



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 03:36 PM EDT

PDB ID : 6OVY / pdb_00006ovy
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter variant -1C
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-08
Resolution : 3.00 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:

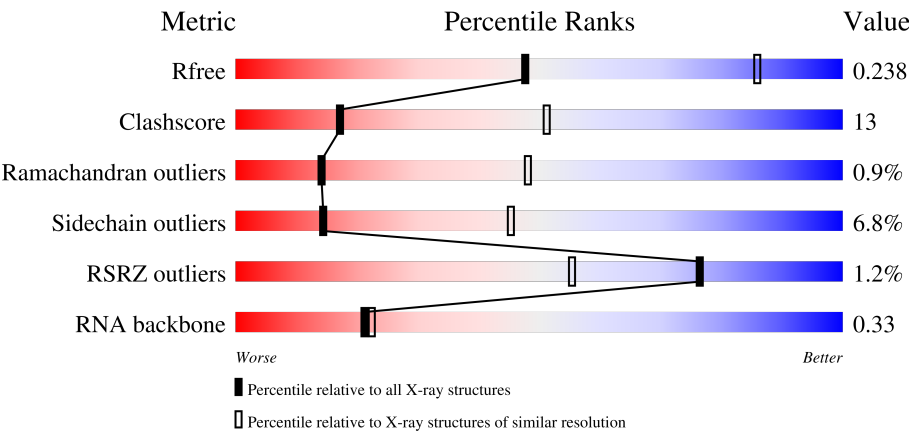
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	315	51% 18% • 28%
1	B	315	% 46% 22% • 30%
2	C	1119	% 64% 31% • •
3	D	1524	% 67% 27% • •

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Mol	Chain	Length	Quality of chain
4	E	99	% 75% 18% • 5%
5	F	423	2% 54% 23% • 20%
6	G	22	23% 41% 5% 32%
7	H	27	33% 26% 41%
8	I	4	25% 50% 25%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28273 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	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	222	Total	C	N	O	S	0	0	0
			1750	1118	304	326	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8760	5543	1561	1632	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11726	7432	2065	2194	35			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	338	Total	C	N	O	S	0	0	0
			2747	1736	500	507	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

- Molecule 6 is a DNA chain called DNA (5'-D(P*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*CP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	15	Total	C	N	O	P	0	0	0
			304	144	60	85	15			

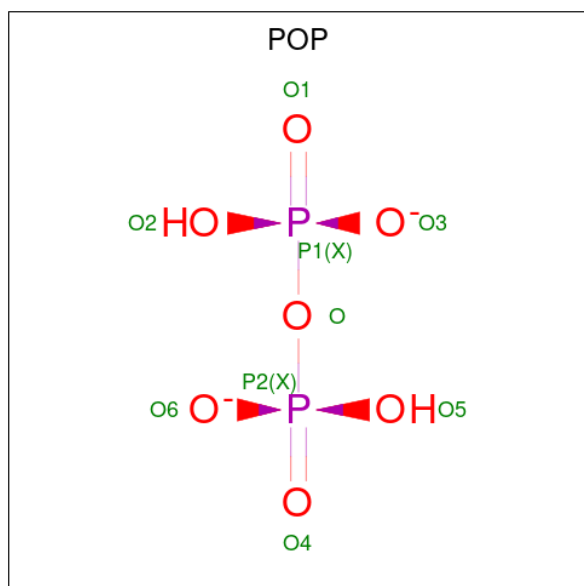
- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*TP*CP*TP*GP*AP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	16	Total	C	N	O	P	0	0	0
			330	159	60	96	15			

- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	4	Total	C	N	O	P	0	0	0
			101	40	20	35	6			

- Molecule 9 is PYROPHOSPHATE 2- (CCD ID: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	P	0	0
			9	7	2		

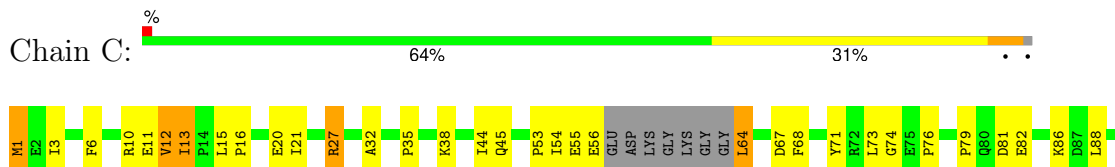
- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

