



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 02:42 pm BST

PDB ID : 5UAC
Title : Escherichia coli RNA polymerase and Rifampin complex, wild-type
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : 2016-12-19
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

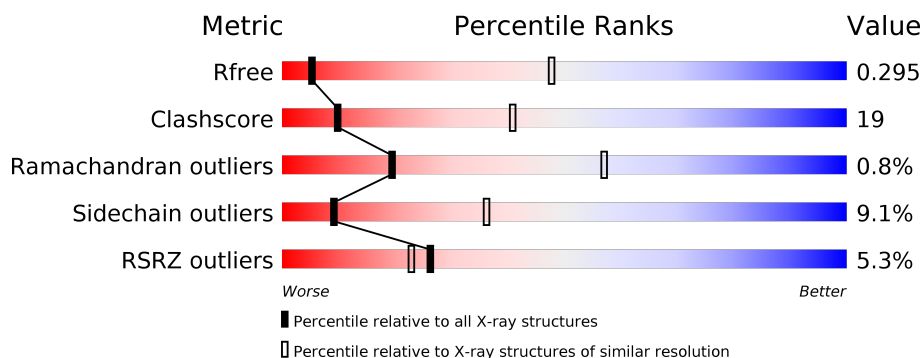
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 on 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	
1	B	329	
1	G	329	
1	H	329	
2	C	1342	
2	I	1342	

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

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
7	MG	J	1501	-	-	-	X
8	ZN	D	1503	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55049 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	227	Total	C	N	O	S	0	0	0
			1753	1091	311	345	6			
1	B	214	Total	C	N	O	S	0	0	0
			1649	1029	290	324	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	215	Total	C	N	O	S	0	0	0
			1659	1037	291	325	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1342	Total	C	N	O	S	0	0	0
			10585	6641	1843	2057	44			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9089	5714	1627	1702	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9001	5659	1612	1684	46			

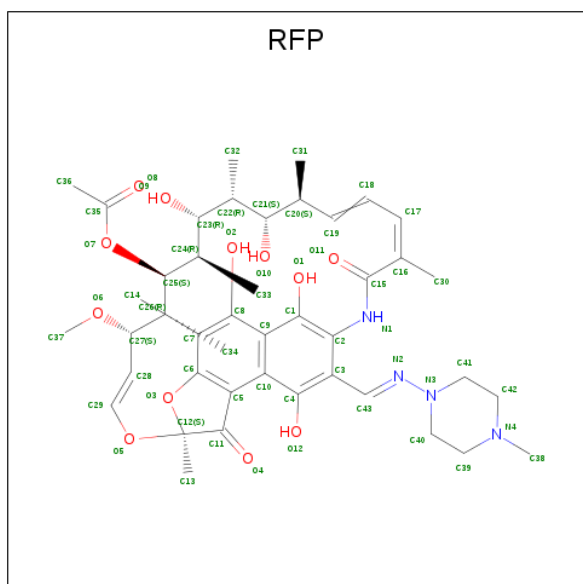
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

Chain G:

39% 25% 32%

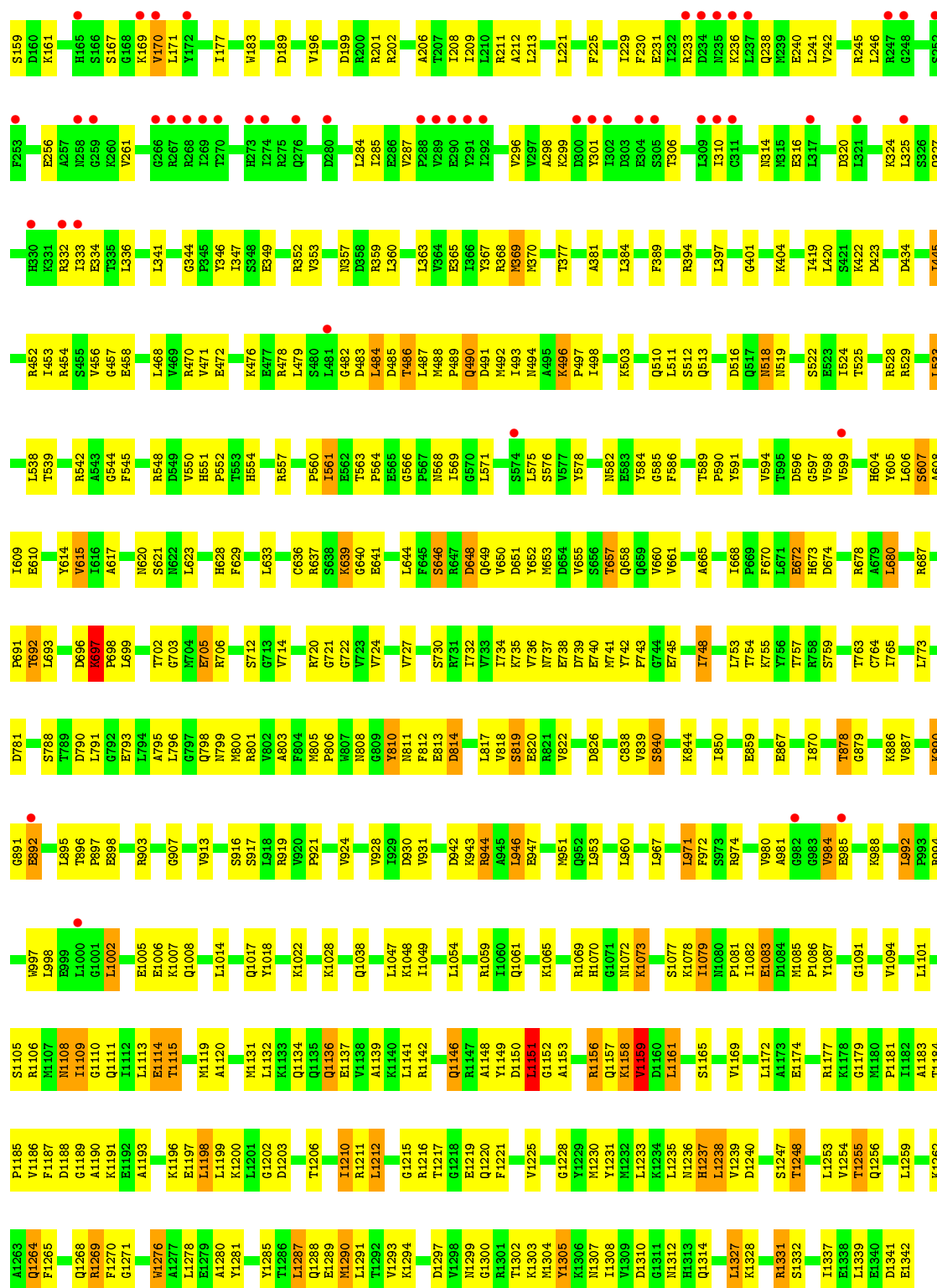
PRO THR VAL ARG SER ILE ALA ASP GLU

MET GLN GLY SER VAL THR L9 K10 P11 R12 L13 V14 D15 V19 S20 H23 V26 E29 P30 G36 H37 T38 R48 I46 L47 S49 S60 E68 V69 E60 I61 D62 H66 S69 T70 G73 V74 Q75 E76 D77 I78 L82 N83 N84 L85 V87

[illegible]

Chain C:

ID	Name	Category
S72	S72	Green
Y73	Y73	Green
R74	R74	Green
L75	L75	Green
V82	V82	Green
C85	C85	Green
Q86	Q86	Green
V90	V90	Green
T91	T91	Green
Y92	Y92	Green
S93	S93	Green
A94	A94	Green
P95	P95	Green
L96	L96	Green
R97	R97	Green
Y98	Y98	Green
K99	K99	Green
L100	L100	Green
R101	R101	Green
L102	L102	Green
V103	V103	Green
Y105	Y105	Green
L106	L106	Green
R107	R107	Green
Y108	Y108	Green
A109	A109	Green
P110	P110	Green
V114	V114	Green
K115	K115	Green
D116	D116	Green
L117	L117	Green
K118	K118	Green
E119	E119	Green
Q120	Q120	Green
E121	E121	Green
D122	D122	Green
I128	I128	Green
N139	N139	Green
G140	G140	Green
T141	T141	Green
E142	E142	Green
L143	L143	Green
V144	V144	Green
I145	I145	Green
V146	V146	Green
L149	L149	Green
H150	H150	Green
R151	R151	Green
P152	P152	Green
Y153	Y153	Green
V158	V158	Green
M1	M1	Green
V2	V2	Green
Y3	Y3	Green
S4	S4	Green
Y5	Y5	Green
T6	T6	Green
E7	E7	Green
K8	K8	Green
K9	K9	Green
R10	R10	Green
I11	I11	Green
A12	A12	Green
K13	K13	Green
D14	D14	Green
F15	F15	Green
G16	G16	Green
K17	K17	Green
A18	A18	Green
L22	L22	Green
D23	D23	Green
V24	V24	Green
P25	P25	Green
T26	T26	Green
L27	L27	Green
S28	S28	Green
I30	I30	Green
S34	S34	Green
K37	K37	Green
F38	F38	Green
I39	I39	Green
E40	E40	Green
Q41	Q41	Green
D42	D42	Green
P43	P43	Green
E44	E44	Green
Y47	Y47	Green
G48	G48	Green
L49	L49	Green
S55	S55	Green
V56	V56	Green
I59	I59	Green
Q60	Q60	Green
S61	S61	Green
Y62	Y62	Green
G63	G63	Green
S64	S64	Green
N65	N65	Green
S66	S66	Green
E67	E67	Green
L68	L68	Green
P69	P69	Green
Y70	Y70	Green
V71	V71	Green

