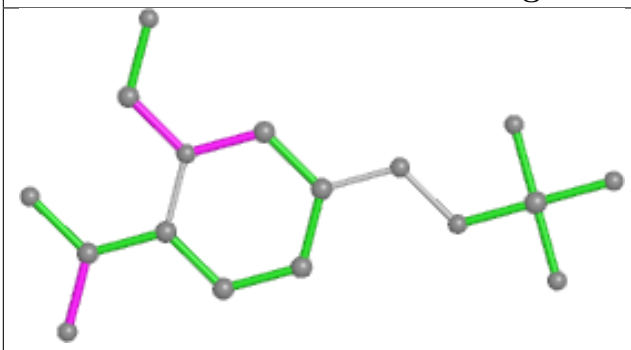
There are no ring outliers.

2 monomers are involved in 2 short contacts:

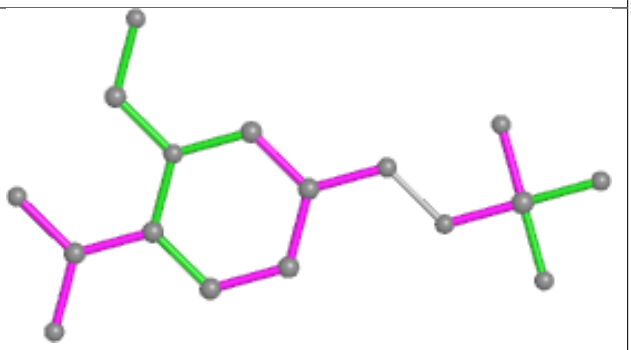
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	NXL	1	0
3	B	301	NXL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

