



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 8, 2022 – 10:29 am BST

PDB ID : 7PCS
Title : Structure of the heterotetrameric SDR family member BbsCD
Authors : Essen, L.-O.; Heider, J.; von Horsten, S.
Deposited on : 2021-08-04
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

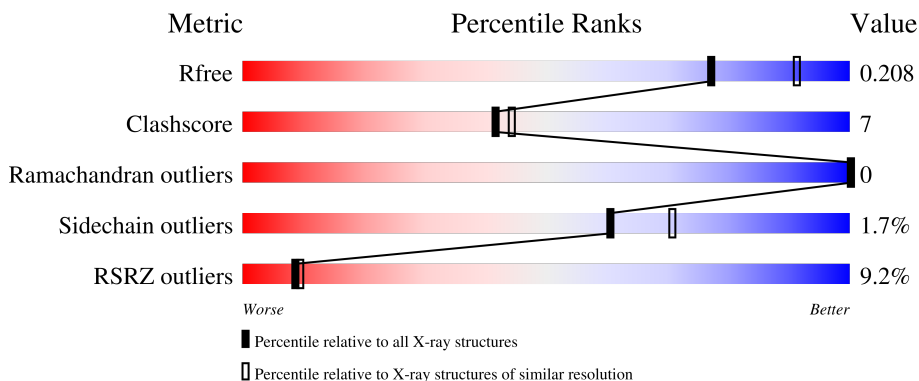
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


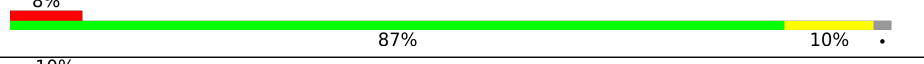


The reported resolution of this entry is 2.25 Å.

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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	250	
1	C	250	
2	B	248	
2	D	248	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	301	-	-	X	-
3	GOL	D	304	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14941 atoms, of which 7349 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 BbsC.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	244	3562	1095	1808	318	336	5	0	3	0
1	C	244	3562	1095	1808	318	336	5	0	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	98	LYS	ASN	engineered mutation	UNP Q9KJF2
A	99	PRO	-	insertion	UNP Q9KJF2
C	98	LYS	ASN	engineered mutation	UNP Q9KJF2
C	99	PRO	-	insertion	UNP Q9KJF2

- Molecule 2 is a protein called BbsD.

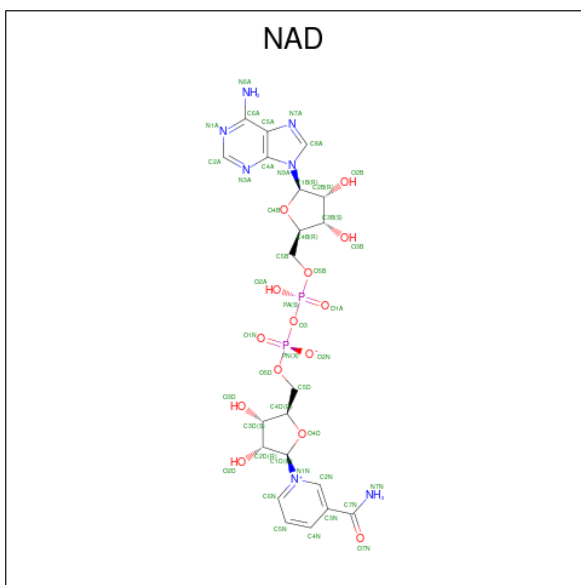
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	247	3637	1134	1818	331	344	10	0	1	0
2	D	247	3668	1141	1836	335	347	9	0	1	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	8	3	2	3	0	0
3	A	1	9	3	3	3	0	0
3	B	1	9	3	3	3	0	0
3	C	1	9	3	3	3	0	0
3	C	1	8	3	2	3	0	0
3	D	1	9	3	3	3	0	0
3	D	1	9	3	3	3	0	0
3	D	1	14	3	8	3	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula: $C_{21}H_{27}N_7O_{14}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	H	N	O			P
4	B	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		
4	D	1	Total	C	H	N	O	P	0	0
			70	21	26	7	14	2		

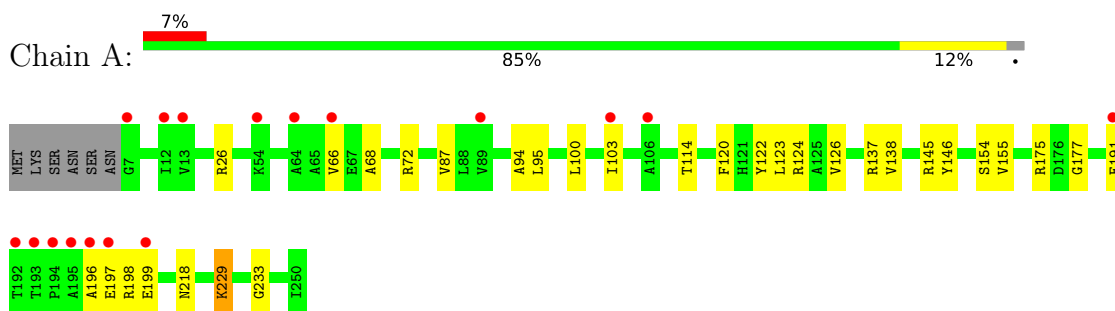
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	86	Total	O	0	0
			86	86		
5	B	80	Total	O	0	0
			80	80		
5	C	68	Total	O	0	0
			68	68		
5	D	63	Total	O	0	0
			63	63		

