



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:04 PM UTC

PDB ID : 4R9U / pdb_00004r9u
Title : Structure of vitamin B12 transporter BtuCD in a nucleotide-bound outward facing state
Authors : Korkhov, V.M.; Mireku, S.A.; Veprintsev, D.B.; Locher, K.P.
Deposited on : 2014-09-08
Resolution : 2.79 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

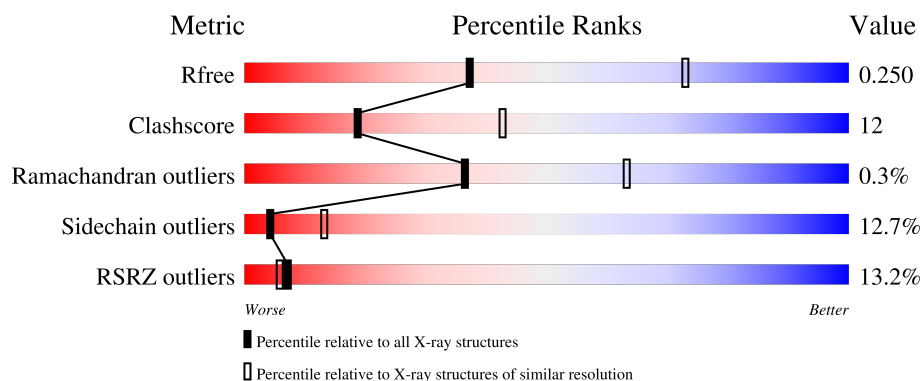
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	333	16% 68% 25% . .
1	B	333	15% 65% 27% 6% .
2	C	249	10% 65% 29% 6%
2	D	249	8% 64% 31% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8792 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 Vitamin B12 import system permease protein BtuC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			
1	B	324	Total	C	N	O	S	0	0	0
			2441	1611	418	400	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP P06609
A	-5	PRO	-	expression tag	UNP P06609
A	-4	SER	-	expression tag	UNP P06609
A	-3	GLY	-	expression tag	UNP P06609
A	-2	THR	-	expression tag	UNP P06609
A	-1	SER	-	expression tag	UNP P06609
A	0	HIS	-	expression tag	UNP P06609
A	18	SER	CYS	engineered mutation	UNP P06609
A	32	SER	CYS	engineered mutation	UNP P06609
A	120	SER	CYS	engineered mutation	UNP P06609
A	156	SER	CYS	engineered mutation	UNP P06609
A	205	SER	CYS	engineered mutation	UNP P06609
A	206	SER	CYS	engineered mutation	UNP P06609
A	267	SER	CYS	engineered mutation	UNP P06609
B	-6	GLY	-	expression tag	UNP P06609
B	-5	PRO	-	expression tag	UNP P06609
B	-4	SER	-	expression tag	UNP P06609
B	-3	GLY	-	expression tag	UNP P06609
B	-2	THR	-	expression tag	UNP P06609
B	-1	SER	-	expression tag	UNP P06609
B	0	HIS	-	expression tag	UNP P06609
B	18	SER	CYS	engineered mutation	UNP P06609
B	32	SER	CYS	engineered mutation	UNP P06609
B	120	SER	CYS	engineered mutation	UNP P06609
B	156	SER	CYS	engineered mutation	UNP P06609

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Chain	Residue	Modelled	Actual	Comment	Reference
B	205	SER	CYS	engineered mutation	UNP P06609
B	206	SER	CYS	engineered mutation	UNP P06609
B	267	SER	CYS	engineered mutation	UNP P06609

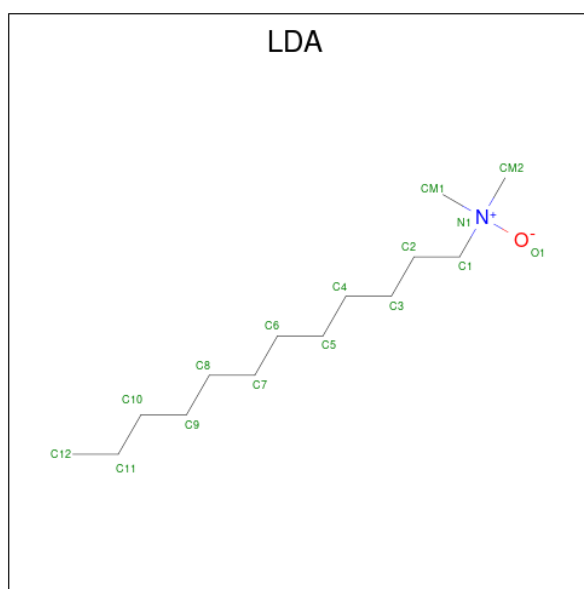
- Molecule 2 is a protein called Vitamin B12 import ATP-binding protein BtuD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	248	Total	C	N	O	S	0	0	0
			1891	1183	351	348	9			
2	D	248	Total	C	N	O	S	0	0	0
			1891	1183	351	348	9			

There are 6 discrepancies between the modelled and reference sequences:

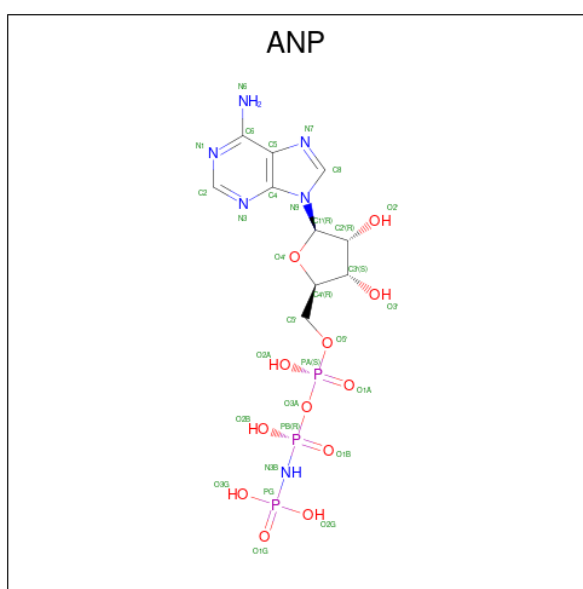
Chain	Residue	Modelled	Actual	Comment	Reference
C	159	GLN	GLU	engineered mutation	UNP P06611
C	162	CYS	ASN	engineered mutation	UNP P06611
C	180	SER	CYS	engineered mutation	UNP P06611
D	159	GLN	GLU	engineered mutation	UNP P06611
D	162	CYS	ASN	engineered mutation	UNP P06611
D	180	SER	CYS	engineered mutation	UNP P06611

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: $C_{14}H_{31}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	A	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		
3	B	1	Total	C	N	O	0	0
			16	14	1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

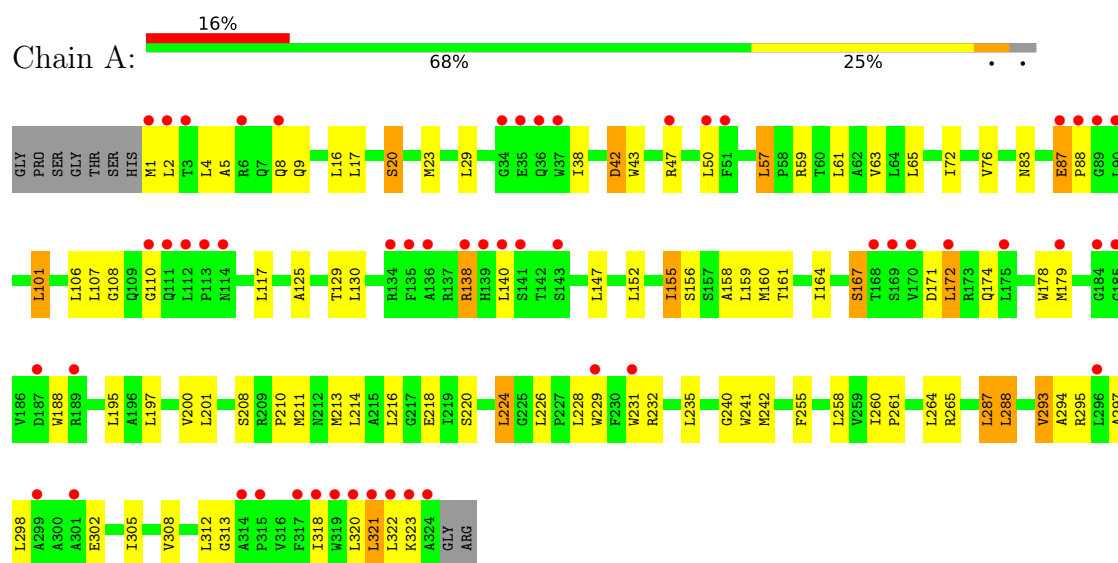
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