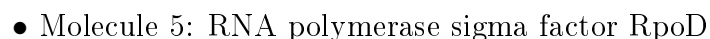


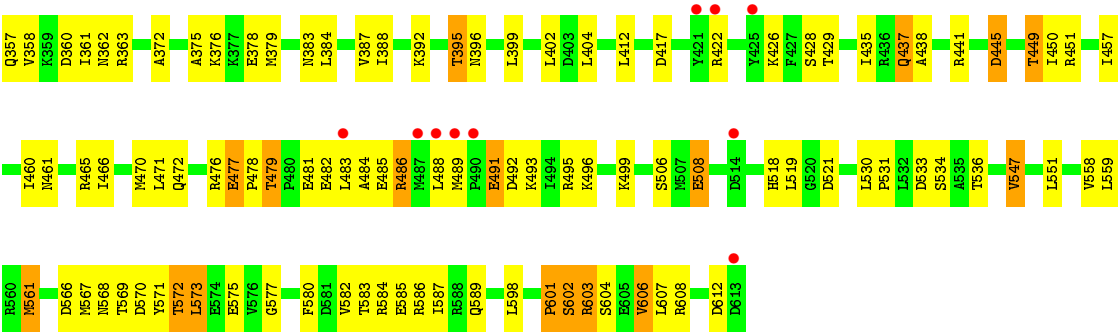
• Molecule 2: DNA-directed RNA polymerase subunit beta











4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.96Å 204.43Å 313.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 3.80 29.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.98-3.80) 99.8 (29.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.75Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.248 , 0.295 0.248 , 0.295	Depositor DCC
R_{free} test set	1991 reflections (1.67%)	wwPDB-VP
Wilson B-factor (Å ²)	159.8	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 102.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55049	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.67% 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: ZN, RFP, 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	2/1774 (0.1%)	0.86	2/2405 (0.1%)
1	B	0.66	0/1668	0.91	1/2260 (0.0%)
1	G	0.54	0/1751	0.77	1/2373 (0.0%)
1	H	0.53	0/1678	0.85	2/2274 (0.1%)
2	C	0.89	12/10754 (0.1%)	0.92	25/14509 (0.2%)
2	I	0.58	4/10735 (0.0%)	0.71	2/14484 (0.0%)
3	D	0.96	20/9229 (0.2%)	0.98	27/12459 (0.2%)
3	J	0.74	4/9140 (0.0%)	0.86	14/12341 (0.1%)
4	E	0.69	0/693	0.81	1/935 (0.1%)
4	K	0.31	0/629	0.55	0/847
5	F	0.50	0/3864	0.69	3/5194 (0.1%)
5	L	0.46	0/3872	0.63	1/5205 (0.0%)
All	All	0.74	42/55787 (0.1%)	0.84	79/75286 (0.1%)

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	B	0	1
2	C	0	6
2	I	0	2
3	D	0	6
3	J	0	2
4	E	0	1
5	F	0	1
5	L	0	1
All	All	0	20