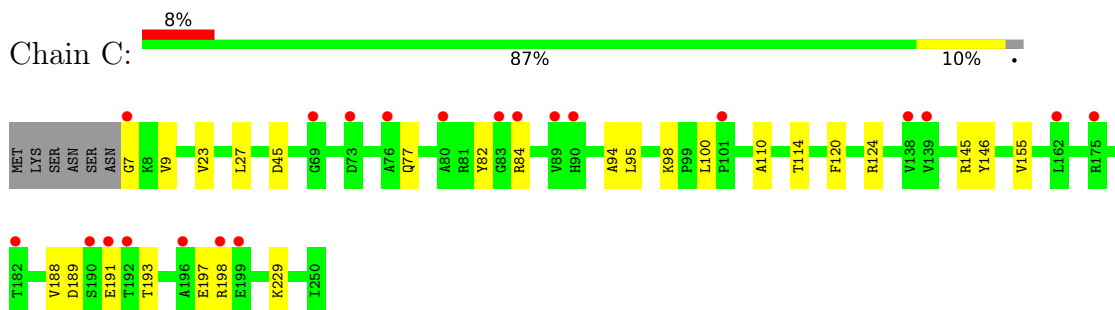
3 Residue-property plots [i](#)

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.

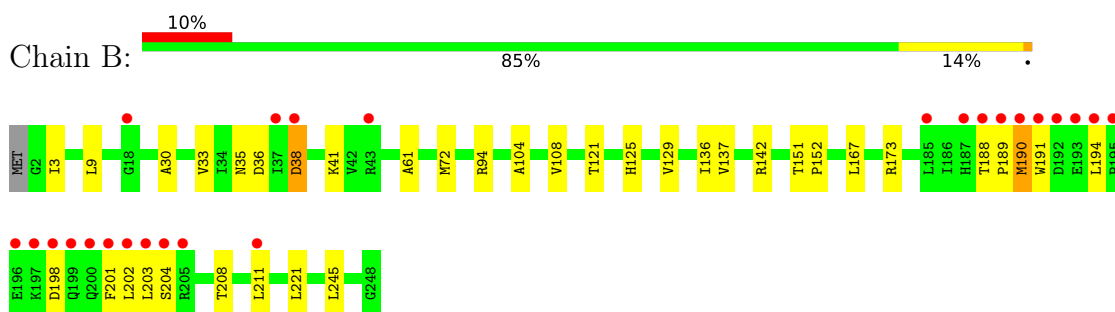
- Molecule 1: BbsC



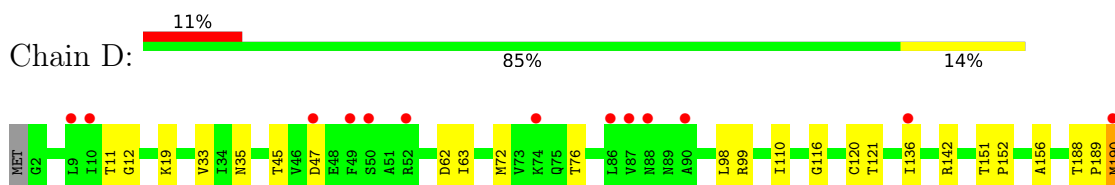
- Molecule 1: BbsC

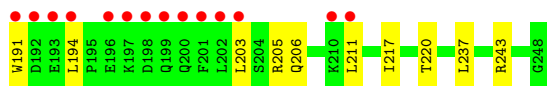


- Molecule 2: BbsD



- Molecule 2: BbsD





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	68.60Å 68.60Å 191.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.70 – 2.25 29.70 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.2 (29.70-2.25) 96.2 (29.70-2.25)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.24Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122, PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.184 , 0.210 0.184 , 0.208	Depositor DCC
R_{free} test set	961 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	37.6	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for -h,-k,l 0.044 for h,-h-k,-l 0.024 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14941	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: GOL, NAD

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	0.31	0/1782	0.56	0/2414
1	C	0.30	0/1782	0.56	0/2414
2	B	0.38	1/1848 (0.1%)	0.71	2/2501 (0.1%)
2	D	0.31	0/1861	0.57	0/2517
All	All	0.33	1/7273 (0.0%)	0.60	2/9846 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	38	ASP	CB-CG	-5.22	1.40	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	38	ASP	CB-CG-OD1	16.12	132.81	118.30
2	B	38	ASP	OD1-CG-OD2	-10.65	103.06	123.30

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	1754	1808	1808	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1754	1808	1808	22	0
2	B	1819	1818	1818	31	0
2	D	1832	1836	1836	31	0
3	A	12	5	16	4	0
3	B	6	3	8	2	0
3	C	12	5	16	4	0
3	D	18	14	24	2	0
4	B	44	26	26	1	0
4	D	44	26	26	5	0
5	A	86	0	0	0	0
5	B	80	0	0	2	0
5	C	68	0	0	3	0
5	D	63	0	0	2	0
All	All	7592	7349	7386	102	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 7.