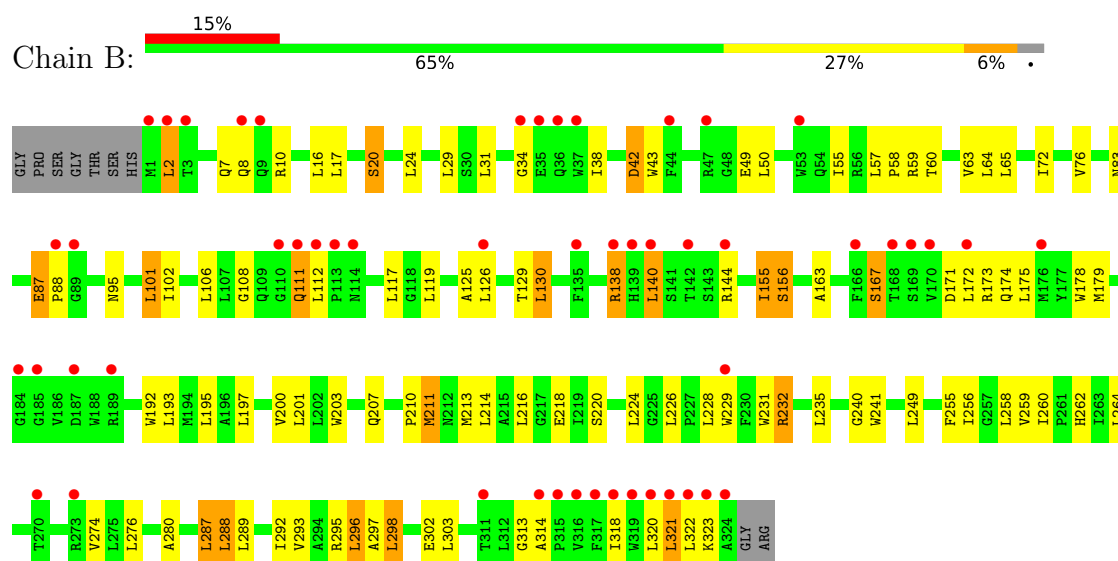
3 Residue-property plots [i](#)

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.

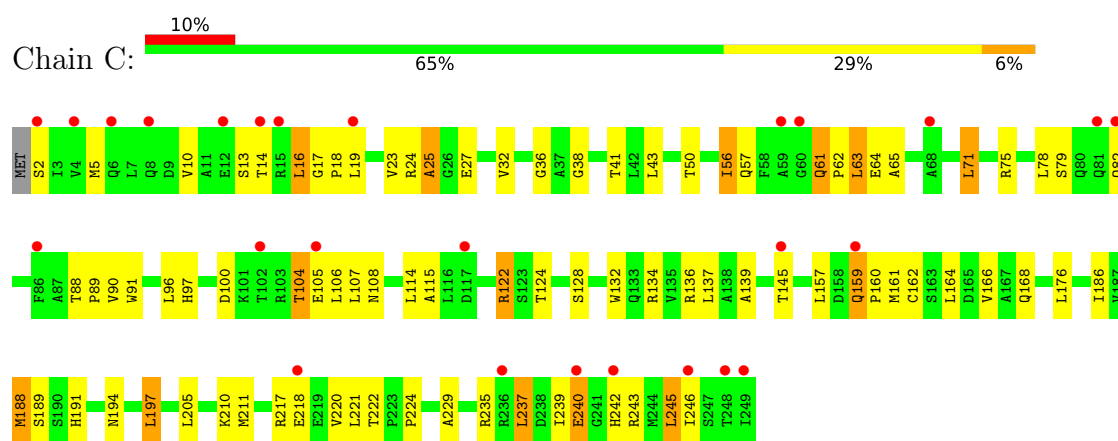
- Molecule 1: Vitamin B12 import system permease protein BtuC



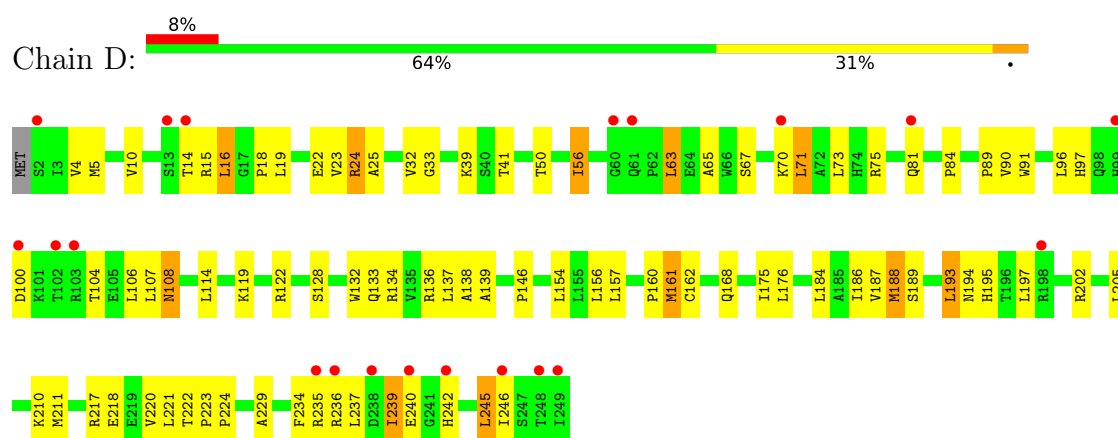
- Molecule 1: Vitamin B12 import system permease protein BtuC



- Molecule 2: Vitamin B12 import ATP-binding protein BtuD



• Molecule 2: Vitamin B12 import ATP-binding protein BtuD



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	372.85Å 113.21Å 69.43Å 90.00° 94.92° 90.00°	Depositor
Resolution (Å)	29.51 – 2.79 29.51 – 2.79	Depositor EDS
% Data completeness (in resolution range)	69.2 (29.51-2.79) 69.1 (29.51-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.80Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.217 , 0.246 0.219 , 0.250	Depositor DCC
R_{free} test set	1972 reflections (2.74%)	wwPDB-VP
Wilson B-factor (Å ²)	63.3	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8792	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LDA, ANP, MG

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	0.73	0/2495	1.14	10/3408 (0.3%)
1	B	0.72	0/2495	1.12	10/3408 (0.3%)
2	C	0.65	0/1925	1.02	8/2608 (0.3%)
2	D	0.66	0/1925	1.05	4/2608 (0.2%)
All	All	0.69	0/8840	1.09	32/12032 (0.3%)