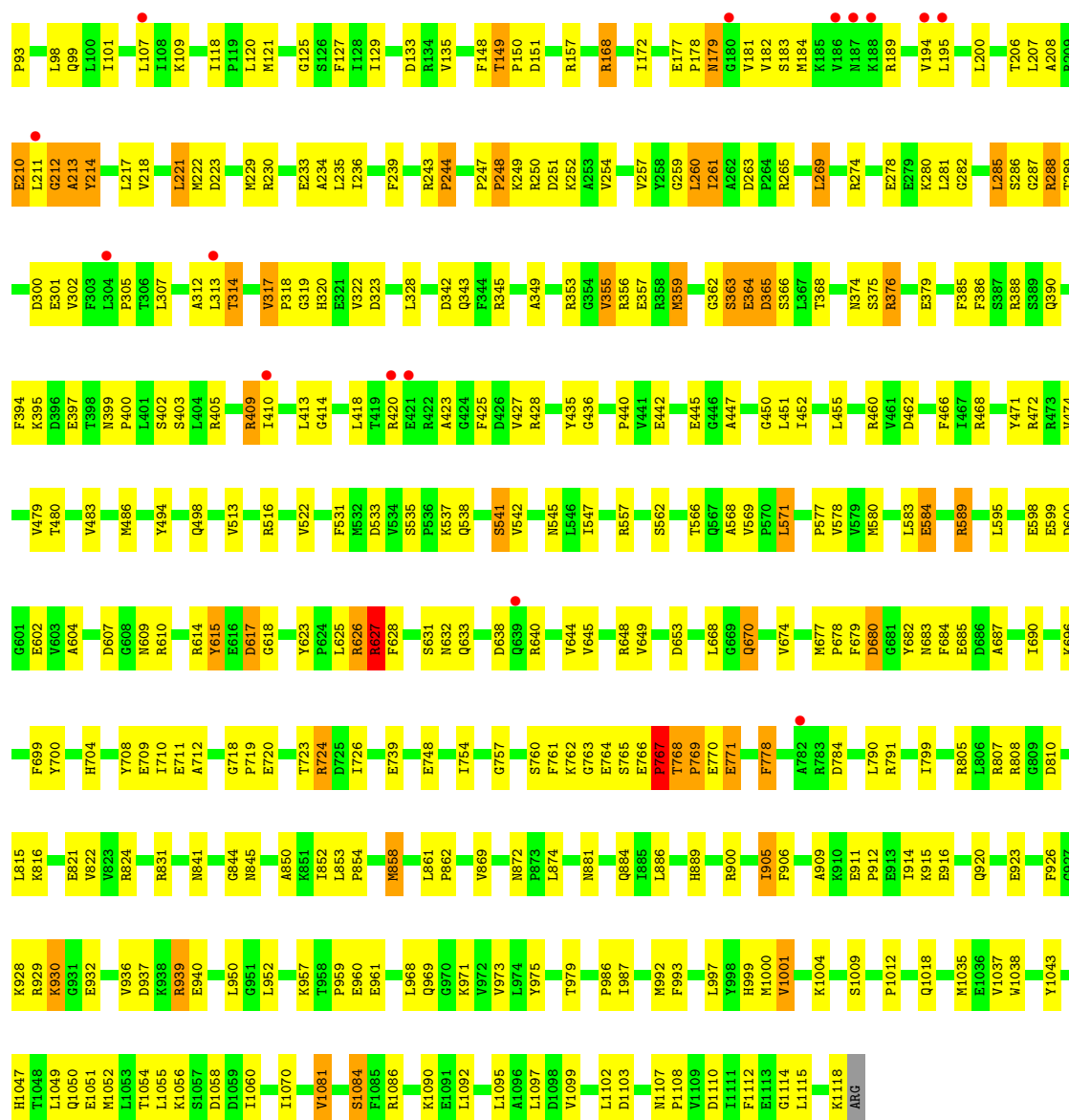
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	1	Total	Mg	0	0
			1	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

