



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 02:13 AM UTC

PDB ID : 5UAH / pdb_00005uah
Title : Escherichia coli RNA polymerase and Rifampin complex, RpoB D516V mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 4.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

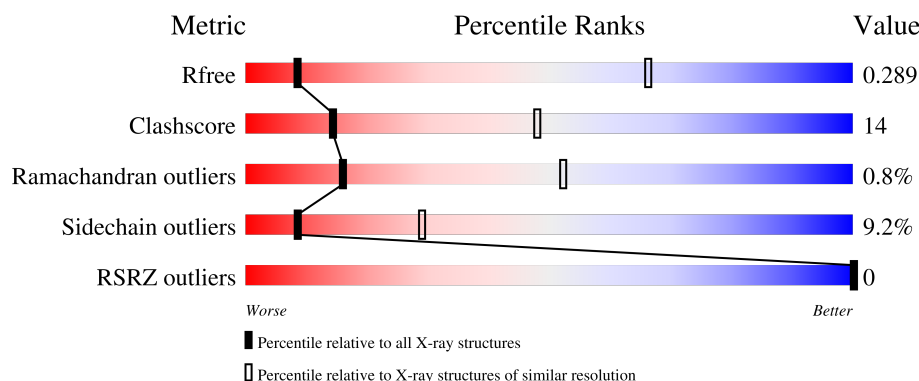
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	329	 47% 21% . 29%
1	B	329	 34% 28% . 34%
1	G	329	 42% 23% . . 31%
1	H	329	 41% 22% . 34%
2	C	1342	 62% 34% .

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55125 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1812	1127	323	356	6			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10569	6632	1841	2053	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10565	6630	1840	2052	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	516	VAL	ASP	engineered mutation	UNP P0A8V2
I	516	VAL	ASP	engineered mutation	UNP P0A8V2

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1167	Total	C	N	O	S	0	0	0
			9065	5700	1622	1697	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

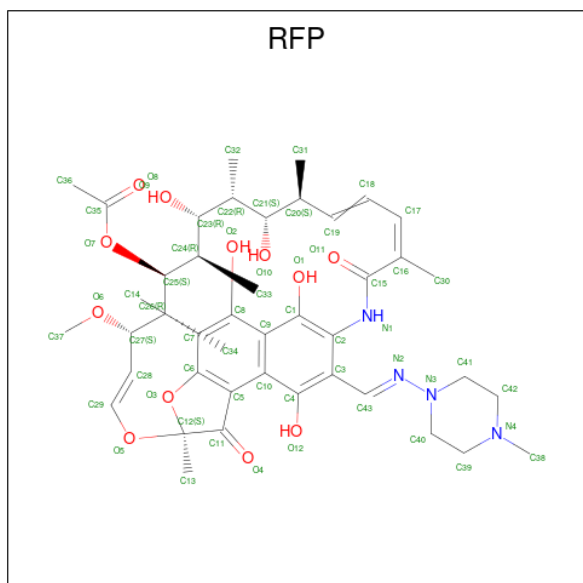
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			59	43	4	12		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total 1	Mg 1	0	0
7	J	1	Total 1	Mg 1	0	0

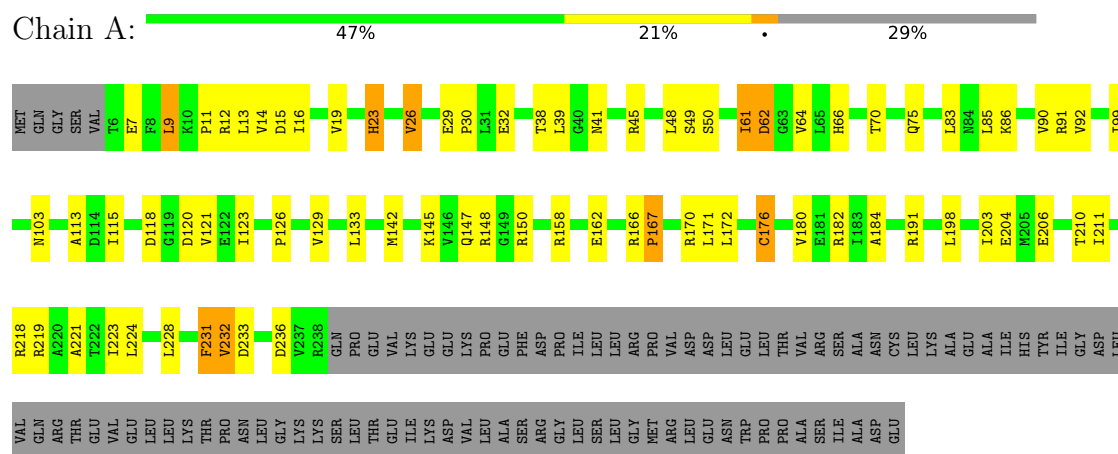
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total 2	Zn 2	0	0
8	J	2	Total 2	Zn 2	0	0