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	260	ILE	CA-C-N	-12.48	107.03	119.64
1	A	260	ILE	C-N-CA	-12.48	107.03	119.64
1	B	260	ILE	CA-C-N	-11.93	107.59	119.64
1	B	260	ILE	C-N-CA	-11.93	107.59	119.64
1	A	57	LEU	CA-C-N	-9.81	109.73	119.64
1	A	57	LEU	C-N-CA	-9.81	109.73	119.64
1	B	57	LEU	CA-C-N	-8.78	110.77	119.64
1	B	57	LEU	C-N-CA	-8.78	110.77	119.64
1	B	87	GLU	CA-C-N	-8.45	109.28	119.84
1	B	87	GLU	C-N-CA	-8.45	109.28	119.84
1	A	87	GLU	CA-C-N	-8.31	109.45	119.84
1	A	87	GLU	C-N-CA	-8.31	109.45	119.84
1	A	83	ASN	CA-C-N	6.77	127.04	119.32
1	A	83	ASN	C-N-CA	6.77	127.04	119.32
2	C	145	THR	CA-C-N	5.96	125.64	119.56
2	C	145	THR	C-N-CA	5.96	125.64	119.56
2	C	161	MET	N-CA-C	-5.76	106.12	114.12
2	D	84	PRO	CA-C-N	5.72	125.70	120.03
2	D	84	PRO	C-N-CA	5.72	125.70	120.03
2	C	61	GLN	CA-C-N	-5.65	113.39	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	61	GLN	C-N-CA	-5.65	113.39	120.51
2	C	13	SER	CB-CA-C	-5.62	109.10	115.79
1	B	155	ILE	CB-CA-C	-5.58	104.83	111.97
1	A	293	VAL	N-CA-C	-5.51	107.61	112.90
1	A	155	ILE	CB-CA-C	-5.48	104.96	111.97
2	C	239	ILE	N-CA-C	5.46	115.82	108.17
1	B	256	ILE	N-CA-C	5.38	115.82	110.23
2	C	25	ALA	N-CA-C	5.27	116.84	111.14
2	D	175	ILE	CB-CA-C	-5.26	105.24	111.97
2	D	161	MET	N-CA-C	-5.21	106.84	114.39
1	B	83	ASN	CA-C-N	5.15	124.77	119.05
1	B	83	ASN	C-N-CA	5.15	124.77	119.05

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	2441	0	2606	57	0
1	B	2441	0	2606	70	0
2	C	1891	0	1924	49	0
2	D	1891	0	1924	50	0
3	A	32	0	62	1	0
3	B	32	0	62	1	0
4	C	31	0	13	3	0
4	D	31	0	13	1	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	8792	0	9210	214	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 12.