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	764	CYS	CB-SG	-11.76	1.62	1.82
3	D	454	CYS	CB-SG	-8.90	1.67	1.82
2	C	636	CYS	CB-SG	-8.85	1.67	1.82
3	J	888	CYS	CB-SG	-8.72	1.67	1.82
2	C	838	CYS	CB-SG	-8.60	1.67	1.82

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	343	LEU	CA-CB-CG	-8.74	95.19	115.30
3	D	807	LEU	CB-CG-CD2	-8.46	96.62	111.00
3	J	327	LEU	CB-CG-CD2	-8.45	96.64	111.00
3	D	888	CYS	CA-CB-SG	-8.38	98.92	114.00
3	J	426	ALA	C-N-CD	-8.01	102.98	120.60

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	GLU	Peptide
2	C	109	ALA	Peptide
2	C	1239	VAL	Mainchain
2	C	236	LYS	Peptide
2	C	646	SER	Mainchain

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	1753	0	1780	90	0
1	B	1649	0	1674	101	0
1	G	1730	0	1756	82	0
1	H	1659	0	1692	91	0
2	C	10585	0	10603	425	0
2	I	10566	0	10576	385	0
3	D	9089	0	9264	449	0
3	J	9001	0	9170	378	0
4	E	691	0	695	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	24	0
5	F	3813	0	3880	132	0
5	L	3821	0	3884	134	0
6	C	59	0	54	14	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	2	0
8	J	2	0	0	1	0
All	All	55049	0	55662	2119	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 19.

The worst 5 of 2119 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)
3:J:343:LEU:CG	3:J:343:LEU:CD2	1.79	1.59
3:D:426:ALA:CB	3:D:427:PRO:CD	2.12	1.26
3:J:426:ALA:CB	3:J:427:PRO:HD3	1.69	1.19
3:D:343:LEU:HD22	3:D:344:GLY:HA3	1.16	1.16
3:D:426:ALA:HB3	3:D:427:PRO:CD	1.70	1.13

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	225/329 (68%)	196 (87%)	25 (11%)	4 (2%)	8	42
1	B	210/329 (64%)	183 (87%)	22 (10%)	5 (2%)	6	37
1	G	222/329 (68%)	193 (87%)	25 (11%)	4 (2%)	8	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	211/329 (64%)	187 (89%)	17 (8%)	7 (3%)	4	32
2	C	1340/1342 (100%)	1233 (92%)	100 (8%)	7 (0%)	29	66
2	I	1338/1342 (100%)	1232 (92%)	101 (8%)	5 (0%)	34	70
3	D	1162/1407 (83%)	1072 (92%)	81 (7%)	9 (1%)	19	57
3	J	1151/1407 (82%)	1056 (92%)	80 (7%)	15 (1%)	12	48
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%)	422 (91%)	39 (8%)	1 (0%)	47	79
5	L	463/613 (76%)	424 (92%)	38 (8%)	1 (0%)	47	79
All	All	6948/8222 (84%)	6354 (92%)	536 (8%)	58 (1%)	19	57

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	162	GLU
1	A	167	PRO
1	B	13	LEU
2	C	1159	VAL
3	D	10	ALA

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	194/286 (68%)	182 (94%)	12 (6%)	18	49
1	B	182/286 (64%)	172 (94%)	10 (6%)	21	53
1	G	191/286 (67%)	179 (94%)	12 (6%)	18	49
1	H	184/286 (64%)	177 (96%)	7 (4%)	33	61
2	C	1157/1157 (100%)	1051 (91%)	106 (9%)	9	35
2	I	1154/1157 (100%)	1050 (91%)	104 (9%)	9	37
3	D	970/1168 (83%)	873 (90%)	97 (10%)	7	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	J	960/1168 (82%)	860 (90%)	100 (10%)	7	30
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	29
4	K	67/75 (89%)	63 (94%)	4 (6%)	19	50
5	F	417/540 (77%)	376 (90%)	41 (10%)	8	33
5	L	418/540 (77%)	376 (90%)	42 (10%)	7	32
All	All	5966/7024 (85%)	5423 (91%)	543 (9%)	9	36

5 of 543 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	395	THR
2	I	116	ASP
5	L	98	VAL
5	F	450	ILE
1	G	13	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	362	ASN
2	I	69	GLN
5	L	131	GLN
5	F	383	ASN
5	F	472	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 7 ligands modelled in this entry, 6 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	2.49	21 (33%)	94,94,94	2.68	36 (38%)