All (102) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:THR:O	1:C:198:ARG:NH1	2.05	0.89
1:A:26[B]:ARG:NH1	1:A:218:ASN:O	2.10	0.84
2:D:47:ASP:OD1	5:D:401:HOH:O	1.98	0.81
1:C:7:GLY:O	1:C:84:ARG:NH2	2.17	0.78
1:C:197:GLU:OE2	5:C:401:HOH:O	2.01	0.77
2:B:173:ARG:NH2	5:B:401:HOH:O	2.19	0.76
2:D:206:GLN:NE2	5:D:402:HOH:O	2.21	0.73
2:D:191:TRP:CE2	2:D:211:LEU:HD11	2.24	0.73
2:B:202:LEU:HD12	2:B:202:LEU:H	1.55	0.71
2:B:191:TRP:CE2	2:B:211:LEU:HD11	2.28	0.69
1:C:77:GLN:O	5:C:402:HOH:O	2.10	0.67
1:C:145[B]:ARG:NH2	3:C:302:GOL:O3	2.28	0.67
1:C:188:VAL:HG23	3:C:302:GOL:H12	1.78	0.65
2:B:201:PHE:O	2:B:204:SER:OG	2.12	0.64
2:B:191:TRP:CZ2	2:B:211:LEU:HD11	2.34	0.63
2:D:11:THR:HB	2:D:63:ILE:CD1	2.30	0.62
1:A:26[A]:ARG:NH2	1:A:218:ASN:OD1	2.33	0.62
2:B:202:LEU:HD12	2:B:202:LEU:N	2.15	0.61
2:D:11:THR:HB	2:D:63:ILE:HD11	1.81	0.61
1:C:145[B]:ARG:NH1	5:C:405:HOH:O	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:MET:SD	2:D:194:LEU:HD11	2.43	0.58
2:B:190:MET:O	2:B:194:LEU:HD13	2.04	0.57
2:B:190:MET:SD	2:B:190:MET:N	2.77	0.56
2:D:142:ARG:HB3	3:D:302:GOL:H2	1.88	0.56
2:D:220:THR:CG2	2:D:237:LEU:HD23	2.37	0.55
2:B:36:ASP:OD1	4:B:301:NAD:O2B	2.21	0.55
1:C:23:VAL:O	1:C:27:LEU:HD23	2.07	0.54
1:A:94:ALA:O	1:A:95:LEU:HD23	2.06	0.54
1:A:122:TYR:O	1:A:126:VAL:HG23	2.08	0.54
2:D:19:LYS:HE3	2:D:45:THR:HG23	1.90	0.54
1:C:95:LEU:HD21	1:C:114:THR:HG23	1.89	0.54
1:A:100:LEU:HD11	1:C:124:ARG:HG2	1.89	0.53
1:C:94:ALA:O	1:C:95:LEU:HD23	2.08	0.53
1:C:189:ASP:OD1	1:C:198:ARG:NE	2.32	0.53
1:A:68:ALA:HB1	1:A:72:ARG:HH12	1.74	0.53
2:B:203:LEU:HD21	2:B:211:LEU:HG	1.91	0.52
1:C:45:ASP:OD1	3:C:301:GOL:H12	2.09	0.52
1:A:233:GLY:HA3	2:B:245:LEU:HD11	1.91	0.52
1:C:191:GLU:H	1:C:198:ARG:HH21	1.58	0.51
1:C:191:GLU:H	1:C:198:ARG:NH2	2.08	0.51
2:B:190:MET:O	2:B:194:LEU:CD1	2.59	0.50
2:B:104:ALA:O	2:B:108:VAL:HG12	2.12	0.50
3:A:301:GOL:H31	2:B:208:THR:HG22	1.93	0.50
2:B:202:LEU:H	2:B:202:LEU:CD1	2.24	0.49
1:C:95:LEU:HD21	1:C:114:THR:CG2	2.43	0.49
2:D:63:ILE:H	4:D:301:NAD:H61A	1.61	0.49
4:D:301:NAD:H2B	4:D:301:NAD:N3A	2.26	0.49
2:D:151:THR:HB	2:D:152:PRO:HD3	1.94	0.49
1:C:9:VAL:HG21	1:C:82:TYR:HB3	1.96	0.48
1:A:123:LEU:HD22	1:A:138:VAL:HG11	1.95	0.48
1:A:177:GLY:HA2	3:A:301:GOL:H32	1.94	0.48
1:A:124:ARG:HG2	1:C:100:LEU:HD11	1.96	0.47
2:D:203:LEU:HD21	2:D:211:LEU:HG	1.97	0.47
2:D:205:ARG:O	2:D:243[B]:ARG:NE	2.48	0.47
1:C:110:ALA:O	1:C:114:THR:HG22	2.16	0.46
1:A:145[A]:ARG:CZ	1:A:155:VAL:HG11	2.45	0.46
2:B:121:THR:HG23	2:B:136:ILE:HD13	1.97	0.46
3:B:302:GOL:H11	5:B:470:HOH:O	2.15	0.46
2:D:62:ASP:OD1	4:D:301:NAD:N6A	2.48	0.46
2:D:190:MET:O	2:D:194:LEU:HD13	2.14	0.46
1:C:145[A]:ARG:CZ	1:C:155:VAL:HG11	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:33:VAL:HG21	2:D:76:THR:HG23	1.97	0.46
1:A:100:LEU:HA	1:A:103:ILE:HG13	1.98	0.46
1:A:229:LYS:O	3:A:301:GOL:H2	2.15	0.46
2:B:137:VAL:HG11	2:B:221:LEU:CD2	2.46	0.46
2:B:142:ARG:HB3	3:B:302:GOL:H31	1.98	0.45
2:B:188:THR:OG1	2:B:189:PRO:HD2	2.16	0.45
1:A:196:ALA:HA	1:A:199:GLU:HG2	1.98	0.45
2:B:3:ILE:HD12	2:B:30:ALA:HB2	1.98	0.45
1:A:87:VAL:HG22	1:A:137:ARG:HB2	1.99	0.45
1:A:191:GLU:HA	1:A:198:ARG:HH21	1.81	0.45
2:D:63:ILE:HG22	2:D:116:GLY:HA3	1.98	0.45
2:B:151:THR:HB	2:B:152:PRO:HD3	1.99	0.44
2:D:19:LYS:HE3	2:D:45:THR:CG2	2.47	0.44
2:D:191:TRP:NE1	2:D:211:LEU:HD11	2.33	0.44
1:A:177:GLY:CA	3:A:301:GOL:H32	2.48	0.44
1:C:188:VAL:CG2	3:C:302:GOL:H12	2.45	0.44
2:D:63:ILE:N	4:D:301:NAD:H61A	2.15	0.44
2:B:61:ALA:HB3	2:B:72:MET:HE3	2.00	0.43
2:D:188:THR:OG1	2:D:189:PRO:HD2	2.18	0.43
2:D:63:ILE:HG22	2:D:116:GLY:CA	2.48	0.43
2:D:217:ILE:N	2:D:217:ILE:HD12	2.32	0.43
1:A:66:VAL:HG11	1:A:114:THR:HG22	1.99	0.43
2:B:38:ASP:CG	2:B:41:LYS:HG3	2.38	0.43
2:B:188:THR:HG21	2:B:190:MET:HG2	2.00	0.43
2:B:198:ASP:O	2:B:202:LEU:CD1	2.67	0.43
2:D:35:ASN:OD1	2:D:72:MET:CE	2.67	0.43
1:A:68:ALA:HB1	1:A:72:ARG:NH1	2.33	0.43
2:D:63:ILE:HD12	4:D:301:NAD:N7A	2.34	0.43
2:B:9:LEU:HD13	2:B:33:VAL:HB	2.00	0.42
1:A:103:ILE:HD12	1:A:154:SER:HB3	2.01	0.42
2:D:12:GLY:H	2:D:35:ASN:HD22	1.67	0.42
2:D:99:ARG:NH1	3:D:304:GOL:H32	2.34	0.42
2:B:35:ASN:HB2	2:B:72:MET:HE2	2.02	0.42
2:B:125:HIS:O	2:B:129:VAL:HG23	2.20	0.42
2:D:121:THR:HG23	2:D:136:ILE:HD13	2.02	0.42
2:B:188:THR:HG23	2:B:191:TRP:H	1.85	0.42
1:C:191:GLU:N	1:C:198:ARG:NH2	2.68	0.41
2:D:63:ILE:HG23	2:D:120:CYS:SG	2.60	0.41
2:B:125:HIS:CG	2:D:98:LEU:HD23	2.56	0.41
2:B:121:THR:HG21	2:B:167:LEU:HD13	2.02	0.41
2:D:110:ILE:HD13	2:D:156:ALA:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	245/250 (98%)	236 (96%)	9 (4%)	0	100	100
1	C	245/250 (98%)	234 (96%)	11 (4%)	0	100	100
2	B	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
2	D	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
All	All	982/996 (99%)	952 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	173/176 (98%)	168 (97%)	5 (3%)	42	51
1	C	173/176 (98%)	169 (98%)	4 (2%)	50	59
2	B	184/187 (98%)	182 (99%)	2 (1%)	73	82
2	D	186/187 (100%)	185 (100%)	1 (0%)	88	92
All	All	716/726 (99%)	704 (98%)	12 (2%)	60	71