All (214) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:71:LEU:HD13	2:D:75:ARG:HH21	1.47	0.79
2:C:157:LEU:HB2	2:C:188:MET:HB3	1.65	0.78
1:B:34:GLY:HA2	1:B:296:LEU:HD22	1.65	0.78
1:A:224:LEU:HD21	2:C:97:HIS:HA	1.68	0.75
1:B:106:LEU:HD21	1:B:167:SER:HB3	1.69	0.74
2:D:205:LEU:HD21	2:D:229:ALA:HB2	1.69	0.74
1:B:129:THR:HG21	1:B:240:GLY:HA3	1.70	0.73
1:A:318:ILE:HG22	1:A:322:LEU:HG	1.69	0.72
2:C:205:LEU:HD21	2:C:229:ALA:HB2	1.70	0.72
1:A:322:LEU:O	1:B:138:ARG:NH1	2.22	0.71
2:D:5:MET:HB3	2:D:23:VAL:HB	1.72	0.71
1:B:200:VAL:HG21	1:B:241:TRP:CD1	2.27	0.70
2:C:71:LEU:HD13	2:C:75:ARG:HH21	1.56	0.69
1:A:106:LEU:HD21	1:A:167:SER:HB3	1.74	0.69
2:D:67:SER:OG	2:D:70:LYS:HG2	1.92	0.68
1:A:129:THR:HG21	1:A:240:GLY:HA3	1.74	0.68
1:A:318:ILE:HA	1:A:321:LEU:HD12	1.76	0.68
2:C:5:MET:HB3	2:C:23:VAL:HB	1.76	0.67
1:B:63:VAL:HG13	1:B:287:LEU:HD13	1.77	0.67
1:A:295:ARG:HA	1:A:302:GLU:HG3	1.76	0.66
1:B:214:LEU:HD21	1:B:228:LEU:HD21	1.78	0.66
2:D:222:THR:HG22	2:D:224:PRO:HD2	1.78	0.66
2:D:67:SER:H	2:D:70:LYS:HE2	1.59	0.65
2:C:17:GLY:HA3	2:C:210:LYS:HE3	1.76	0.65
1:B:60:THR:HG23	1:B:288:LEU:HD21	1.79	0.64
1:B:295:ARG:HA	1:B:302:GLU:HG3	1.78	0.64
1:A:57:LEU:HD23	1:A:188:TRP:HZ2	1.61	0.64
1:B:101:LEU:HD21	1:B:117:LEU:HB3	1.79	0.63
1:B:171:ASP:OD2	1:B:173:ARG:NH1	2.30	0.63
2:C:56:ILE:HD11	2:C:63:LEU:HD22	1.81	0.63
1:A:255:PHE:CZ	1:A:313:GLY:HA3	2.35	0.62
1:A:294:ALA:HB2	1:A:308:VAL:HG11	1.81	0.62
1:A:322:LEU:HB3	1:A:323:LYS:HE3	1.82	0.61
1:A:101:LEU:HD21	1:A:117:LEU:HB3	1.82	0.61
1:B:318:ILE:HA	1:B:321:LEU:HD12	1.83	0.60
1:B:193:LEU:HD12	1:B:249:LEU:HD13	1.84	0.60
1:A:42:ASP:OD2	1:A:42:ASP:N	2.35	0.60
2:D:137:LEU:HD21	2:D:160:PRO:HB2	1.83	0.59
1:B:318:ILE:HG22	1:B:322:LEU:HG	1.85	0.59
1:A:63:VAL:HG11	1:A:288:LEU:HA	1.86	0.58
2:C:137:LEU:HD21	2:C:160:PRO:HB2	1.84	0.58
1:B:108:GLY:HA3	1:B:112:LEU:HD11	1.83	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:197:LEU:HD13	2:C:221:LEU:HD12	1.85	0.58
2:C:218:GLU:OE2	2:C:243:ARG:NH1	2.37	0.57
1:B:111:GLN:O	1:B:111:GLN:NE2	2.38	0.57
1:B:322:LEU:HB3	1:B:323:LYS:HE3	1.86	0.57
2:C:19:LEU:HD22	2:C:211:MET:HB2	1.86	0.56
1:A:200:VAL:HG21	1:A:241:TRP:CD1	2.40	0.56
1:A:213:MET:HE3	1:A:224:LEU:HB3	1.88	0.56
2:D:157:LEU:HB2	2:D:188:MET:HB3	1.88	0.55
2:C:222:THR:HG22	2:C:224:PRO:HD2	1.88	0.55
2:C:166:VAL:HG21	2:D:193:LEU:HD21	1.88	0.55
1:B:87:GLU:HG3	1:B:258:LEU:HB2	1.89	0.55
1:A:59:ARG:O	1:A:63:VAL:HG23	2.07	0.54
1:A:218:GLU:HG2	1:A:228:LEU:HD11	1.90	0.54
1:B:95:ASN:HB3	1:B:156:SER:HB2	1.89	0.54
1:B:102:ILE:HG21	1:B:163:ALA:HB1	1.90	0.54
2:D:114:LEU:HD12	2:D:138:ALA:HB2	1.90	0.53
2:D:119:LYS:HG2	2:D:122:ARG:HH21	1.73	0.53
1:A:138:ARG:NH1	1:B:322:LEU:O	2.38	0.53
1:A:155:ILE:HD11	1:B:318:ILE:HG13	1.89	0.53
2:C:97:HIS:CG	2:C:139:ALA:HB1	2.42	0.53
2:C:246:ILE:HD13	2:D:242:HIS:CG	2.44	0.53
1:B:288:LEU:O	1:B:292:ILE:HG13	2.07	0.53
1:B:42:ASP:N	1:B:42:ASP:OD2	2.41	0.53
2:D:161:MET:HE3	2:D:195:HIS:NE2	2.24	0.53
1:A:318:ILE:HG13	1:B:155:ILE:HD11	1.91	0.53
2:D:239:ILE:HD13	2:D:239:ILE:N	2.24	0.52
1:B:65:LEU:HB3	1:B:197:LEU:HD23	1.92	0.52
2:D:176:LEU:HD22	2:D:186:ILE:HD13	1.93	0.51
2:C:194:ASN:OD1	2:C:245:LEU:N	2.43	0.51
2:D:132:TRP:CE2	2:D:136:ARG:HD2	2.45	0.51
1:B:72:ILE:HD11	1:B:280:ALA:HB2	1.92	0.51
1:A:59:ARG:NH2	1:A:302:GLU:OE2	2.35	0.51
2:C:240:GLU:CD	2:D:235:ARG:HH12	2.18	0.50
1:B:108:GLY:HA3	1:B:112:LEU:CD1	2.41	0.50
1:A:5:ALA:O	1:A:9:GLN:HB2	2.11	0.50
1:A:308:VAL:O	1:A:312:LEU:HG	2.12	0.50
2:D:22:GLU:OE1	2:D:24:ARG:NH2	2.45	0.50
1:A:16:LEU:O	1:A:20:SER:OG	2.30	0.49
2:C:63:LEU:C	2:C:65:ALA:H	2.20	0.49
1:A:38:ILE:HG22	1:A:43:TRP:HD1	1.77	0.49
1:B:213:MET:HE3	1:B:224:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:PHE:CZ	1:B:313:GLY:HA3	2.48	0.49
2:D:157:LEU:HB3	2:D:160:PRO:HG3	1.93	0.49
1:A:87:GLU:HG3	1:A:258:LEU:HB2	1.95	0.49
2:D:133:GLN:OE1	2:D:136:ARG:NH1	2.43	0.49
1:A:125:ALA:O	1:A:129:THR:HG23	2.13	0.48
1:B:178:TRP:HE3	1:B:179:MET:HG2	1.78	0.48
2:D:18:PRO:HD2	2:D:210:LYS:HZ2	1.78	0.48
2:D:4:VAL:HG23	2:D:25:ALA:HB2	1.94	0.48
2:C:36:GLY:HA2	4:C:301:ANP:H3'	1.94	0.48
2:D:33:GLY:O	2:D:39:LYS:NZ	2.45	0.48
1:B:7:GLN:O	1:B:10:ARG:HG2	2.13	0.48
2:C:16:LEU:HD12	2:C:41:THR:HG22	1.95	0.48
2:D:22:GLU:O	2:D:202:ARG:NH2	2.47	0.48
1:A:4:LEU:HD13	2:C:91:TRP:CD1	2.49	0.47
1:B:87:GLU:CG	1:B:258:LEU:HB2	2.44	0.47
1:A:171:ASP:HB3	1:A:174:GLN:HB2	1.96	0.47
1:A:201:LEU:HG	1:A:242:MET:HE3	1.96	0.47
1:B:289:LEU:O	1:B:293:VAL:HG23	2.14	0.47
2:C:2:SER:O	2:C:25:ALA:HB2	2.15	0.47
2:C:61:GLN:HG2	2:C:62:PRO:HD2	1.95	0.47
2:D:220:VAL:HG12	2:D:221:LEU:HD23	1.96	0.47
1:A:38:ILE:HG22	1:A:43:TRP:CD1	2.50	0.47
2:C:197:LEU:HD22	2:C:245:LEU:HD12	1.97	0.47
1:A:261:PRO:HB2	1:A:265:ARG:HH21	1.80	0.47
2:D:134:ARG:HD3	2:D:168:GLN:HG3	1.97	0.47
1:A:214:LEU:HD21	1:A:228:LEU:HD21	1.97	0.46
1:A:210:PRO:HG3	1:A:231:TRP:CZ2	2.50	0.46
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.66	0.46
1:A:76:VAL:HG13	1:A:235:LEU:HD13	1.98	0.46
1:A:287:LEU:HD23	1:A:287:LEU:HA	1.71	0.46
2:C:237:LEU:HD21	2:C:246:ILE:HD12	1.98	0.46
1:B:210:PRO:HG3	1:B:231:TRP:CZ2	2.51	0.46
2:C:24:ARG:HB2	2:C:27:GLU:HG2	1.98	0.46
2:C:38:GLY:HA2	4:C:301:ANP:H5'1	1.98	0.46
2:D:70:LYS:O	2:D:73:LEU:HB2	2.15	0.46
2:D:205:LEU:HD21	2:D:229:ALA:CB	2.44	0.46
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.71	0.45
1:B:218:GLU:HG2	1:B:228:LEU:HD11	1.99	0.45
2:D:19:LEU:HD22	2:D:211:MET:HB2	1.96	0.45
1:B:140:LEU:O	1:B:232:ARG:NH2	2.43	0.45
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ALA:O	1:B:318:ILE:HG12	2.16	0.45
2:C:114:LEU:O	2:C:134:ARG:NH1	2.42	0.45
2:D:10:VAL:O	2:D:18:PRO:HA	2.17	0.45
1:A:160:MET:O	1:A:164:ILE:HG13	2.16	0.45
1:B:298:LEU:HB2	1:B:303:LEU:HD11	1.97	0.45
1:A:178:TRP:HE3	1:A:179:MET:HG2	1.81	0.45
3:A:501:LDA:HM12	3:A:501:LDA:H22	1.66	0.45
1:B:59:ARG:NH2	1:B:302:GLU:OE2	2.36	0.45
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.64	0.45
2:D:97:HIS:CG	2:D:139:ALA:HB1	2.52	0.45
1:A:158:ALA:HA	1:A:161:THR:HG22	1.99	0.45
1:A:213:MET:CE	1:A:226:LEU:HB2	2.47	0.45
1:B:76:VAL:HG13	1:B:235:LEU:HD13	1.98	0.45
1:B:125:ALA:O	1:B:129:THR:HG23	2.17	0.45
1:B:293:VAL:O	1:B:297:ALA:HB2	2.17	0.45
2:D:194:ASN:OD1	2:D:245:LEU:N	2.50	0.45
1:B:55:ILE:O	1:B:58:PRO:HD2	2.16	0.45
1:B:119:LEU:HD12	1:B:119:LEU:HA	1.76	0.45
1:B:16:LEU:O	1:B:20:SER:OG	2.33	0.44
1:B:224:LEU:HD23	1:B:224:LEU:HA	1.64	0.44
2:C:88:THR:O	2:C:124:THR:HG23	2.17	0.44
2:C:90:VAL:HG23	2:C:122:ARG:O	2.16	0.44
2:C:134:ARG:HD3	2:C:168:GLN:HG3	1.98	0.44
1:A:108:GLY:C	1:A:110:GLY:H	2.26	0.44
1:B:255:PHE:CE1	1:B:259:VAL:HG21	2.53	0.44
1:B:192:TRP:CE3	3:B:501:LDA:H52	2.53	0.44
1:A:218:GLU:HG2	1:A:228:LEU:CD1	2.47	0.44
1:B:2:LEU:HD23	2:D:108:ASN:HD21	1.83	0.44
2:C:132:TRP:CE2	2:C:136:ARG:HD2	2.53	0.44
2:D:16:LEU:HD12	2:D:41:THR:HG22	2.00	0.44
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.73	0.44
1:B:126:LEU:O	1:B:130:LEU:HB2	2.18	0.44
1:B:211:MET:HE3	1:B:214:LEU:HD12	2.00	0.44
2:C:36:GLY:H	4:C:301:ANP:HNB1	1.66	0.44
2:D:146:PRO:HG3	2:D:184:LEU:HD13	1.99	0.44
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.82	0.44
2:D:67:SER:N	2:D:70:LYS:HE2	2.31	0.43
2:D:156:LEU:HD23	2:D:187:VAL:HB	2.00	0.43
1:B:276:LEU:HD23	1:B:276:LEU:HA	1.85	0.43
1:B:59:ARG:O	1:B:63:VAL:HG23	2.18	0.43
1:A:65:LEU:HB3	1:A:197:LEU:HD23	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:236:ARG:HE	2:D:236:ARG:HB3	1.63	0.43
1:A:172:LEU:H	1:A:172:LEU:HG	1.54	0.43
1:B:38:ILE:HG22	1:B:43:TRP:HD1	1.83	0.43
1:B:140:LEU:HD23	1:B:144:ARG:HB3	2.00	0.43
2:D:71:LEU:HD13	2:D:75:ARG:NH2	2.25	0.43
2:D:63:LEU:C	2:D:65:ALA:H	2.26	0.43
1:B:235:LEU:HD23	1:B:235:LEU:HA	1.82	0.42
1:A:264:LEU:HD23	1:A:264:LEU:HA	1.77	0.42
1:A:305:ILE:HG21	1:A:305:ILE:HD13	1.74	0.42
2:C:10:VAL:O	2:C:18:PRO:HA	2.19	0.42
2:D:75:ARG:HD2	2:D:75:ARG:C	2.45	0.42
2:D:89:PRO:HB2	2:D:91:TRP:CD1	2.54	0.42
1:B:102:ILE:HG21	1:B:163:ALA:CB	2.49	0.42
2:C:63:LEU:O	2:C:65:ALA:N	2.46	0.42
2:D:15:ARG:HB2	4:D:301:ANP:O4'	2.20	0.42
1:A:16:LEU:HD23	1:A:16:LEU:HA	1.94	0.42
1:B:31:LEU:HD23	1:B:31:LEU:HA	1.84	0.41
1:B:38:ILE:HG22	1:B:43:TRP:CD1	2.55	0.41
1:B:64:LEU:HD21	1:B:288:LEU:HD12	2.01	0.41
2:D:56:ILE:HD11	2:D:63:LEU:HD22	2.02	0.41
2:D:154:LEU:HD21	2:D:156:LEU:HD21	2.02	0.41
2:D:223:PRO:HB3	2:D:234:PHE:O	2.19	0.41
2:C:242:HIS:CG	2:D:246:ILE:HD13	2.55	0.41
2:D:70:LYS:HA	2:D:73:LEU:HD12	2.02	0.41
2:C:82:GLN:HE21	2:C:136:ARG:HH21	1.67	0.41
2:C:197:LEU:HD12	2:C:197:LEU:HA	1.84	0.41
1:A:293:VAL:O	1:A:297:ALA:HB2	2.21	0.41
2:C:164:LEU:HA	2:C:164:LEU:HD23	1.74	0.41
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.85	0.41
1:B:203:TRP:O	1:B:207:GLN:HG2	2.21	0.41
2:C:115:ALA:HB3	2:C:134:ARG:NH1	2.36	0.41
2:C:159:GLN:NE2	2:C:191:HIS:HD2	2.19	0.41
2:C:235:ARG:NH1	2:D:240:GLU:OE2	2.54	0.41
2:C:78:LEU:HD23	2:C:79:SER:O	2.21	0.41
2:C:89:PRO:HB2	2:C:91:TRP:CD1	2.56	0.41
2:C:176:LEU:HD22	2:C:186:ILE:HD13	2.03	0.41
1:A:1:MET:H3	2:C:104:THR:HG22	1.85	0.41
2:C:71:LEU:HD23	2:C:71:LEU:HA	1.84	0.41
1:A:23:MET:HE2	1:A:23:MET:HB3	1.90	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.82	0.40
1:B:293:VAL:O	1:B:293:VAL:HG12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:220:VAL:HG12	2:C:221:LEU:HD23	2.03	0.40
2:D:90:VAL:HG23	2:D:122:ARG:O	2.21	0.40
1:B:197:LEU:HD12	1:B:197:LEU:HA	1.77	0.40
1:A:72:ILE:HD12	1:A:201:LEU:HD23	2.04	0.40
1:B:213:MET:HE2	1:B:226:LEU:HB2	2.03	0.40
2:C:205:LEU:HD21	2:C:229:ALA:CB	2.45	0.40
1:B:173:ARG:HG3	1:B:174:GLN:N	2.36	0.40
1:B:287:LEU:HD23	1:B:287:LEU:HA	1.88	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	322/333 (97%)	293 (91%)	28 (9%)	1 (0%)	36	63
1	B	322/333 (97%)	294 (91%)	27 (8%)	1 (0%)	36	63
2	C	246/249 (99%)	232 (94%)	13 (5%)	1 (0%)	30	57
2	D	246/249 (99%)	234 (95%)	12 (5%)	0	100	100
All	All	1136/1164 (98%)	1053 (93%)	80 (7%)	3 (0%)	36	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	64	GLU
1	A	88	PRO
1	B	88	PRO