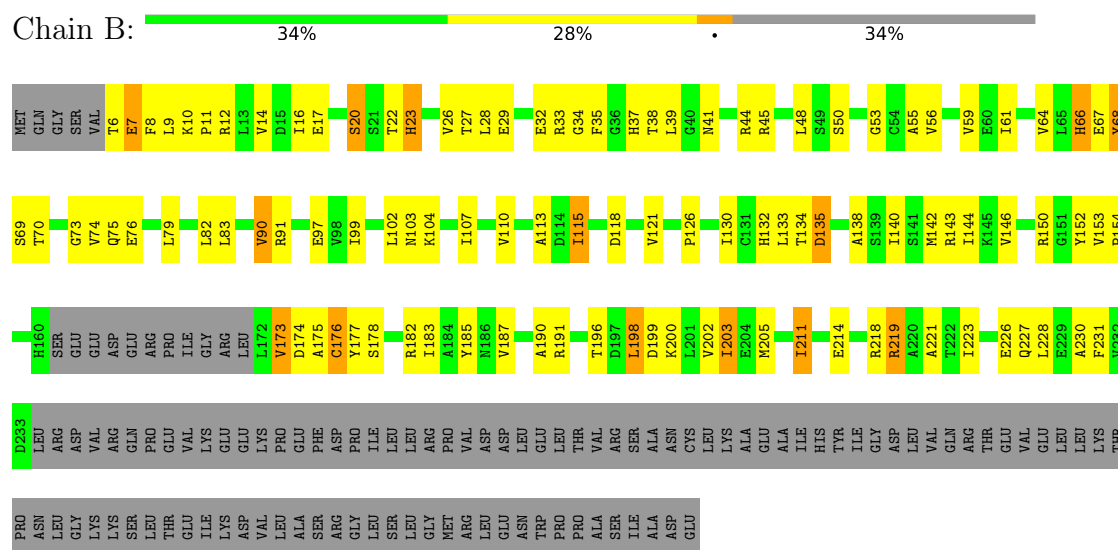
3 Residue-property plots

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: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	187.81Å 206.67Å 310.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.74 – 4.10 29.74 – 4.10	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.74-4.10) 99.0 (29.74-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 4.11Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.243 , 0.287 0.247 , 0.289	Depositor DCC
R_{free} test set	2000 reflections (2.05%)	wwPDB-VP
Wilson B-factor (Å ²)	184.9	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 179.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55125	wwPDB-VP
Average B, all atoms (Å ²)	233.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% 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: MG, ZN, RFP

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	1/1834 (0.1%)	0.71	1/2485 (0.0%)
1	B	0.31	0/1697	0.97	1/2300 (0.0%)
1	G	0.29	0/1777	0.73	1/2408 (0.0%)
1	H	0.32	0/1681	1.01	1/2278 (0.0%)
2	C	0.26	2/10738 (0.0%)	0.71	5/14488 (0.0%)
2	I	0.25	1/10734 (0.0%)	0.72	5/14483 (0.0%)
3	D	0.22	0/9205	0.69	5/12430 (0.0%)
3	J	0.23	0/9140	0.73	7/12341 (0.1%)
4	E	0.19	0/693	0.61	0/935
4	K	0.25	0/629	0.69	0/847
5	F	0.22	0/3864	0.74	0/5194
5	L	0.23	0/3872	0.73	4/5205 (0.1%)
All	All	0.25	4/55864 (0.0%)	0.73	30/75394 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	C	0	3
2	I	0	3
3	D	0	2
3	J	0	3
5	F	0	1
All	All	0	14