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	PHE
1	A	146	TYR
1	A	175	ARG
1	A	197	GLU
1	A	229	LYS
2	B	94	ARG
2	B	190	MET
1	C	98	LYS
1	C	120	PHE
1	C	146	TYR
1	C	229	LYS
2	D	190	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	187	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
3	GOL	D	304	-	5,5,5	0.56	0	5,5,5	1.43	1 (20%)
4	NAD	B	301	-	42,48,48	4.91	13 (30%)	50,73,73	1.77	7 (14%)
3	GOL	B	302	-	5,5,5	0.62	0	5,5,5	1.01	0
3	GOL	A	301	-	5,5,5	1.00	0	5,5,5	1.05	1 (20%)
3	GOL	D	303	-	5,5,5	0.81	0	5,5,5	1.05	0
3	GOL	A	302	-	5,5,5	0.82	0	5,5,5	1.01	0
3	GOL	C	302	-	5,5,5	0.69	0	5,5,5	1.14	1 (20%)
3	GOL	D	302	-	5,5,5	0.78	0	5,5,5	1.08	0
4	NAD	D	301	-	42,48,48	4.98	12 (28%)	50,73,73	1.68	7 (14%)
3	GOL	C	301	-	5,5,5	0.79	0	5,5,5	1.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	304	-	-	2/4/4/4	-
4	NAD	B	301	-	-	4/26/62/62	0/5/5/5
3	GOL	B	302	-	-	0/4/4/4	-
3	GOL	A	301	-	-	2/4/4/4	-
3	GOL	D	303	-	-	0/4/4/4	-
3	GOL	A	302	-	-	2/4/4/4	-
3	GOL	C	302	-	-	2/4/4/4	-
3	GOL	D	302	-	-	3/4/4/4	-
4	NAD	D	301	-	-	2/26/62/62	0/5/5/5
3	GOL	C	301	-	-	2/4/4/4	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	301	NAD	O4D-C1D	15.29	1.62	1.41
4	B	301	NAD	O4D-C1D	15.24	1.62	1.41
4	D	301	NAD	O4B-C1B	14.92	1.61	1.41
4	B	301	NAD	O4B-C1B	14.50	1.61	1.41
4	D	301	NAD	C2B-C1B	-13.92	1.32	1.53
4	B	301	NAD	C2B-C1B	-13.52	1.33	1.53
4	D	301	NAD	C2D-C1D	-12.94	1.34	1.53
4	B	301	NAD	C2D-C1D	-12.61	1.34	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	NAD	C7N-N7N	8.15	1.48	1.33
4	D	301	NAD	C7N-N7N	7.99	1.48	1.33
4	B	301	NAD	O4B-C4B	-6.26	1.31	1.45
4	D	301	NAD	O4B-C4B	-6.06	1.31	1.45
4	B	301	NAD	O4D-C4D	-5.91	1.31	1.45
4	D	301	NAD	O4D-C4D	-5.91	1.31	1.45
4	D	301	NAD	C4N-C3N	-3.65	1.33	1.39
4	B	301	NAD	C4N-C3N	-3.63	1.33	1.39
4	B	301	NAD	C2N-C3N	3.13	1.43	1.39
4	D	301	NAD	C2N-C3N	3.10	1.43	1.39
4	B	301	NAD	C5A-C4A	-2.78	1.33	1.40
4	B	301	NAD	PA-O5B	2.75	1.70	1.59
4	D	301	NAD	PA-O5B	2.75	1.70	1.59
4	D	301	NAD	C5A-C4A	-2.68	1.33	1.40
4	B	301	NAD	O2B-C2B	2.25	1.48	1.43
4	D	301	NAD	C6N-C5N	2.07	1.43	1.38
4	B	301	NAD	C6N-C5N	2.00	1.43	1.38