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	249/255 (98%)	220 (88%)	29 (12%)	5	16
1	B	249/255 (98%)	217 (87%)	32 (13%)	4	13
2	C	200/201 (100%)	173 (86%)	27 (14%)	4	11
2	D	200/201 (100%)	174 (87%)	26 (13%)	4	12
All	All	898/912 (98%)	784 (87%)	114 (13%)	4	13

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	8	GLN
1	A	17	LEU
1	A	20	SER
1	A	29	LEU
1	A	42	ASP
1	A	47	ARG
1	A	50	LEU
1	A	101	LEU
1	A	130	LEU
1	A	138	ARG
1	A	140	LEU
1	A	156	SER
1	A	159	LEU
1	A	167	SER
1	A	172	LEU
1	A	195	LEU
1	A	208	SER
1	A	211	MET
1	A	216	LEU
1	A	220	SER
1	A	224	LEU
1	A	229	TRP
1	A	232	ARG

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Mol	Chain	Res	Type
1	A	287	LEU
1	A	288	LEU
1	A	298	LEU
1	A	320	LEU
1	A	321	LEU
1	B	2	LEU
1	B	8	GLN
1	B	17	LEU
1	B	20	SER
1	B	24	LEU
1	B	29	LEU
1	B	42	ASP
1	B	49	GLU
1	B	50	LEU
1	B	101	LEU
1	B	111	GLN
1	B	130	LEU
1	B	138	ARG
1	B	140	LEU
1	B	156	SER
1	B	167	SER
1	B	172	LEU
1	B	195	LEU
1	B	201	LEU
1	B	211	MET
1	B	216	LEU
1	B	220	SER
1	B	229	TRP
1	B	232	ARG
1	B	262	HIS
1	B	274	VAL
1	B	287	LEU
1	B	288	LEU
1	B	296	LEU
1	B	298	LEU
1	B	320	LEU
1	B	321	LEU
2	C	14	THR
2	C	16	LEU
2	C	32	VAL
2	C	43	LEU
2	C	50	THR

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Mol	Chain	Res	Type
2	C	56	ILE
2	C	57	GLN
2	C	63	LEU
2	C	71	LEU
2	C	96	LEU
2	C	100	ASP
2	C	104	THR
2	C	105	GLU
2	C	106	LEU
2	C	107	LEU
2	C	108	ASN
2	C	122	ARG
2	C	128	SER
2	C	159	GLN
2	C	162	CYS
2	C	188	MET
2	C	189	SER
2	C	197	LEU
2	C	217	ARG
2	C	237	LEU
2	C	240	GLU
2	C	245	LEU
2	D	14	THR
2	D	16	LEU
2	D	24	ARG
2	D	32	VAL
2	D	50	THR
2	D	56	ILE
2	D	63	LEU
2	D	71	LEU
2	D	81	GLN
2	D	96	LEU
2	D	100	ASP
2	D	104	THR
2	D	106	LEU
2	D	107	LEU
2	D	108	ASN
2	D	128	SER
2	D	162	CYS
2	D	188	MET
2	D	189	SER
2	D	193	LEU