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	513	GLN	CA-C	6.27	1.60	1.52
1	A	29	GLU	CA-C	6.15	1.60	1.52
2	C	373	GLY	C-N	5.59	1.45	1.33
2	I	373	GLY	C-N	5.16	1.44	1.33

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1183	SER	CA-C-N	8.10	129.69	120.06
3	D	1183	SER	C-N-CA	8.10	129.69	120.06
2	I	1137	GLU	CA-CB-CG	7.80	129.69	114.10
3	J	425	ARG	NE-CZ-NH2	7.72	126.14	119.20
1	G	29	GLU	N-CA-C	7.20	125.72	109.81

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	ASN	Sidechain
1	B	135	ASP	Sidechain
2	C	107	ARG	Peptide
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide

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	1812	0	1839	72	0
1	B	1677	0	1703	95	0
1	G	1755	0	1773	75	0
1	H	1662	0	1687	69	0
2	C	10569	0	10587	335	0
2	I	10565	0	10581	269	0
3	D	9065	0	9210	308	0
3	J	9001	0	9165	287	0
4	E	691	0	695	20	0
4	K	627	0	634	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	3813	0	3880	105	0
5	L	3821	0	3884	98	0
6	C	59	0	56	5	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	55125	0	55694	1557	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 14.

The worst 5 of 1557 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:C:1271:GLY:HA2	3:D:343:LEU:HD21	1.23	1.11
2:C:1269:ARG:HG2	3:D:343:LEU:HD12	1.36	1.07
5:L:97:PRO:HA	5:L:100:MET:HG3	1.45	0.97
5:L:456:MET:HE1	5:L:497:VAL:HG13	1.51	0.91
2:C:18:ARG:NH1	2:C:621:SER:O	2.04	0.91

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	231/329 (70%)	198 (86%)	29 (13%)	4 (2%)	7	36
1	B	213/329 (65%)	187 (88%)	24 (11%)	2 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	225/329 (68%)	191 (85%)	28 (12%)	6 (3%)	4	28
1	H	212/329 (64%)	187 (88%)	24 (11%)	1 (0%)	24	61
2	C	1338/1342 (100%)	1230 (92%)	102 (8%)	6 (0%)	30	65
2	I	1338/1342 (100%)	1230 (92%)	100 (8%)	8 (1%)	21	58
3	D	1163/1407 (83%)	1071 (92%)	83 (7%)	9 (1%)	16	52
3	J	1151/1407 (82%)	1060 (92%)	78 (7%)	13 (1%)	11	44
4	E	87/91 (96%)	82 (94%)	5 (6%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	462/613 (75%)	421 (91%)	34 (7%)	7 (2%)	8	39
5	L	463/613 (76%)	424 (92%)	37 (8%)	2 (0%)	30	65
All	All	6960/8222 (85%)	6355 (91%)	547 (8%)	58 (1%)	16	52

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	170	VAL
2	C	484	LEU
2	C	1159	VAL
3	D	10	ALA
3	D	1274	PHE

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	201/286 (70%)	190 (94%)	11 (6%)	19	44
1	B	186/286 (65%)	164 (88%)	22 (12%)	5	21
1	G	193/286 (68%)	177 (92%)	16 (8%)	10	32
1	H	183/286 (64%)	162 (88%)	21 (12%)	5	21
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	8	28
2	I	1154/1157 (100%)	1047 (91%)	107 (9%)	8	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	962/1168 (82%)	876 (91%)	86 (9%)	9	30
3	J	960/1168 (82%)	874 (91%)	86 (9%)	9	30
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	22
4	K	67/75 (89%)	62 (92%)	5 (8%)	12	35
5	F	417/540 (77%)	376 (90%)	41 (10%)	7	26
5	L	418/540 (77%)	381 (91%)	37 (9%)	9	30
All	All	5968/7024 (85%)	5419 (91%)	549 (9%)	8	29