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	NAD	C5A-C6A-N6A	6.55	130.31	120.35
4	D	301	NAD	C5A-C6A-N6A	6.44	130.13	120.35
4	B	301	NAD	N3A-C2A-N1A	-5.64	119.86	128.68
4	D	301	NAD	N3A-C2A-N1A	-5.42	120.21	128.68
4	B	301	NAD	N6A-C6A-N1A	-4.36	109.52	118.57
4	D	301	NAD	N6A-C6A-N1A	-4.13	109.99	118.57
4	B	301	NAD	PN-O3-PA	-3.16	121.99	132.83
4	B	301	NAD	C3B-C2B-C1B	2.98	105.46	100.98
4	D	301	NAD	PN-O3-PA	-2.95	122.71	132.83
4	D	301	NAD	O4B-C1B-C2B	-2.83	102.80	106.93
3	D	304	GOL	C3-C2-C1	-2.78	100.91	111.70
4	B	301	NAD	C1B-N9A-C4A	-2.76	121.79	126.64
4	B	301	NAD	C3N-C7N-N7N	2.39	120.62	117.75
4	D	301	NAD	C6N-N1N-C2N	-2.32	119.86	121.97
4	D	301	NAD	C3N-C7N-N7N	2.27	120.47	117.75
3	C	302	GOL	C3-C2-C1	-2.13	103.41	111.70
3	A	301	GOL	C3-C2-C1	-2.02	103.84	111.70

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
4	D	301	NAD	O4D-C1D-N1N-C2N
4	B	301	NAD	O4D-C4D-C5D-O5D
3	D	302	GOL	O1-C1-C2-O2
3	A	302	GOL	O1-C1-C2-C3
3	C	301	GOL	C1-C2-C3-O3
3	C	302	GOL	C1-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	A	301	GOL	O1-C1-C2-O2
3	C	302	GOL	O2-C2-C3-O3
4	B	301	NAD	C3D-C4D-C5D-O5D
3	A	302	GOL	O1-C1-C2-O2
3	D	302	GOL	O2-C2-C3-O3
3	D	304	GOL	O2-C2-C3-O3
4	B	301	NAD	PN-O3-PA-O1A
3	C	301	GOL	O2-C2-C3-O3
4	D	301	NAD	O4B-C4B-C5B-O5B
4	B	301	NAD	PA-O3-PN-O2N
3	D	304	GOL	C1-C2-C3-O3

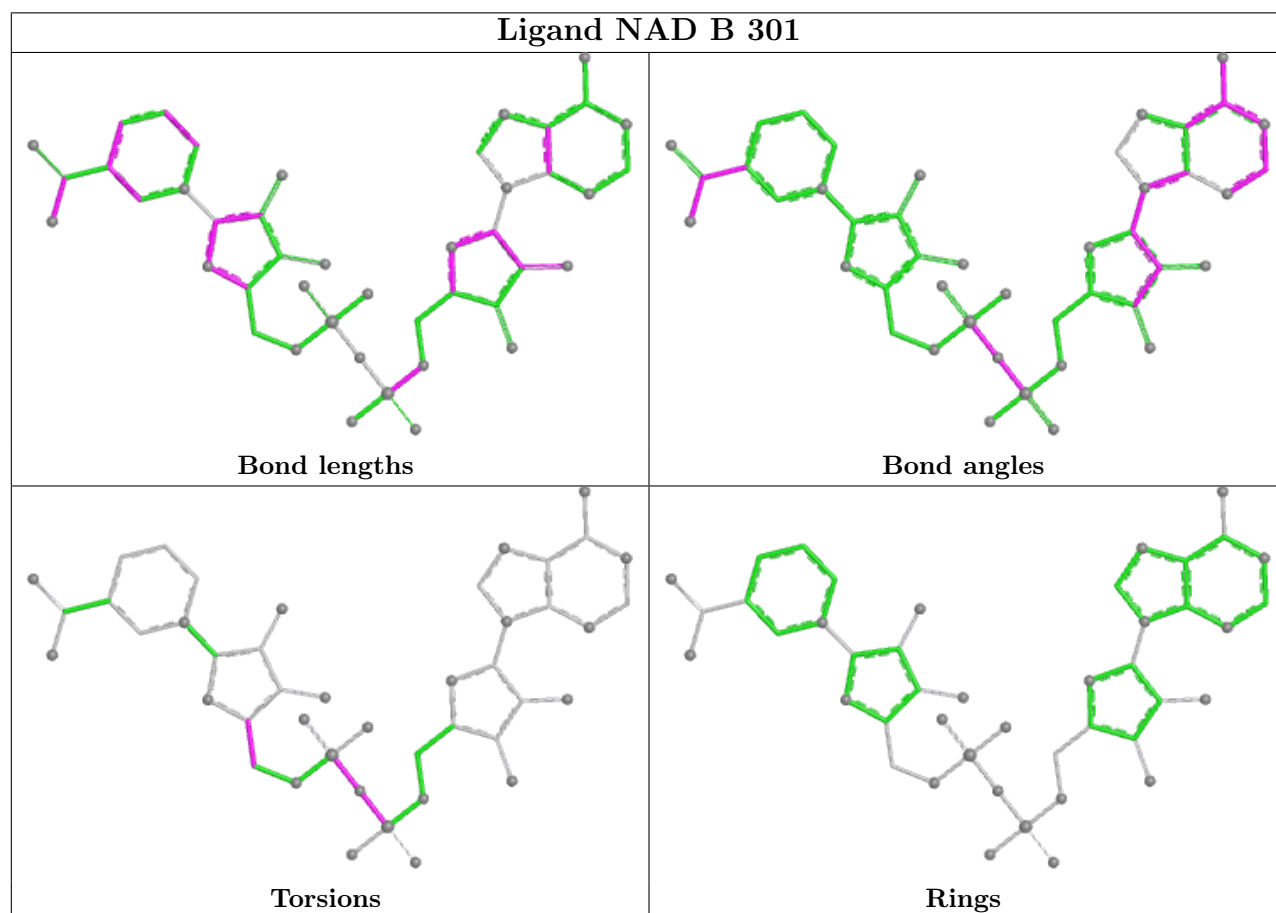
There are no ring outliers.