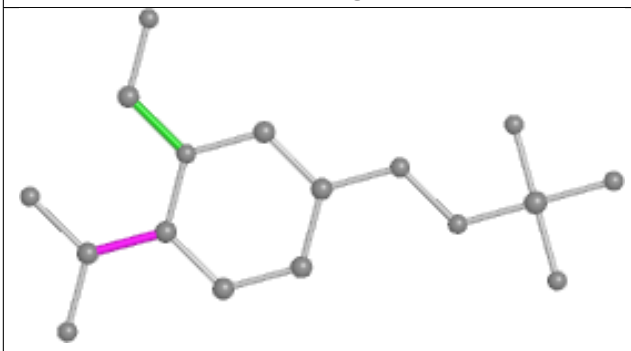
Ligand NXL A 301



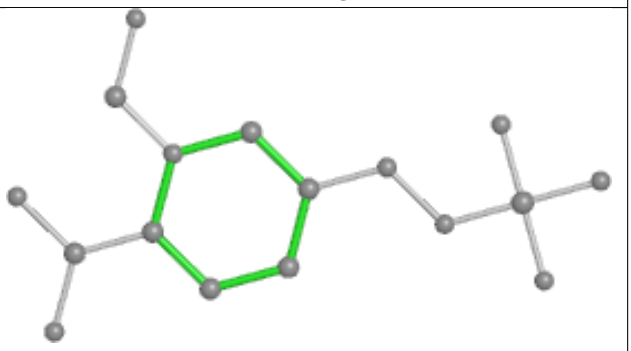
Bond lengths



Bond angles

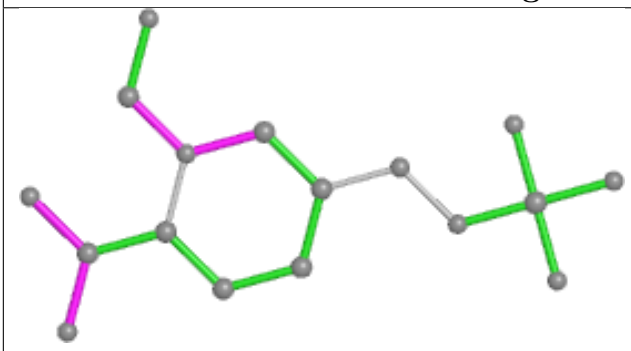


Torsions

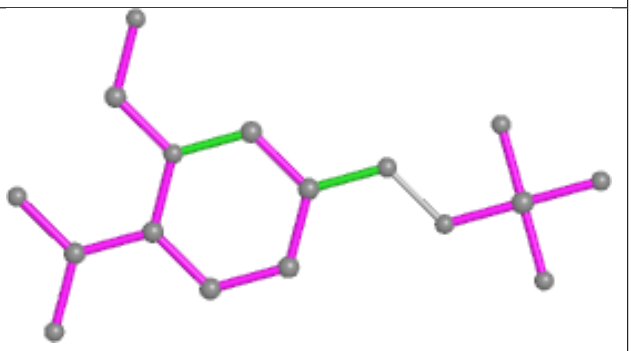


Rings

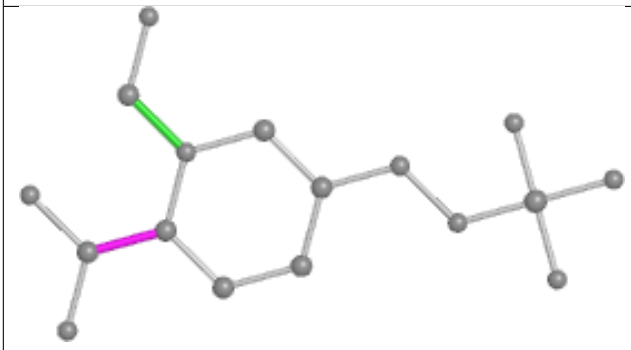
Ligand NXL D 301



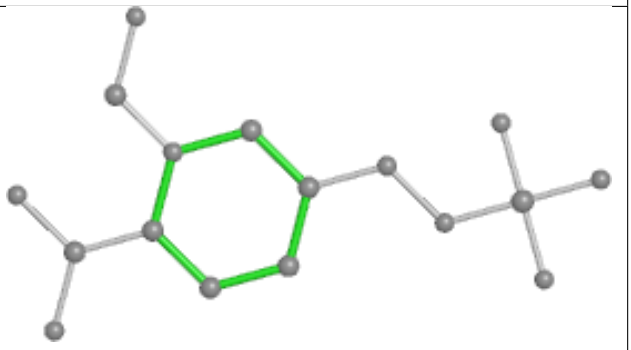
Bond lengths



Bond angles

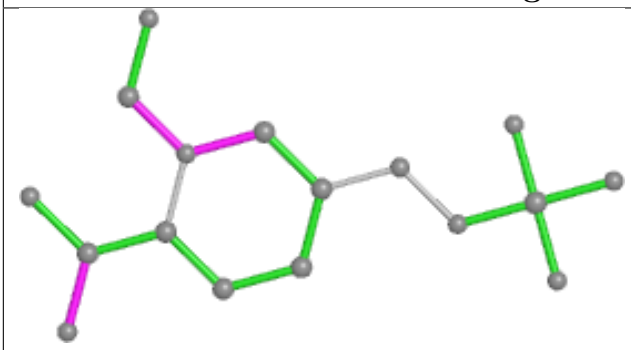


Torsions

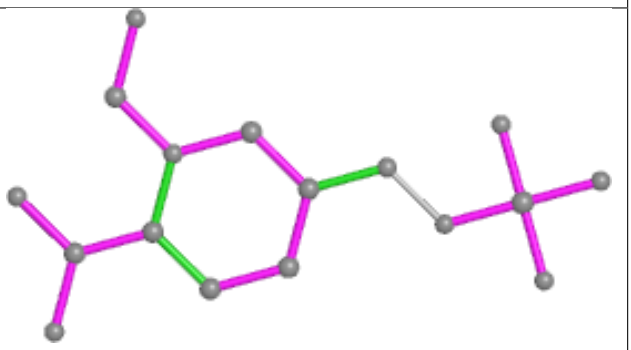


Rings

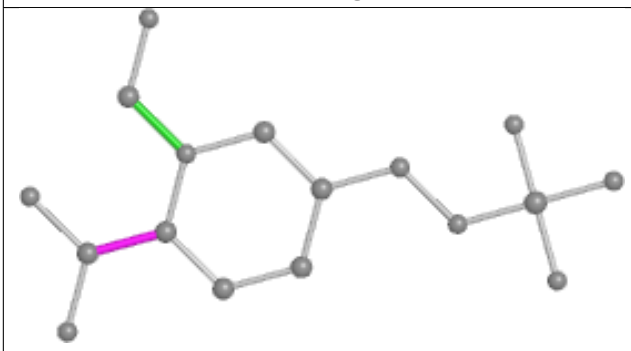
Ligand NXL C 301



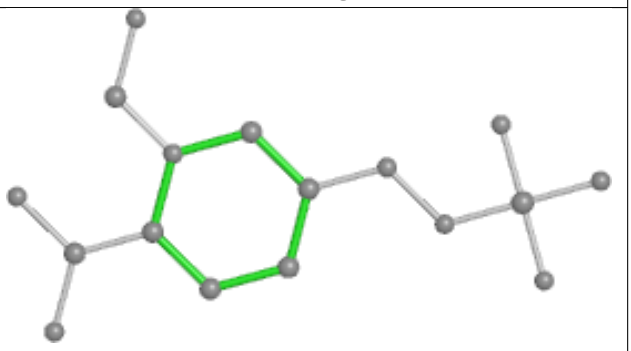
Bond lengths



Bond angles

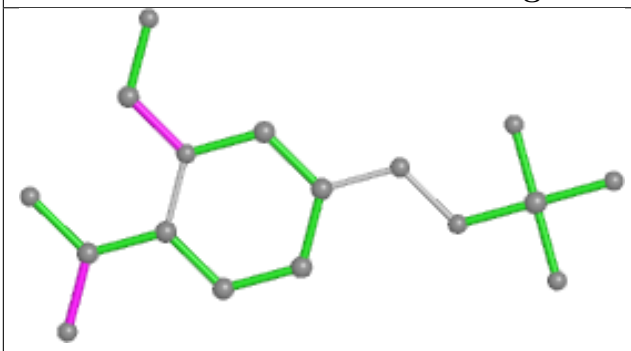