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Mol	Chain	Res	Type
2	D	197	LEU
2	D	217	ARG
2	D	218	GLU
2	D	237	LEU
2	D	239	ILE
2	D	245	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	81	GLN
2	C	98	GLN
2	C	153	GLN
2	C	159	GLN
2	D	35	ASN
2	D	57	GLN
2	D	81	GLN
2	D	191	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	ANP	C	301	5	33,33,33	0.90	2 (6%)	45,52,52	1.05	4 (8%)
3	LDA	A	502	-	13,15,15	2.19	2 (15%)	14,17,17	0.55	0
3	LDA	A	501	-	13,15,15	2.27	2 (15%)	14,17,17	0.62	0
3	LDA	B	501	-	13,15,15	2.23	2 (15%)	14,17,17	0.54	0
3	LDA	B	502	-	13,15,15	2.27	2 (15%)	14,17,17	0.72	0
4	ANP	D	301	5	33,33,33	0.89	3 (9%)	45,52,52	1.09	4 (8%)

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
4	ANP	C	301	5	-	9/18/38/38	0/3/3/3
3	LDA	A	502	-	-	8/13/13/13	-
3	LDA	A	501	-	-	7/13/13/13	-
3	LDA	B	501	-	-	8/13/13/13	-
3	LDA	B	502	-	-	3/13/13/13	-
4	ANP	D	301	5	-	4/18/38/38	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	LDA	O1-N1	-6.68	1.25	1.42
3	B	501	LDA	O1-N1	-6.59	1.26	1.42
3	A	501	LDA	O1-N1	-6.58	1.26	1.42
3	A	502	LDA	O1-N1	-6.43	1.26	1.42
3	A	501	LDA	C1-N1	-4.78	1.46	1.51
3	B	502	LDA	C1-N1	-4.58	1.46	1.51
3	A	502	LDA	C1-N1	-4.42	1.46	1.51
3	B	501	LDA	C1-N1	-4.39	1.47	1.51
4	C	301	ANP	PG-O1G	2.82	1.50	1.46
4	D	301	ANP	PB-O1B	2.81	1.50	1.46
4	C	301	ANP	PG-N3B	2.76	1.70	1.63
4	D	301	ANP	PG-N3B	2.42	1.69	1.63
4	D	301	ANP	PB-N3B	2.10	1.68	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	301	ANP	O1B-PB-N3B	-3.58	106.49	111.77
4	D	301	ANP	O3G-PG-O1G	-3.18	105.47	113.45
4	D	301	ANP	O2G-PG-O1G	-2.87	106.25	113.45
4	C	301	ANP	O2B-PB-O3A	2.87	114.22	104.64
4	D	301	ANP	O2G-PG-O3G	2.68	114.79	107.59
4	C	301	ANP	O2G-PG-O1G	-2.48	107.22	113.45
4	C	301	ANP	O3G-PG-O1G	-2.37	107.50	113.45
4	D	301	ANP	O1G-PG-N3B	2.04	114.78	111.77

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	301	ANP	PB-N3B-PG-O1G
4	C	301	ANP	PG-N3B-PB-O1B
4	C	301	ANP	PA-O3A-PB-O2B
4	C	301	ANP	C5'-O5'-PA-O1A
4	C	301	ANP	C5'-O5'-PA-O3A
4	D	301	ANP	PB-N3B-PG-O1G
4	D	301	ANP	PG-N3B-PB-O1B
4	D	301	ANP	PA-O3A-PB-O2B
3	A	502	LDA	C11-C10-C9-C8
3	B	501	LDA	C3-C4-C5-C6
3	B	501	LDA	C5-C6-C7-C8
3	A	502	LDA	C7-C8-C9-C10
3	A	502	LDA	C2-C3-C4-C5
3	A	501	LDA	C7-C8-C9-C10
3	B	501	LDA	C1-C2-C3-C4
3	A	501	LDA	C3-C4-C5-C6
3	B	501	LDA	C11-C10-C9-C8
3	A	502	LDA	C1-C2-C3-C4
3	A	501	LDA	C1-C2-C3-C4
3	B	502	LDA	C4-C5-C6-C7
3	B	501	LDA	C7-C8-C9-C10
3	A	502	LDA	C6-C7-C8-C9
4	C	301	ANP	O4'-C4'-C5'-O5'
3	A	502	LDA	C9-C10-C11-C12
3	B	501	LDA	C4-C5-C6-C7
3	A	501	LDA	C2-C3-C4-C5
3	A	502	LDA	C5-C6-C7-C8
3	B	502	LDA	C5-C6-C7-C8

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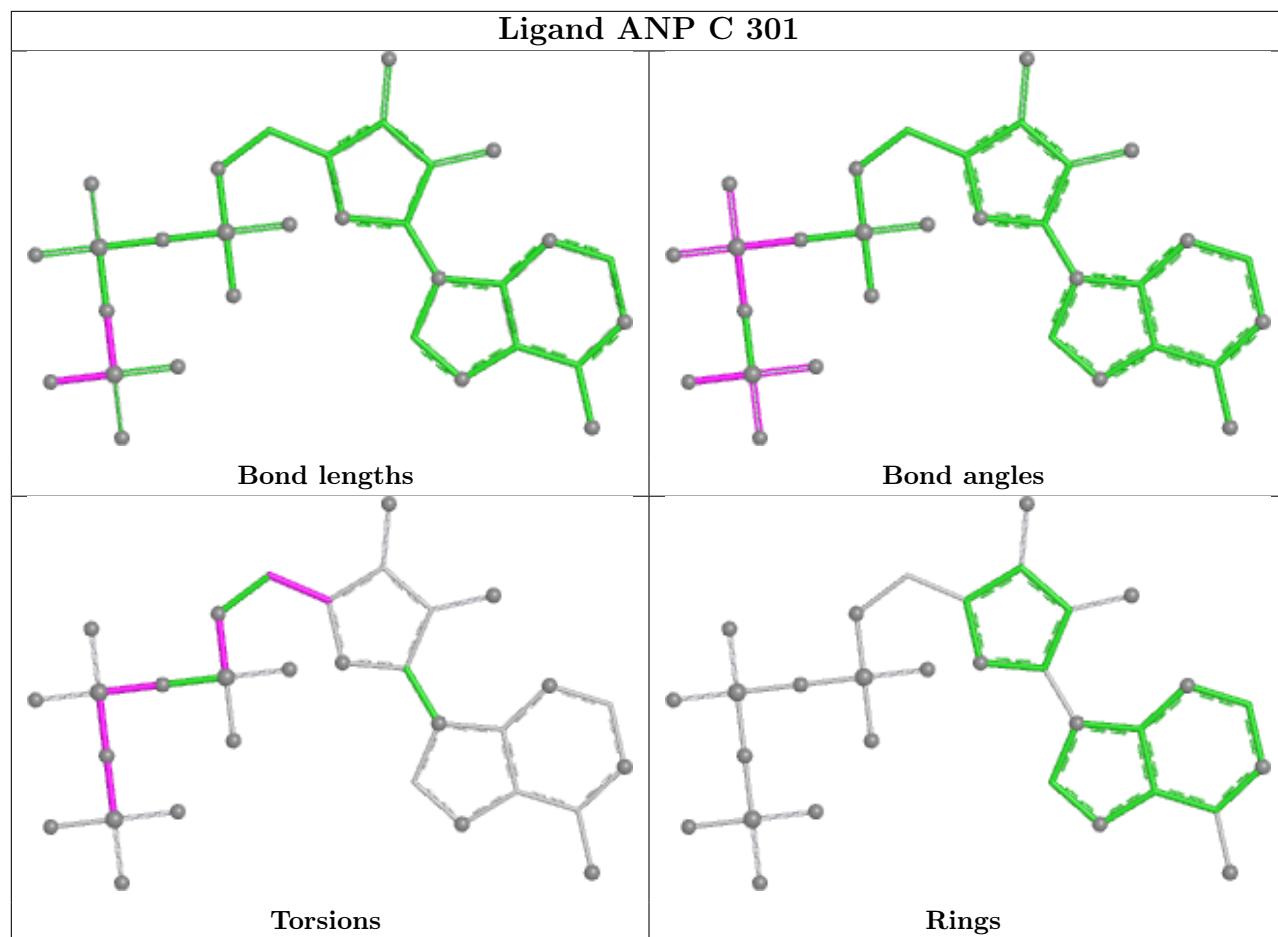
Mol	Chain	Res	Type	Atoms
3	A	501	LDA	C4-C5-C6-C7
3	B	501	LDA	C2-C3-C4-C5
3	B	502	LDA	C6-C7-C8-C9
4	C	301	ANP	C5'-O5'-PA-O2A
3	A	501	LDA	N1-C1-C2-C3
3	A	502	LDA	N1-C1-C2-C3
4	C	301	ANP	C3'-C4'-C5'-O5'
3	A	501	LDA	C5-C6-C7-C8
3	B	501	LDA	C2-C1-N1-CM1
4	C	301	ANP	PA-O3A-PB-O1B
4	D	301	ANP	PA-O3A-PB-O1B