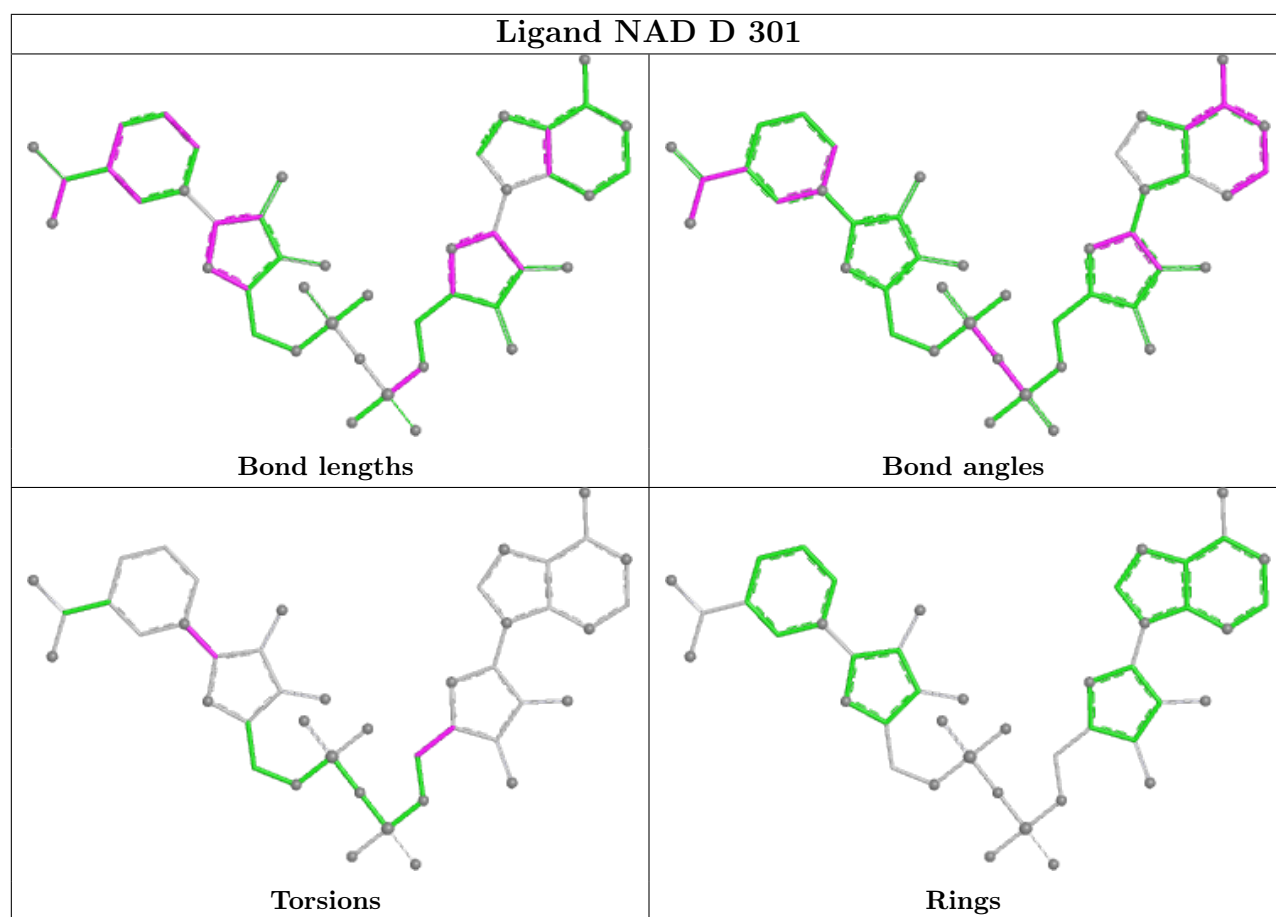
8 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	304	GOL	1	0
4	B	301	NAD	1	0
3	B	302	GOL	2	0
3	A	301	GOL	4	0
3	C	302	GOL	3	0
3	D	302	GOL	1	0
4	D	301	NAD	5	0
3	C	301	GOL	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	244/250 (97%)	0.25	17 (6%) 16 17	35, 52, 86, 112	0
1	C	244/250 (97%)	0.38	21 (8%) 10 11	36, 58, 86, 119	0
2	B	247/248 (99%)	0.33	25 (10%) 7 7	32, 46, 129, 176	0
2	D	247/248 (99%)	0.43	27 (10%) 5 5	33, 51, 119, 170	0
All	All	982/996 (98%)	0.35	90 (9%) 9 9	32, 52, 97, 176	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	195	PRO	5.7
2	D	190	MET	5.7
2	B	189	PRO	5.7
2	B	199	GLN	5.6
2	D	193	GLU	5.6
2	B	193	GLU	5.3
2	B	201	PHE	4.9
2	B	198	ASP	4.6
1	A	196	ALA	4.6
2	B	197	LYS	4.6
2	B	211	LEU	4.6
2	D	200	GLN	4.5
2	D	201	PHE	4.1
2	D	194	LEU	4.1
2	D	196	GLU	4.0
1	C	192	THR	4.0
2	B	205	ARG	3.8
2	B	196	GLU	3.8
1	A	64	ALA	3.8
1	C	76	ALA	3.7
2	D	203	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	191	GLU	3.6
1	A	66	VAL	3.5
1	A	197	GLU	3.5
2	D	197	LYS	3.5
1	A	7	GLY	3.5
1	A	194	PRO	3.5
2	B	202	LEU	3.4
2	B	38	ASP	3.4
1	A	191	GLU	3.4
2	B	194	LEU	3.3
2	B	188	THR	3.2
2	D	52	ARG	3.2
1	C	198	ARG	3.1
1	A	193	THR	3.1
1	C	73	ASP	3.1
2	D	49	PHE	3.1
2	D	87	VAL	3.0
1	A	199	GLU	3.0
2	B	43	ARG	3.0
2	D	202	LEU	3.0
1	C	139	VAL	3.0
2	D	86	LEU	2.9
1	C	182	THR	2.9
2	D	192	ASP	2.9
2	B	203	LEU	2.7
1	A	195	ALA	2.7
1	C	199	GLU	2.7
2	B	185	LEU	2.7
2	B	190	MET	2.7
1	C	89	VAL	2.7
1	C	83	GLY	2.6
2	B	191	TRP	2.6
1	C	101	PRO	2.5
2	D	9	LEU	2.5
2	B	187	HIS	2.5
1	A	13	VAL	2.5
2	D	50	SER	2.5
2	D	211	LEU	2.4
1	A	106	ALA	2.4
2	B	192	ASP	2.4
1	C	190	SER	2.4
1	C	69	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	89	VAL	2.4
1	A	103	ILE	2.3
2	D	10	ILE	2.3
1	C	7	GLY	2.3
1	A	192	THR	2.3
2	D	199	GLN	2.3
1	A	12	ILE	2.3
2	D	210	LYS	2.3
2	D	88	ASN	2.3
1	C	196	ALA	2.3
1	C	90	HIS	2.3
1	C	175	ARG	2.3
2	D	136	ILE	2.2
2	D	74	LYS	2.2
1	C	162	LEU	2.2
1	C	138	VAL	2.2
1	A	54	LYS	2.2
2	D	198	ASP	2.1
2	B	18	GLY	2.1
2	B	37	ILE	2.1
2	B	200	GLN	2.1
1	C	80	ALA	2.1
2	D	191	TRP	2.1
2	B	204	SER	2.0
2	D	90	ALA	2.0
1	C	84	ARG	2.0
2	D	47	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