Torsions

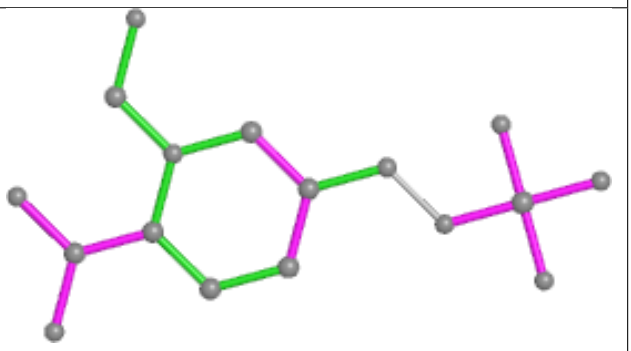


Rings

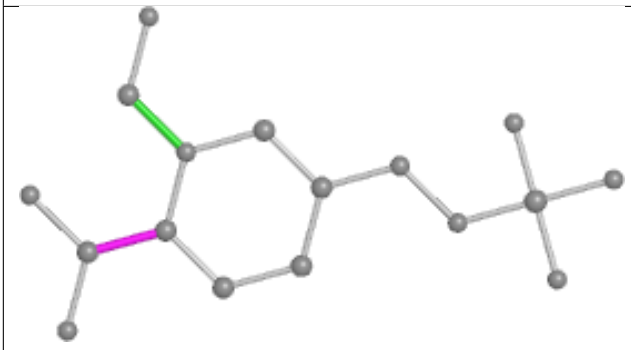
Ligand NXL B 301



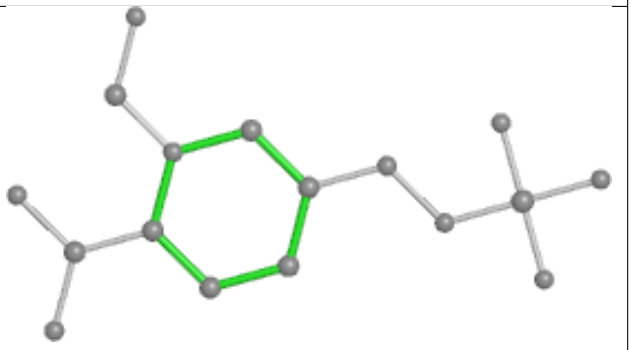
Bond lengths



Bond angles



Torsions



Rings

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, 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	233/265 (87%)	0.12	13 (5%)	24	23	18, 29, 61, 91	2 (0%)
1	C	231/265 (87%)	0.10	8 (3%)	44	41	19, 30, 59, 105	6 (2%)
2	B	241/265 (90%)	0.02	8 (3%)	46	44	17, 29, 54, 78	4 (1%)
2	D	241/265 (90%)	-0.06	5 (2%)	63	61	17, 30, 51, 75	5 (2%)
All	All	946/1060 (89%)	0.04	34 (3%)	42	40	17, 30, 56, 105	17 (1%)