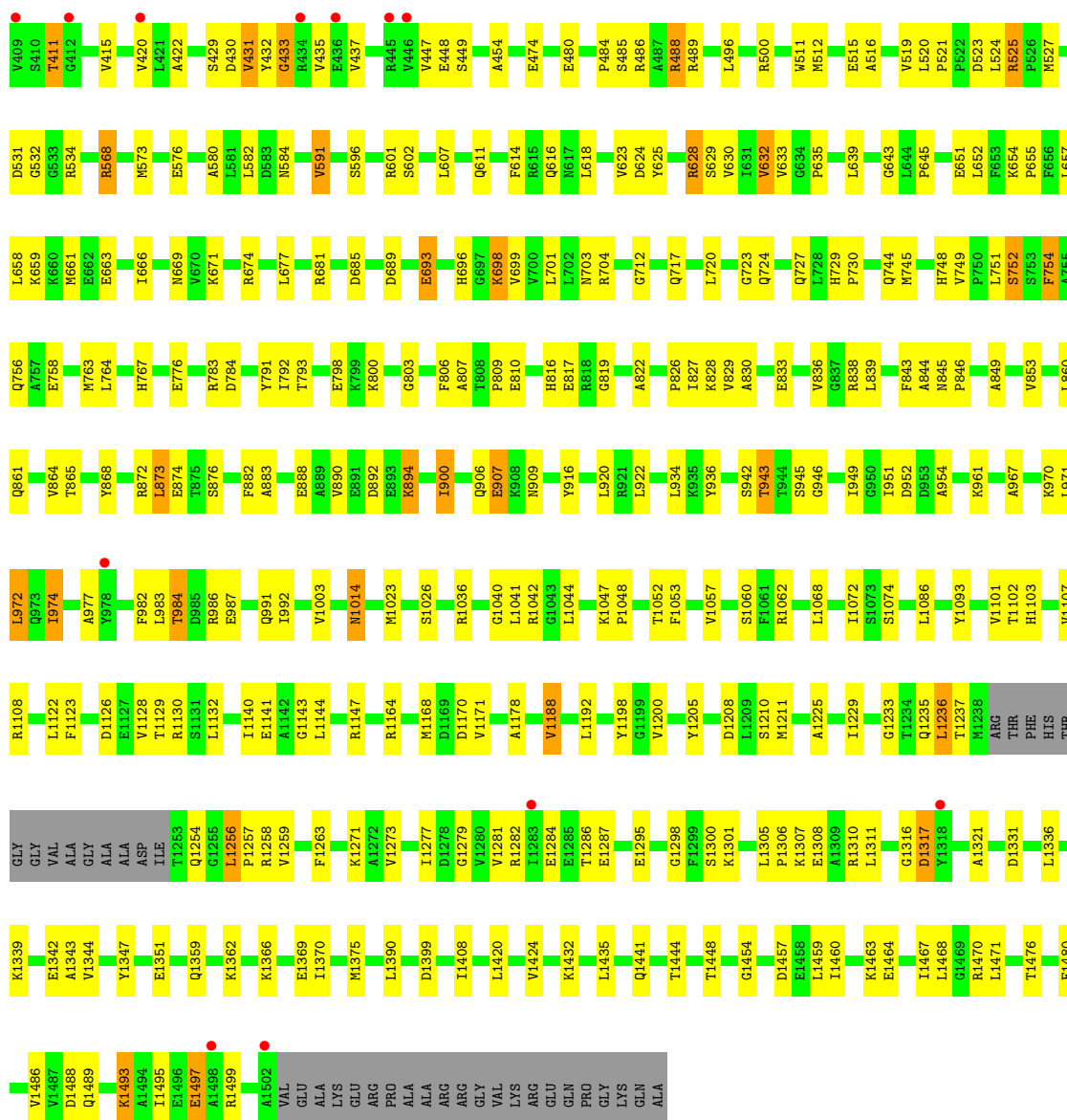
- Molecule 1: DNA-directed RNA polymerase subunit alpha



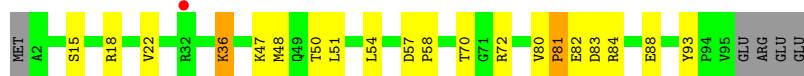
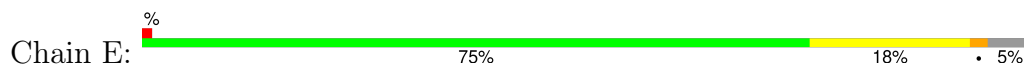