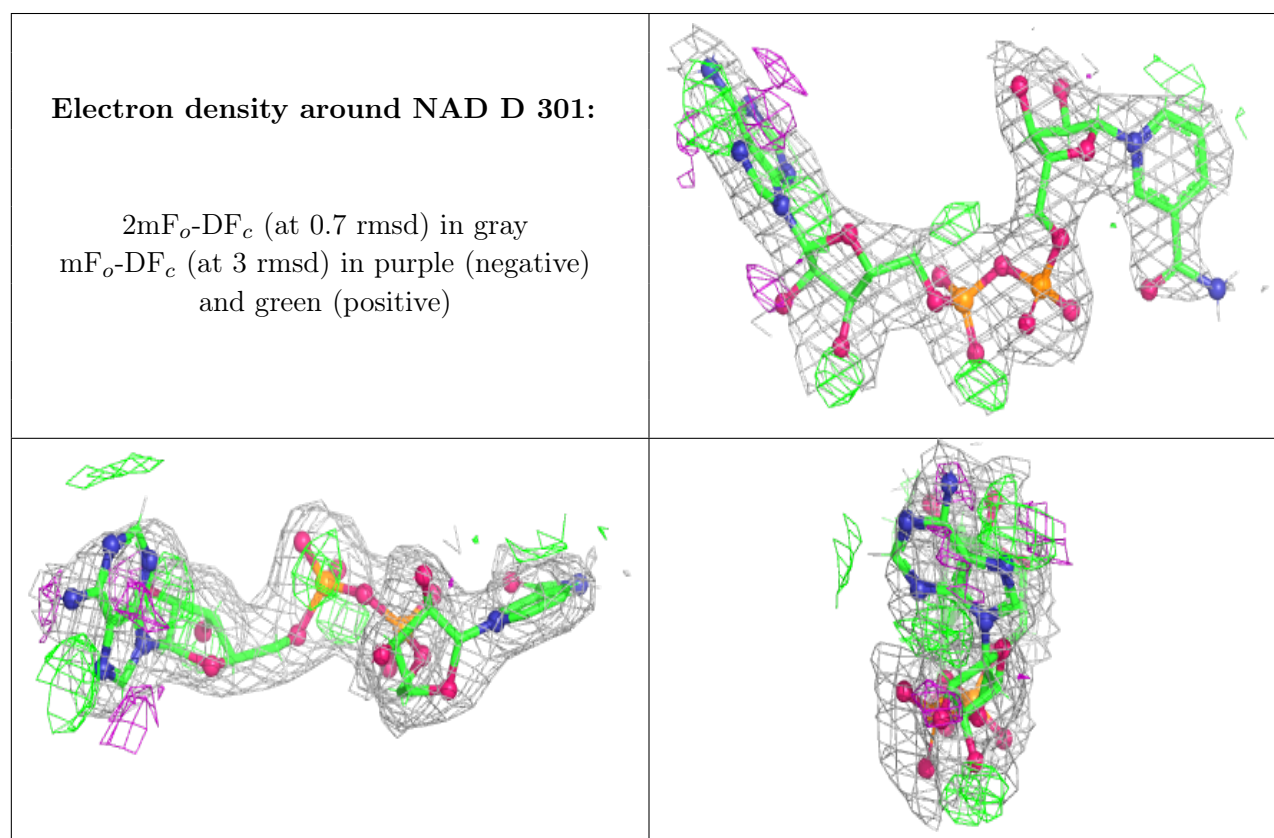
6.4 Ligands [i](#)