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	148	ASP	5.5
1	A	149	ILE	4.1
2	B	101	ASP	4.0
1	A	243	THR	3.9
1	C	36	THR	3.7
1	C	160	GLY	3.6
1	A	161	GLY	3.5
2	D	103	ALA	3.1
1	C	140	HIS	3.1
1	A	147	GLU	3.0
1	A	137	LYS	3.0
1	C	243	THR	3.0
2	B	236	ALA	2.9
1	A	159	ASP	2.9
1	A	236	ALA	2.8
1	A	245	ASP	2.8
2	B	44	VAL	2.7
2	B	245	ASP	2.6
1	A	36	THR	2.5
2	B	103	ALA	2.5
1	A	140	HIS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	40	SER	2.5
1	C	128	ARG	2.3
1	A	235	PHE	2.3
2	B	265	PRO	2.3
2	D	235	PHE	2.3
2	D	101	ASP	2.3
1	A	195	MET	2.2
2	D	254	THR	2.2
2	B	237	MET	2.1
1	C	25	TRP	2.1
2	B	37	GLU	2.0
1	C	38	HIS	2.0
2	D	236	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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	KCX	B	73	12/13	0.93	0.19	19,29,38,46	0
2	KCX	D	73	12/13	0.95	0.19	18,29,35,47	0

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
4	CO2	C	302	3/3	0.84	0.22	38,38,54,57	0
5	CL	B	302	1/1	0.87	0.08	54,54,54,54	0
6	SO4	C	304	5/5	0.89	0.23	34,37,44,60	5

Continued on next page...

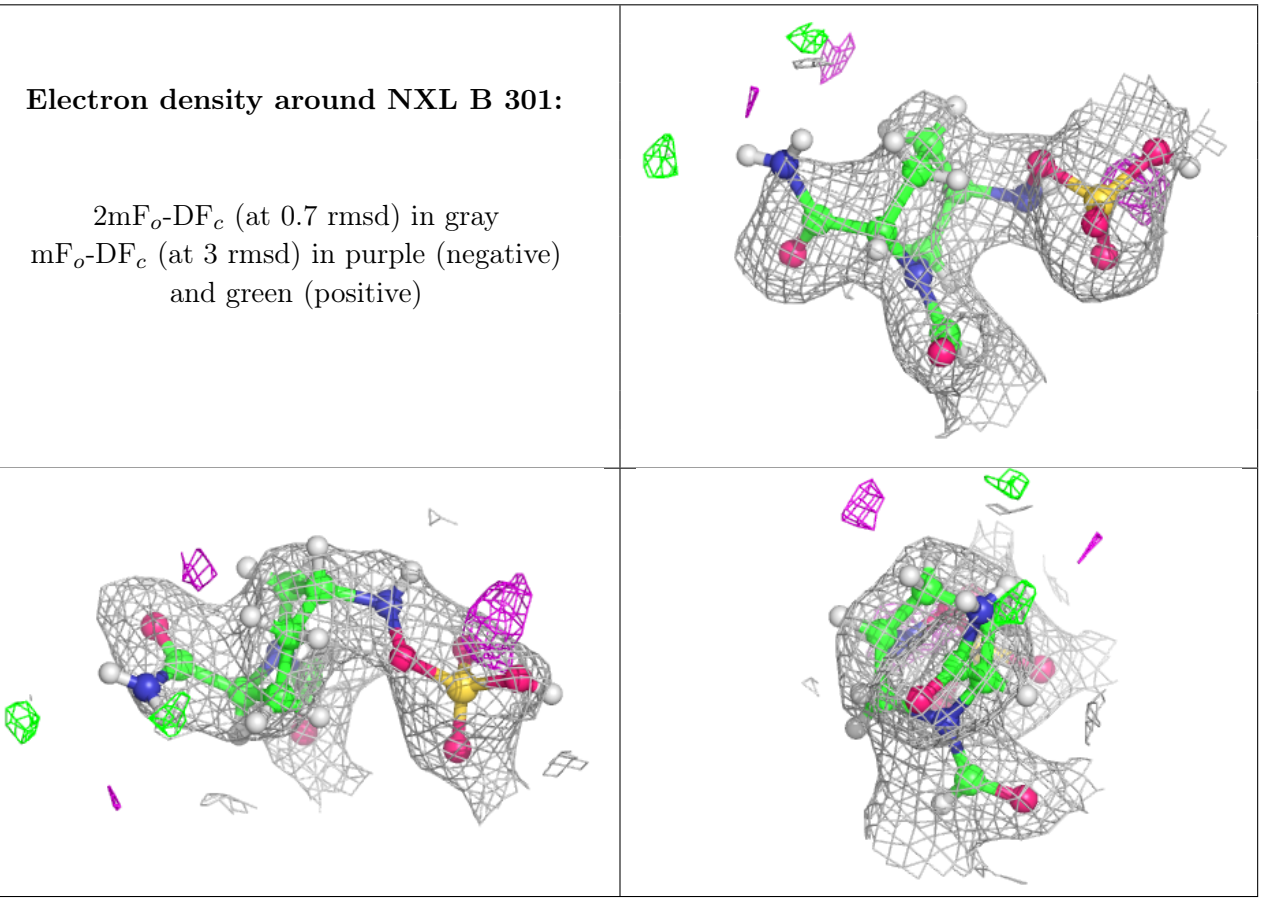
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CO2	A	302	3/3	0.92	0.34	32,32,49,62	0
3	NXL	B	301	17/17	0.93	0.15	23,33,50,54	0
3	NXL	D	301	17/17	0.94	0.15	27,34,43,51	0
3	NXL	C	301	17/17	0.96	0.12	24,33,44,48	0
3	NXL	A	301	17/17	0.96	0.12	26,34,42,49	0
5	CL	A	304	1/1	0.98	0.08	47,47,47,47	0
5	CL	A	303	1/1	0.99	0.13	23,23,23,23	0
5	CL	C	303	1/1	1.00	0.11	21,21,21,21	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.