5 of 549 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	680	ASN
3	J	740	LEU
3	J	678	ARG
5	L	301	ASN
3	D	710	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 105 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	23	HIS
2	I	688	GLN
5	L	128	ASN
1	G	117	HIS
2	I	165	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 8 are monoatomic - leaving 1 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
6	RFP	C	3001	-	63,63,63	2.20	12 (19%)	94,94,94	1.92	21 (22%)

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
6	RFP	C	3001	-	-	9/60/85/85	0/5/5/5

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	10.62	1.57	1.37
6	C	3001	RFP	C15-N1	6.91	1.49	1.35
6	C	3001	RFP	C12-C11	-4.45	1.37	1.54
6	C	3001	RFP	C18-C17	3.77	1.54	1.43
6	C	3001	RFP	O7-C25	-3.72	1.39	1.44

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C2-C3-C43	-5.23	118.44	123.99
6	C	3001	RFP	O4-C11-C5	-5.14	122.15	131.63
6	C	3001	RFP	C41-N3-N2	4.86	139.53	113.99
6	C	3001	RFP	O7-C35-C36	4.85	119.73	111.09
6	C	3001	RFP	C12-C11-C5	4.75	116.48	107.30

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

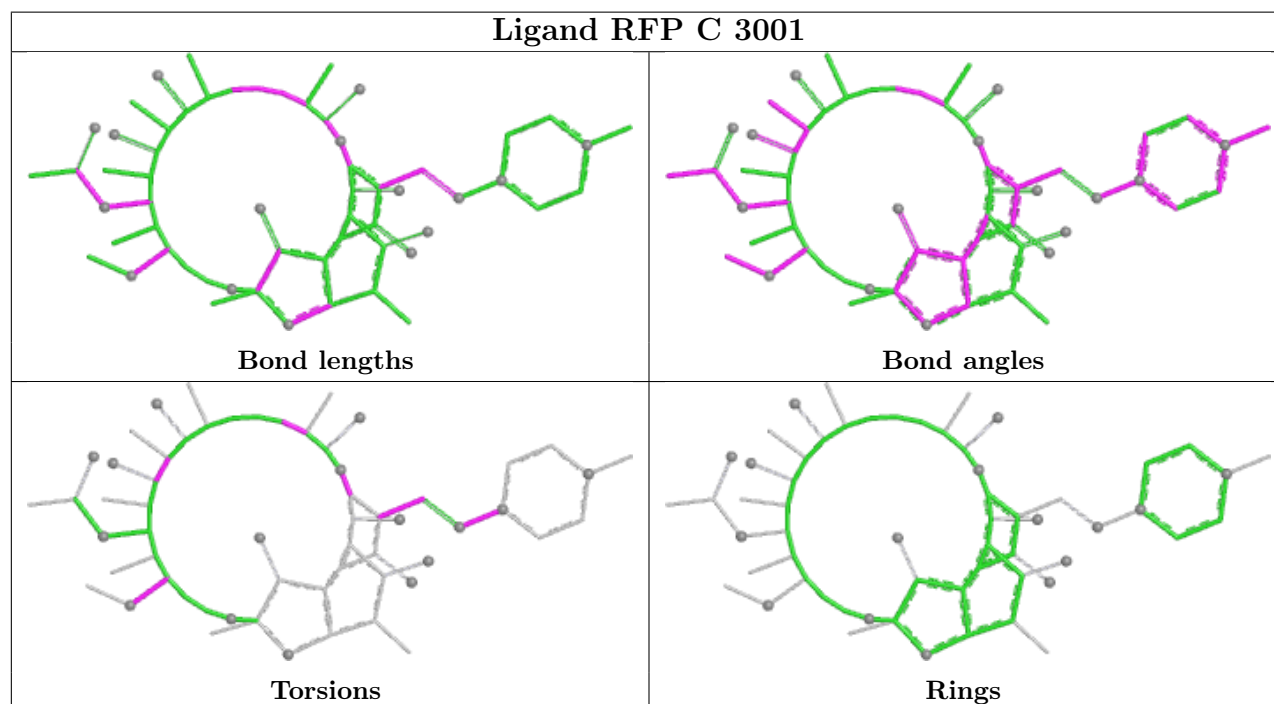
Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C43-N2-N3-C40
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C43-N2-N3-C41
6	C	3001	RFP	C1-C2-N1-C15