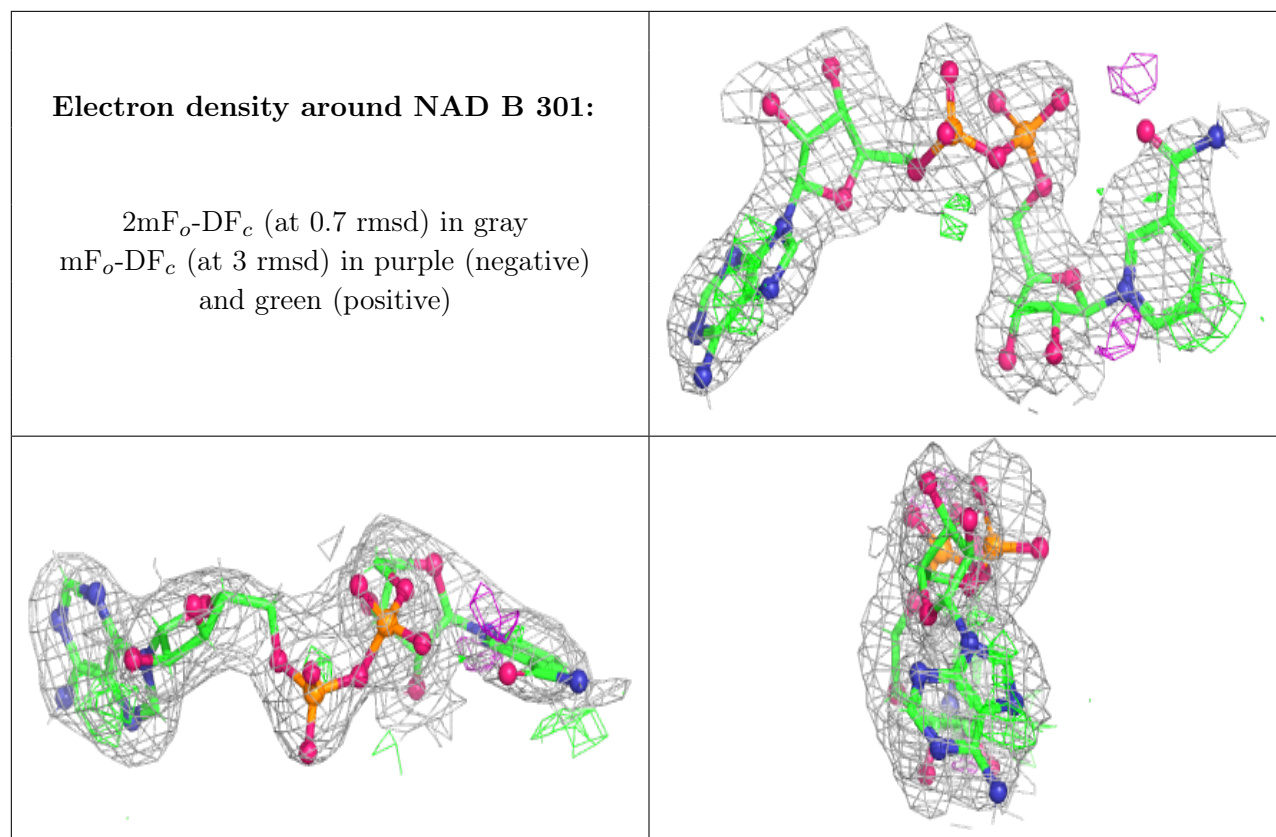
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 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
3	GOL	D	303	6/6	0.69	0.33	49,63,87,87	0
3	GOL	D	304	6/6	0.76	0.42	134,161,186,187	0
3	GOL	B	302	6/6	0.79	0.24	44,55,66,70	0
3	GOL	A	301	6/6	0.84	0.29	55,57,67,67	0
3	GOL	C	302	6/6	0.85	0.31	56,61,80,80	0
3	GOL	A	302	6/6	0.87	0.21	64,70,85,85	0
4	NAD	D	301	44/44	0.89	0.14	53,67,82,102	0
3	GOL	D	302	6/6	0.90	0.15	55,61,73,73	0
4	NAD	B	301	44/44	0.91	0.17	44,63,84,97	70
3	GOL	C	301	6/6	0.93	0.13	66,73,90,90	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.