• Molecule 3: DNA-directed RNA polymerase subunit beta'

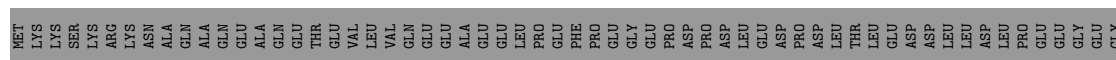


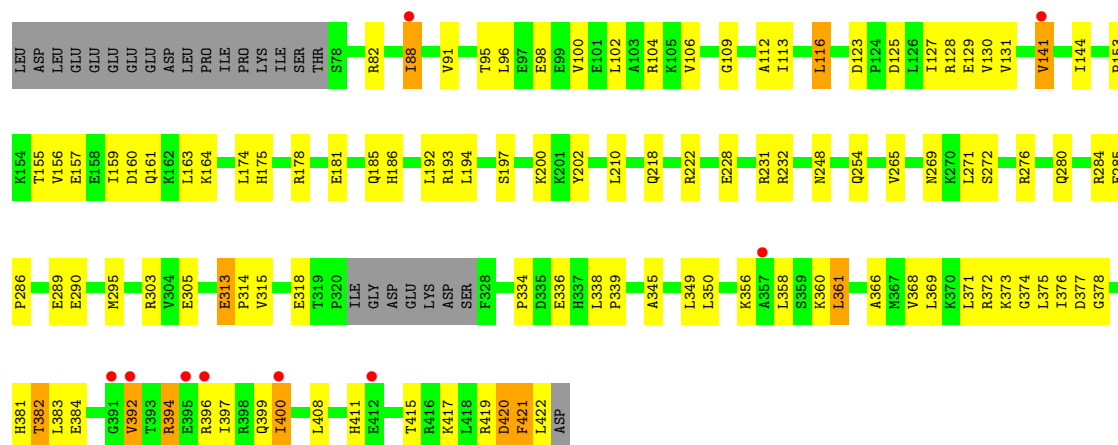


- Molecule 4: DNA-directed RNA polymerase subunit omega

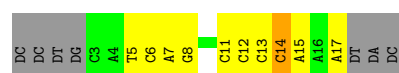
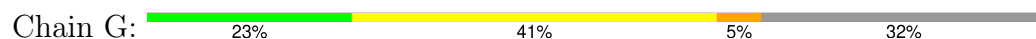


- Molecule 5: RNA polymerase sigma factor SigA

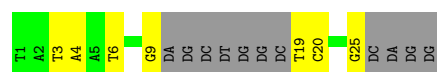




- Molecule 6: DNA (5'-D(P*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*CP*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*TP*CP*TP*GP*AP*TP*G)-3')



- Molecule 8: RNA (5'-D(*(GTP))-R(P*GP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.83Å 102.48Å 295.60Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	45.66 – 3.00 45.66 – 3.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (45.66-3.00) 96.6 (45.66-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.213 , 0.237 0.212 , 0.238	Depositor DCC
R_{free} test set	1991 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	80.3	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28273	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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: MG, ZN, POP, GTP

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	0.54	0/1814	0.91	4/2466 (0.2%)
1	B	0.54	0/1782	0.93	1/2424 (0.0%)
2	C	0.54	0/8927	0.93	9/12075 (0.1%)
3	D	0.57	0/11932	0.92	8/16134 (0.0%)
4	E	0.48	0/775	0.87	0/1045
5	F	0.46	0/2791	0.83	1/3754 (0.0%)
6	G	0.65	1/341 (0.3%)	0.71	0/522
7	H	0.45	0/369	0.58	0/567
8	I	0.99	0/77	1.16	0/119
All	All	0.54	1/28808 (0.0%)	0.91	23/39106 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	14	DC	O3'-P	-5.36	1.53	1.61

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1256	LEU	CA-C-N	-8.26	109.52	119.84
3	D	1256	LEU	C-N-CA	-8.26	109.52	119.84
3	D	35	ARG	NE-CZ-NH1	-7.45	114.05	121.50
3	D	35	ARG	NE-CZ-NH2	7.35	125.81	119.20
2	C	409	ARG	CG-CD-NE	7.26	127.97	112.00

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	1782	0	1834	42	0
1	B	1750	0	1797	61	0
2	C	8760	0	8859	284	0
3	D	11726	0	11949	308	0
4	E	761	0	778	14	0
5	F	2747	0	2831	70	0
6	G	304	0	167	10	0
7	H	330	0	185	6	0
8	I	101	0	43	5	0
9	D	9	0	0	0	0
10	D	1	0	0	0	0
11	D	2	0	0	0	0
All	All	28273	0	28443	713	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 13.