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	-	-	15/60/85/85	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	3001	RFP	O3-C6	9.15	1.55	1.37
6	C	3001	RFP	O7-C25	-8.17	1.32	1.44
6	C	3001	RFP	C12-C11	-5.59	1.32	1.54
6	C	3001	RFP	C15-N1	4.86	1.46	1.35
6	C	3001	RFP	C18-C17	4.05	1.56	1.43

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3001	RFP	C32-C22-C23	-7.21	96.82	111.39
6	C	3001	RFP	C33-C24-C23	-6.90	97.45	111.39
6	C	3001	RFP	C38-N4-C42	6.63	120.58	110.66
6	C	3001	RFP	O7-C25-C26	-6.57	92.21	107.50
6	C	3001	RFP	O4-C11-C5	-5.55	121.23	131.81

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

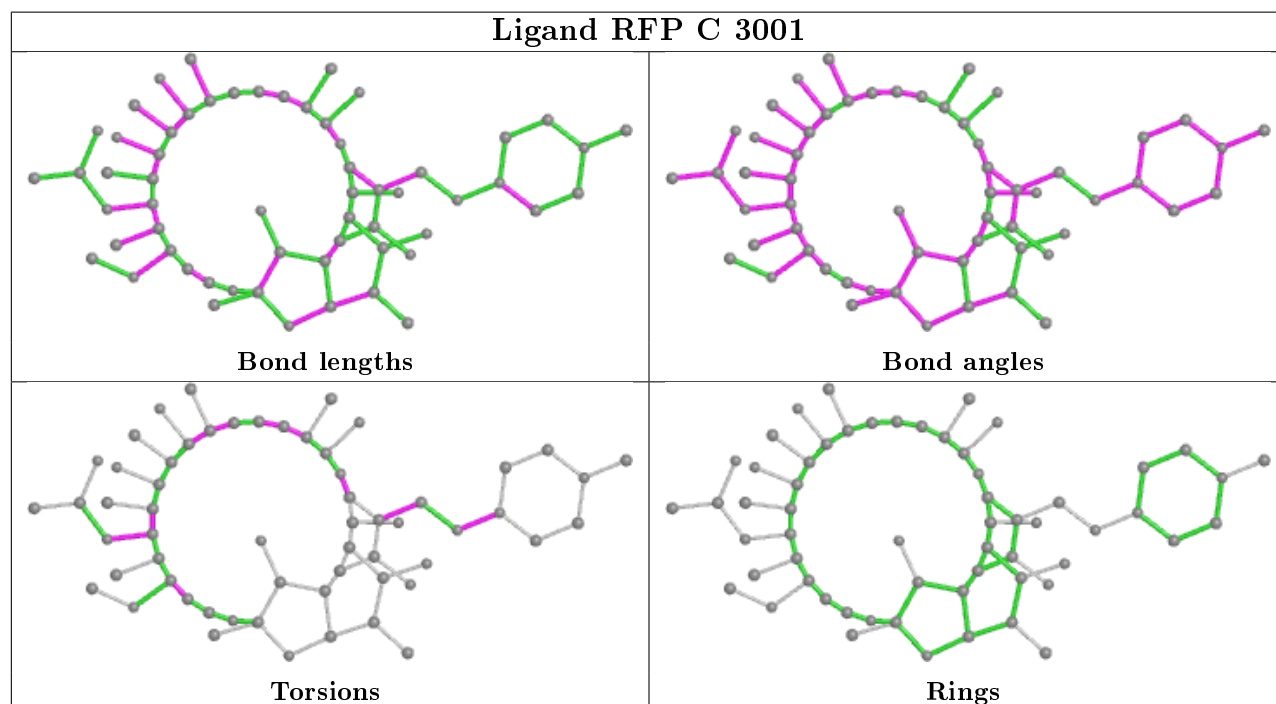
Mol	Chain	Res	Type	Atoms
6	C	3001	RFP	C3-C2-N1-C15
6	C	3001	RFP	C4-C3-C43-N2
6	C	3001	RFP	C19-C20-C21-O10
6	C	3001	RFP	O6-C27-C28-C29
6	C	3001	RFP	C43-N2-N3-C40

There are no ring outliers.