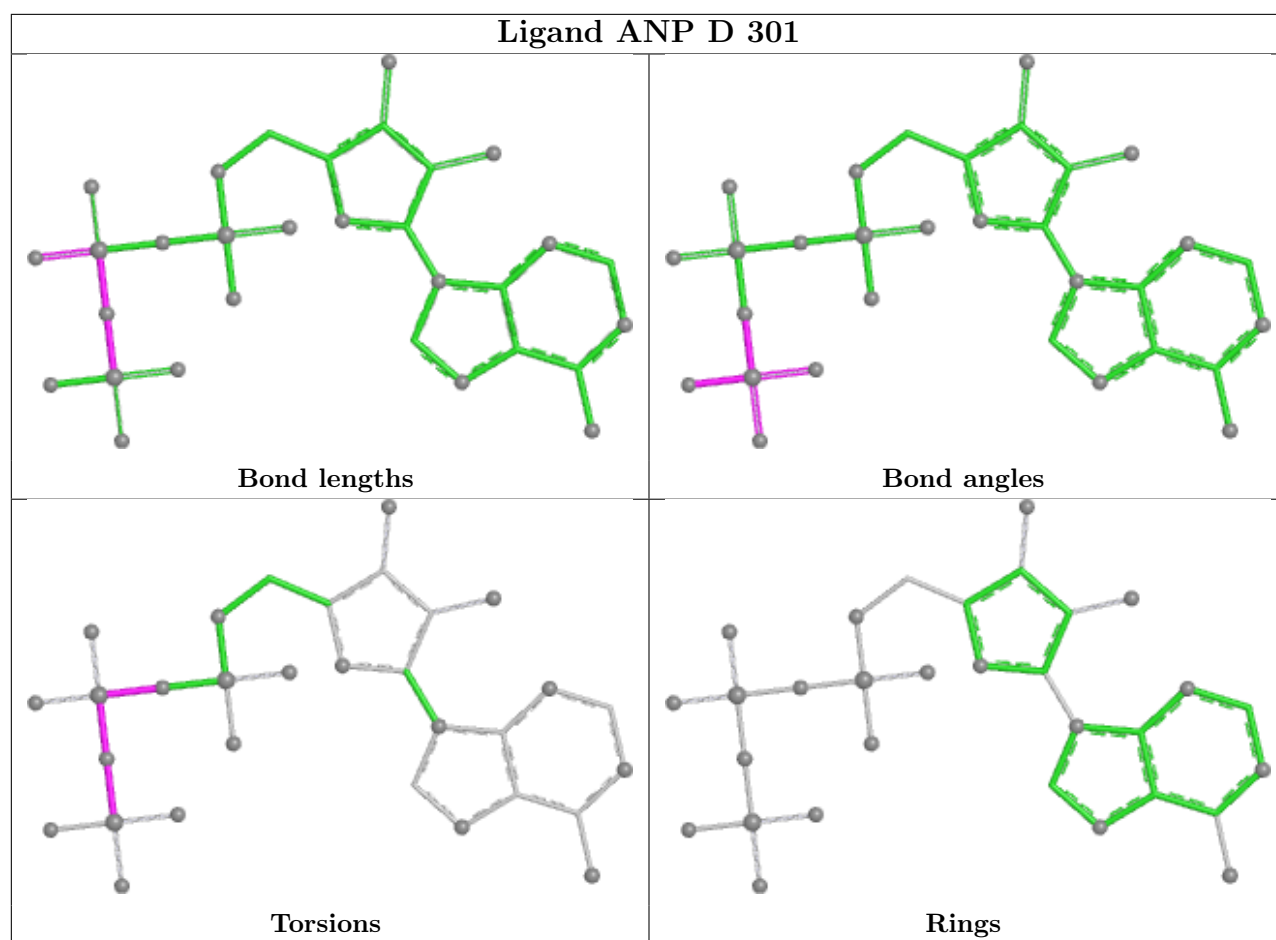
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	ANP	3	0
3	A	501	LDA	1	0
3	B	501	LDA	1	0
4	D	301	ANP	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	324/333 (97%)	0.81	54 (16%) 4 3	41, 74, 140, 187	0
1	B	324/333 (97%)	0.68	51 (15%) 5 4	37, 70, 137, 178	0
2	C	248/249 (99%)	0.76	26 (10%) 11 9	45, 88, 131, 193	0
2	D	248/249 (99%)	0.55	20 (8%) 18 14	47, 76, 119, 200	0
All	All	1144/1164 (98%)	0.71	151 (13%) 7 6	37, 75, 134, 200	0