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	5	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	233/329 (70%)	-0.68	0 100 100	171, 206, 261, 301	0
1	B	217/329 (65%)	-0.64	0 100 100	179, 243, 300, 333	0
1	G	227/329 (68%)	-0.76	0 100 100	223, 269, 305, 330	0
1	H	216/329 (65%)	-0.66	0 100 100	213, 288, 312, 327	0
2	C	1340/1342 (99%)	-0.61	0 100 100	126, 197, 326, 418	0
2	I	1340/1342 (99%)	-0.62	0 100 100	174, 254, 341, 465	0
3	D	1167/1407 (82%)	-0.56	0 100 100	137, 186, 259, 335	0
3	J	1155/1407 (82%)	-0.57	0 100 100	163, 218, 292, 350	0
4	E	89/91 (97%)	-0.66	0 100 100	180, 221, 256, 264	0
4	K	79/91 (86%)	-0.68	0 100 100	244, 325, 377, 395	0
5	F	468/613 (76%)	-0.60	0 100 100	185, 234, 373, 416	0
5	L	469/613 (76%)	-0.64	0 100 100	219, 257, 379, 441	0
All	All	7000/8222 (85%)	-0.61	0 100 100	126, 229, 321, 465	0

There are no RSRZ outliers to report.

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

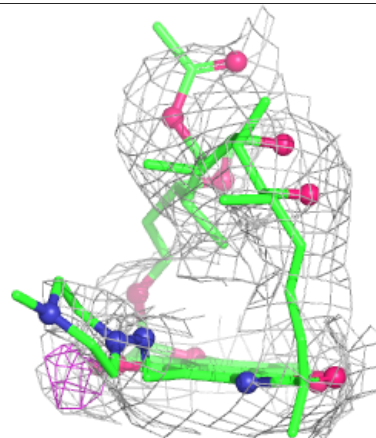
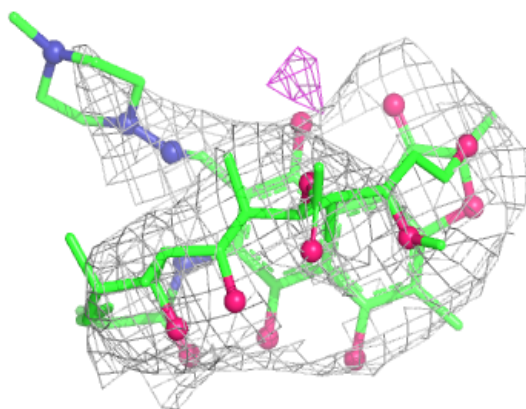
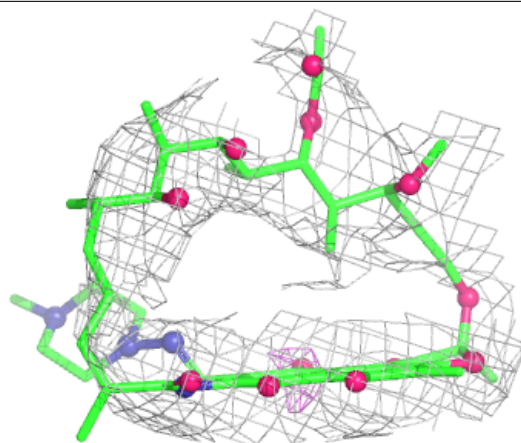
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	MG	I	1401	1/1	-0.04	0.16	216,216,216,216	0
7	MG	C	3002	1/1	0.30	0.13	216,216,216,216	0
7	MG	D	2001	1/1	0.56	0.07	216,216,216,216	0
7	MG	J	2001	1/1	0.72	0.08	216,216,216,216	0
8	ZN	J	2002	1/1	0.82	0.08	222,222,222,222	0
8	ZN	D	2002	1/1	0.89	0.09	216,216,216,216	0
6	RFP	C	3001	59/59	0.94	0.08	136,178,213,228	0
8	ZN	D	2003	1/1	0.96	0.15	216,216,216,216	0
8	ZN	J	2003	1/1	0.97	0.11	216,216,216,216	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 RFP C 3001:

$2mF_o-DF_c$ (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.