1 monomer is involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	3001	RFP	14	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	227/329 (68%)	-0.20	4 (1%) 68 61	128, 159, 207, 262	0
1	B	214/329 (65%)	0.12	7 (3%) 46 38	115, 179, 246, 259	0
1	G	224/329 (68%)	-0.20	1 (0%) 92 89	162, 193, 225, 245	0
1	H	215/329 (65%)	0.10	9 (4%) 36 30	165, 218, 246, 265	0
2	C	1342/1342 (100%)	-0.04	57 (4%) 36 30	96, 152, 303, 368	0
2	I	1340/1342 (99%)	0.24	90 (6%) 17 14	129, 200, 287, 371	0
3	D	1166/1407 (82%)	-0.14	25 (2%) 63 55	94, 140, 215, 278	0
3	J	1155/1407 (82%)	-0.07	30 (2%) 56 47	118, 164, 225, 300	0
4	E	89/91 (97%)	-0.16	0 100 100	131, 170, 200, 214	0
4	K	79/91 (86%)	1.01	19 (24%) 0 0	221, 276, 310, 318	0
5	F	468/613 (76%)	0.50	62 (13%) 3 3	139, 216, 432, 522	0
5	L	469/613 (76%)	0.71	67 (14%) 2 3	144, 239, 458, 518	0
All	All	6988/8222 (84%)	0.09	371 (5%) 26 23	94, 176, 295, 522	0

The worst 5 of 371 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	14.7
5	L	319	ALA	13.8
5	L	321	ALA	13.7
5	F	312	SER	13.5
5	L	327	SER	12.4

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

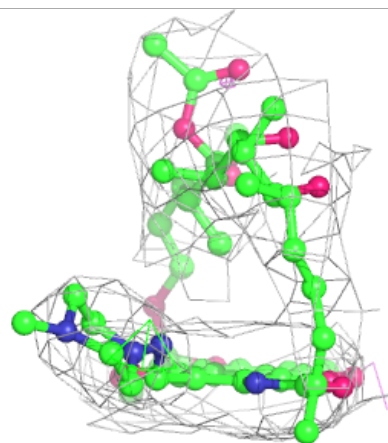
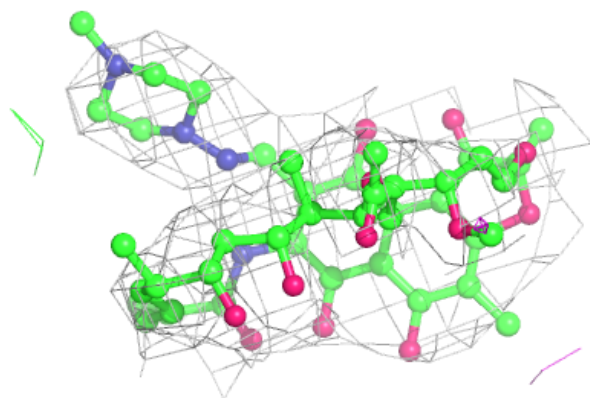
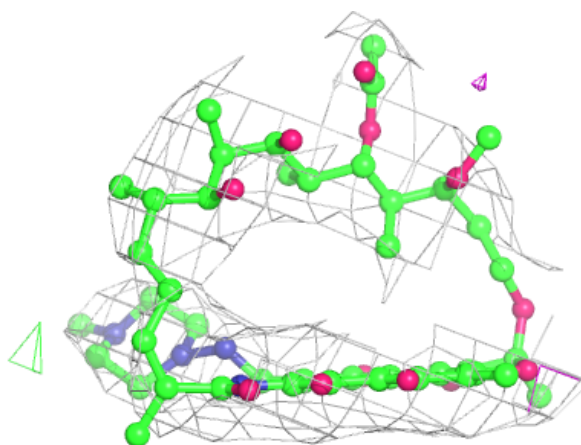
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MG	J	1501	1/1	0.51	0.51	290,290,290,290	0
8	ZN	D	1502	1/1	0.58	0.25	324,324,324,324	0
8	ZN	J	1502	1/1	0.61	0.18	322,322,322,322	0
8	ZN	D	1503	1/1	0.71	0.37	274,274,274,274	0
7	MG	D	1501	1/1	0.80	0.41	264,264,264,264	0
8	ZN	J	1503	1/1	0.86	0.42	281,281,281,281	0
6	RFP	C	3001	59/59	0.92	0.22	88,136,160,162	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.