The worst 5 of 713 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:D:260:GLU:OE1	3:D:273:ARG:NH1	1.86	1.07
6:G:17:DA:C8	6:G:17:DA:H5''	1.94	1.01
3:D:1256:LEU:O	3:D:1257:PRO:C	2.10	0.93
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.35	0.91
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.07	0.86

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	224/315 (71%)	203 (91%)	20 (9%)	1 (0%)	30	65
1	B	220/315 (70%)	201 (91%)	18 (8%)	1 (0%)	24	60
2	C	1107/1119 (99%)	1021 (92%)	71 (6%)	15 (1%)	9	36
3	D	1481/1524 (97%)	1387 (94%)	86 (6%)	8 (0%)	24	60
4	E	92/99 (93%)	87 (95%)	3 (3%)	2 (2%)	5	26
5	F	334/423 (79%)	314 (94%)	16 (5%)	4 (1%)	10	40
All	All	3458/3795 (91%)	3213 (93%)	214 (6%)	31 (1%)	14	48

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLY
1	B	16	GLN
2	C	213	ALA
2	C	248	PRO
2	C	365	ASP

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	199/273 (73%)	190 (96%)	9 (4%)	24	59
1	B	195/273 (71%)	185 (95%)	10 (5%)	21	55
2	C	934/941 (99%)	868 (93%)	66 (7%)	13	43
3	D	1251/1279 (98%)	1159 (93%)	92 (7%)	13	42
4	E	83/88 (94%)	78 (94%)	5 (6%)	17	50
5	F	294/371 (79%)	275 (94%)	19 (6%)	15	47
All	All	2956/3225 (92%)	2755 (93%)	201 (7%)	14	45

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	394	LEU
3	D	873	LEU
5	F	400	ILE
3	D	429	SER
3	D	611	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	350	HIS
5	F	175	HIS
3	D	703	ASN
5	F	254	GLN
3	D	1359	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	2/4 (50%)	1 (50%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	4	G

There are no RNA pucker outliers to report.

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 4 ligands modelled in this entry, 3 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$
9	POP	D	1601	-	6,8,8	1.36	1 (16%)	12,13,13	1.02	1 (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
9	POP	D	1601	-	-	0/6/6/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1601	POP	P1-O3	-2.15	1.46	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1601	POP	O6-P2-O5	2.39	116.77	107.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	226/315 (71%)	-0.07	1 (0%) 88 76	64, 86, 106, 116	0
1	B	222/315 (70%)	-0.02	2 (0%) 81 61	61, 89, 112, 133	0
2	C	1111/1119 (99%)	-0.02	15 (1%) 73 51	50, 83, 147, 176	0
3	D	1485/1524 (97%)	-0.09	14 (0%) 81 61	42, 79, 137, 179	0
4	E	94/99 (94%)	0.09	1 (1%) 78 57	59, 90, 130, 148	0
5	F	338/423 (79%)	0.16	9 (2%) 56 33	58, 95, 165, 201	0
6	G	15/22 (68%)	-0.06	0 100 100	56, 92, 222, 239	0
7	H	16/27 (59%)	-0.00	0 100 100	84, 108, 189, 199	0
8	I	3/4 (75%)	-0.40	0 100 100	58, 58, 66, 71	0
All	All	3510/3848 (91%)	-0.04	42 (1%) 76 55	42, 85, 144, 239	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	434	ARG	3.5
5	F	396	ARG	3.2
3	D	446	VAL	3.1
3	D	412	GLY	3.0
2	C	188	LYS	2.7

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
9	POP	D	1601	9/9	0.71	0.09	84,92,116,124	0
10	MG	D	1602	1/1	0.95	0.12	59,59,59,59	0
11	ZN	D	1603	1/1	1.00	0.04	101,101,101,101	0
11	ZN	D	1604	1/1	1.00	0.02	74,74,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.