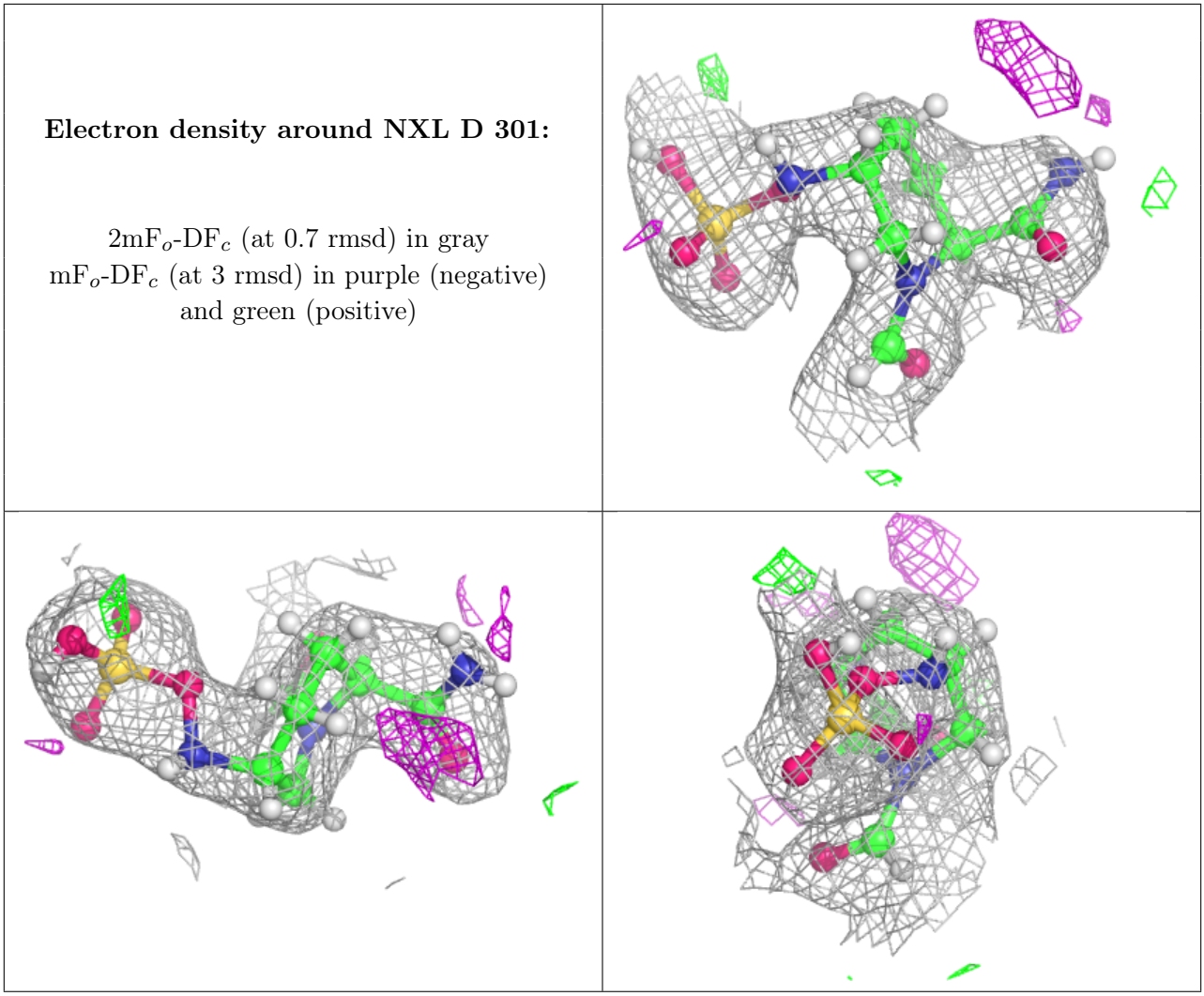
Electron density around NXL B 301:

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



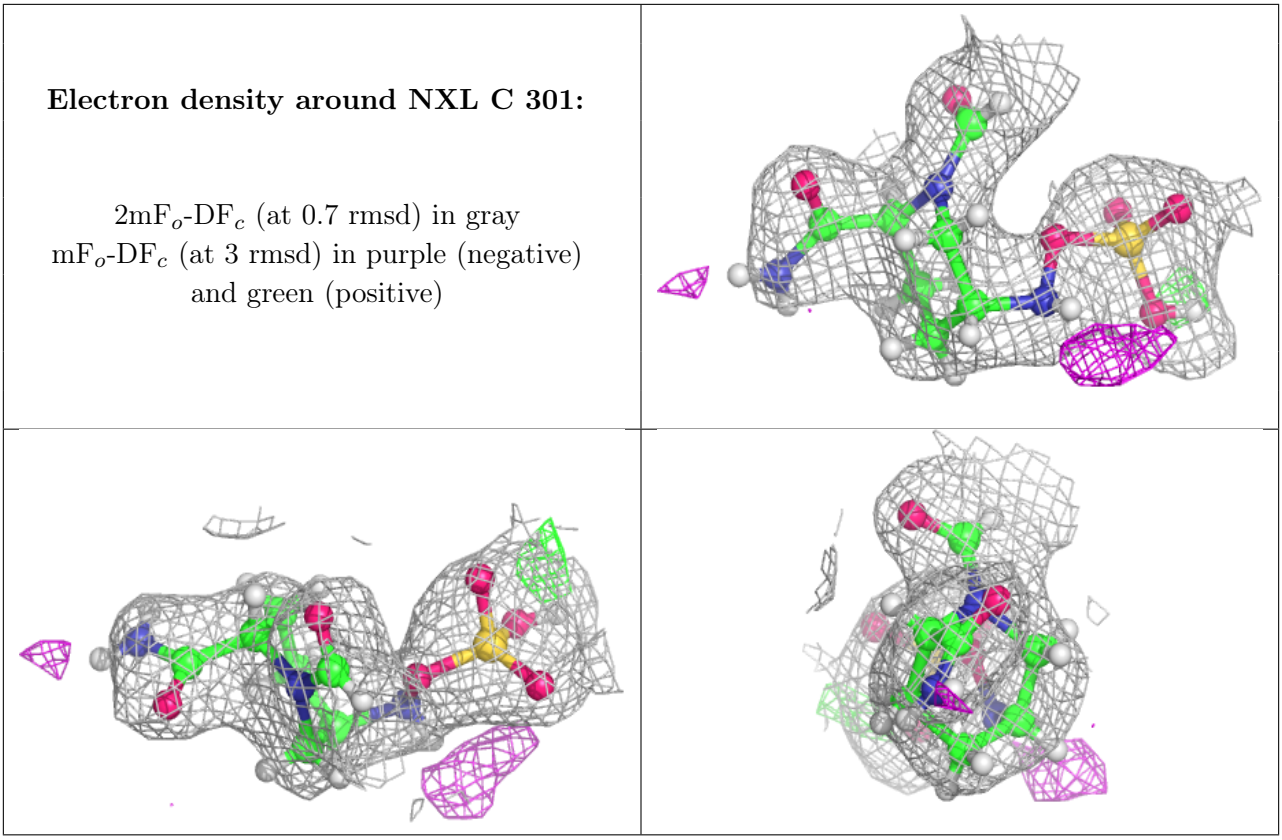
Electron density around NXL D 301:

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



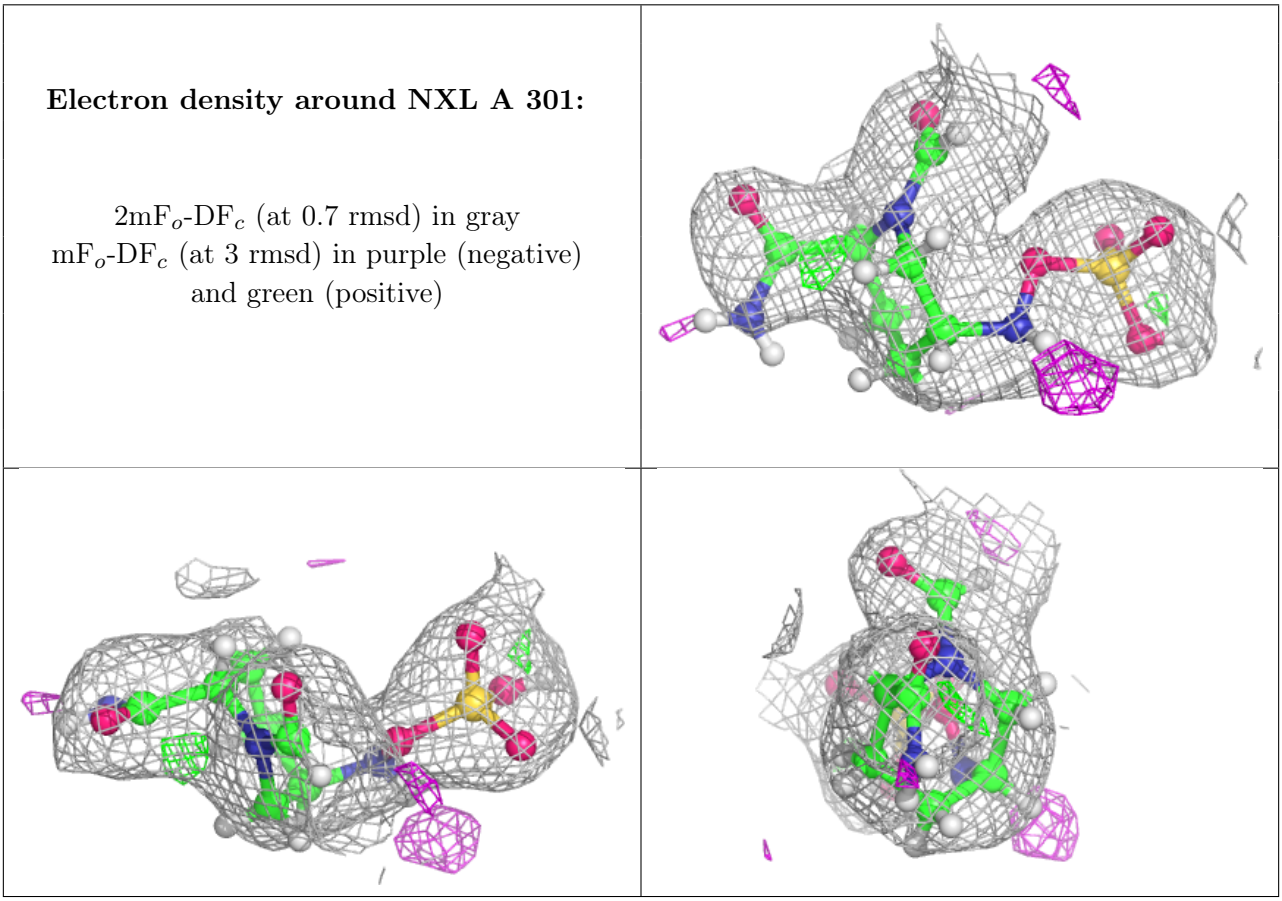
Electron density around NXL C 301:

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



Electron density around NXL A 301:

$2mF_o$-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.