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	LEU	8.5
1	A	184	GLY	7.9
2	C	249	ILE	7.6
2	C	2	SER	6.6
2	D	249	ILE	6.4
1	A	35	GLU	6.2
1	A	322	LEU	5.6
1	A	113	PRO	5.5
1	B	35	GLU	5.5
1	B	322	LEU	5.2
2	C	81	GLN	4.9
2	D	60	GLY	4.9
1	B	324	ALA	4.8
1	B	1	MET	4.6
1	B	321	LEU	4.6
1	B	88	PRO	4.6
1	A	229	TRP	4.5
1	A	140	LEU	4.5
1	B	2	LEU	4.5
1	A	172	LEU	4.4
2	D	2	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	1	MET	4.1
1	A	170	VAL	4.1
1	A	319	TRP	4.1
1	A	51	PHE	4.1
2	D	14	THR	4.0
1	A	89	GLY	3.9
1	B	112	LEU	3.9
1	B	113	PRO	3.9
1	B	169	SER	3.8
1	B	34	GLY	3.8
1	B	184	GLY	3.8
1	B	89	GLY	3.7
1	A	6	ARG	3.7
1	B	142	THR	3.7
1	A	34	GLY	3.7
1	B	317	PHE	3.7
2	C	248	THR	3.7
1	A	136	ALA	3.7
1	B	3	THR	3.7
2	D	246	ILE	3.7
1	B	168	THR	3.6
1	A	3	THR	3.6
2	C	159	GLN	3.6
2	D	248	THR	3.6
1	A	88	PRO	3.6
1	A	110	GLY	3.5
1	B	8	GLN	3.5
1	A	318	ILE	3.5
2	C	14	THR	3.4
1	A	317	PHE	3.4
1	B	318	ILE	3.4
1	B	189	ARG	3.4
2	C	86	PHE	3.4
1	A	47	ARG	3.3
1	B	111	GLN	3.3
1	A	112	LEU	3.3
1	A	321	LEU	3.2
1	A	185	GLY	3.2
1	A	135	PHE	3.2
1	B	172	LEU	3.1
1	A	36	GLN	3.1
2	C	218	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	140	LEU	3.0
2	C	6	GLN	3.0
1	B	323	LYS	3.0
1	B	314	ALA	3.0
1	B	229	TRP	2.9
1	B	315	PRO	2.9
2	C	102	THR	2.9
1	A	111	GLN	2.9
1	A	169	SER	2.9
2	C	8	GLN	2.9
1	A	187	ASP	2.9
2	D	70	LYS	2.9
2	D	240	GLU	2.8
2	C	236	ARG	2.8
1	A	323	LYS	2.8
2	C	246	ILE	2.8
1	B	170	VAL	2.8
1	B	273	ARG	2.8
1	B	110	GLY	2.7
1	A	114	ASN	2.7
1	B	37	TRP	2.7
1	B	319	TRP	2.7
2	D	242	HIS	2.7
2	C	15	ARG	2.7
2	D	236	ARG	2.7
1	A	324	ALA	2.7
2	C	59	ALA	2.7
1	A	139	HIS	2.6
1	B	138	ARG	2.6
2	D	99	HIS	2.6
1	A	314	ALA	2.6
1	B	270	THR	2.5
1	A	37	TRP	2.5
1	A	168	THR	2.5
1	B	176	MET	2.5
1	B	187	ASP	2.5
2	C	105	GLU	2.5
1	A	231	TRP	2.5
2	C	240	GLU	2.5
1	B	316	VAL	2.5
2	C	82	GLN	2.5
2	D	102	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	139	HIS	2.5
2	D	61	GLN	2.4
1	A	301	ALA	2.4
1	B	320	LEU	2.4
2	C	19	LEU	2.4
1	B	135	PHE	2.4
2	D	198	ARG	2.4
1	A	320	LEU	2.4
2	C	12	GLU	2.3
1	B	47	ARG	2.3
1	A	90	LEU	2.3
1	A	50	LEU	2.3
1	B	9	GLN	2.2
2	D	13	SER	2.2
2	D	100	ASP	2.2
2	C	60	GLY	2.2
1	B	53	TRP	2.2
1	A	299	ALA	2.2
1	B	126	LEU	2.2
2	D	81	GLN	2.2
1	A	296	LEU	2.2
1	A	179	MET	2.2
2	C	242	HIS	2.2
1	B	311	THR	2.2
1	A	138	ARG	2.2
1	A	189	ARG	2.2
1	B	114	ASN	2.2
2	D	103	ARG	2.1
1	A	141	SER	2.1
1	A	143	SER	2.1
1	B	166	PHE	2.1
2	C	145	THR	2.1
1	B	185	GLY	2.1
1	A	87	GLU	2.1
1	B	144	ARG	2.1
2	D	235	ARG	2.1
1	B	44	PHE	2.1
1	A	134	ARG	2.1
1	A	315	PRO	2.1
1	A	8	GLN	2.1
2	C	4	VAL	2.1
2	C	117	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	238	ASP	2.0
1	A	175	LEU	2.0
1	B	36	GLN	2.0
2	C	68	ALA	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

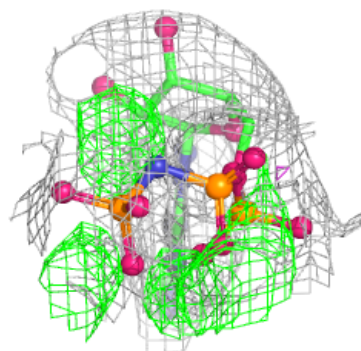
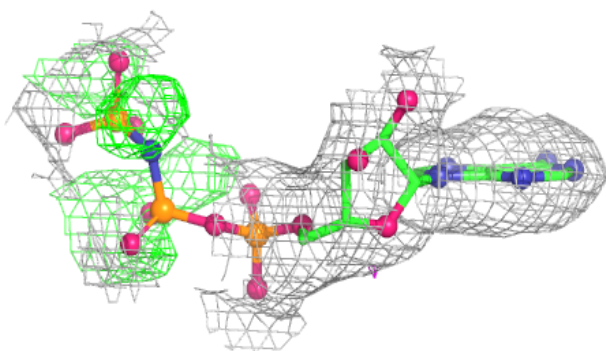
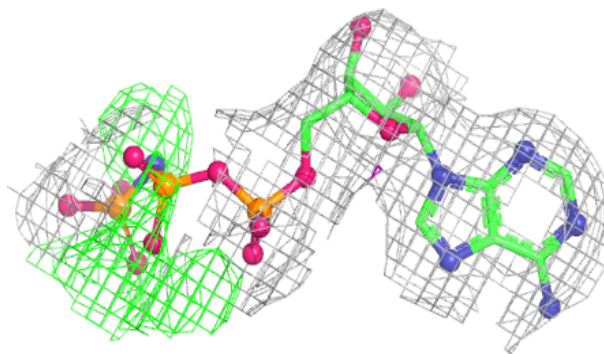
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	LDA	A	502	16/16	0.78	0.31	83,113,130,132	0
3	LDA	A	501	16/16	0.82	0.19	71,81,111,115	0
3	LDA	B	501	16/16	0.83	0.17	60,66,114,119	0
3	LDA	B	502	16/16	0.87	0.24	83,95,120,123	0
5	MG	C	302	1/1	0.93	0.14	44,44,44,44	0
4	ANP	C	301	31/31	0.96	0.10	45,78,100,106	0
4	ANP	D	301	31/31	0.97	0.10	20,69,100,111	0
5	MG	D	302	1/1	0.97	0.12	48,48,48,48	0

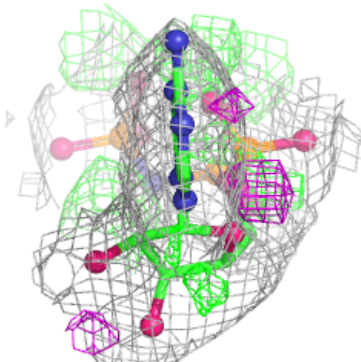
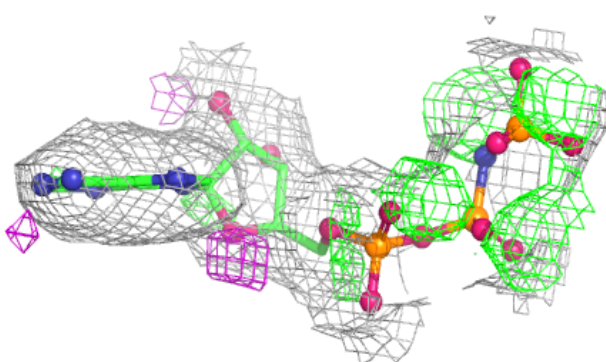
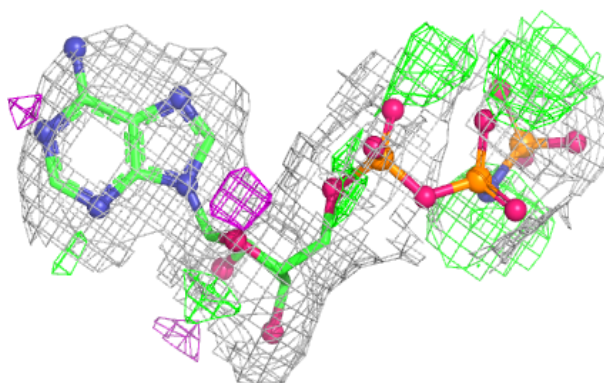
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ANP 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 ANP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.