



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TU3
Title : Crystal Structure of Rab5 complex with Rabaptin5 C-terminal Domain
Authors : Zhu, G.; Zhai, P.; Liu, J.; Terzyan, S.; Li, G.; Zhang, X.C.
Deposited on : 2004-06-24
Resolution : 2.31 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

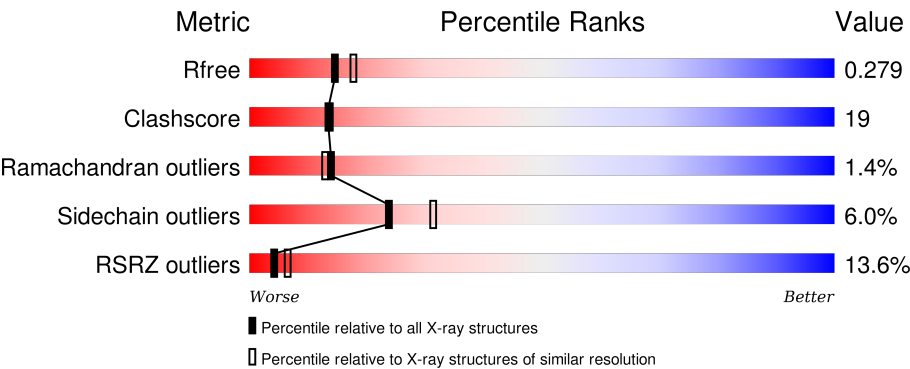
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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. 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	171	<div><div>9%</div><div>65%</div><div>29%</div><div>.</div><div>.</div></div>
1	B	171	<div><div>9%</div><div>65%</div><div>28%</div><div>.</div><div>.</div></div>
1	C	171	<div><div>13%</div><div>57%</div><div>37%</div><div>.</div><div>.</div></div>
1	D	171	<div><div>22%</div><div>39%</div><div>41%</div><div>6%</div><div>14%</div></div>
1	E	171	<div><div>6%</div><div>74%</div><div>22%</div><div>.</div><div>.</div></div>

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Mol	Chain	Length	Quality of chain
2	F	79	<div><div><div></div><div></div><div></div><div></div></div><div>5%35%19%•42%</div></div>
2	G	79	<div><div><div></div><div></div><div></div><div></div></div><div>5%42%19%••35%</div></div>
2	H	79	<div><div><div></div><div></div><div></div><div></div></div><div>15%20%29%6%44%</div></div>
2	I	79	<div><div><div></div><div></div><div></div><div></div></div><div>19%22%34%•43%</div></div>
2	J	79	<div><div><div></div><div></div><div></div><div></div></div><div>10%49%16%•33%</div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8735 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 Ras-related protein Rab-5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total 1296	C 825	N 218	O 247	S 6	0	0	0
1	B	166	Total 1305	C 831	N 220	O 248	S 6	0	0	0
1	C	166	Total 1305	C 829	N 221	O 249	S 6	0	0	0
1	D	147	Total 1141	C 726	N 190	O 220	S 5	0	0	0
1	E	167	Total 1313	C 835	N 222	O 250	S 6	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	MET	-	CLONING ARTIFACT	UNP P20339
B	14	MET	-	CLONING ARTIFACT	UNP P20339
C	14	MET	-	CLONING ARTIFACT	UNP P20339
D	14	MET	-	CLONING ARTIFACT	UNP P20339
E	14	MET	-	CLONING ARTIFACT	UNP P20339

- Molecule 2 is a protein called Rab GTPase binding effector protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	46	Total	C	N	O	0	0	0
			381	233	74	74			
2	G	51	Total	C	N	O	0	0	0
			422	257	82	83			
2	H	44	Total	C	N	O	0	0	0
			367	225	71	71			
2	I	45	Total	C	N	O	0	0	0
			375	230	73	72			
2	J	53	Total	C	N	O	0	0	0
			437	267	84	86			

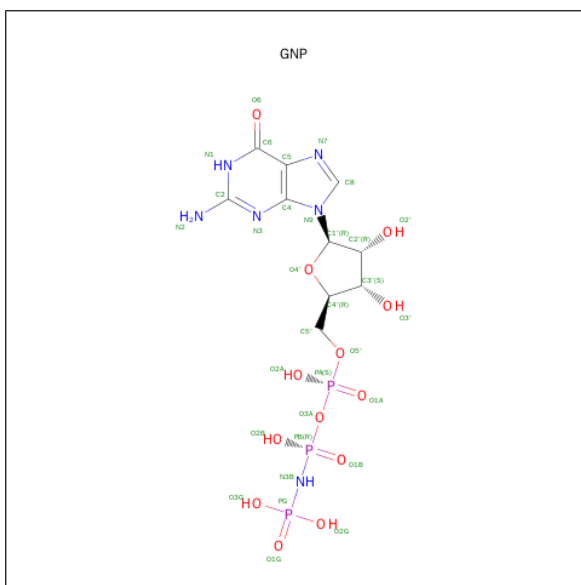
There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	784	GLY	-	CLONING ARTIFACT	UNP Q15276
F	785	PRO	-	CLONING ARTIFACT	UNP Q15276
F	786	LEU	-	CLONING ARTIFACT	UNP Q15276
F	787	GLY	-	CLONING ARTIFACT	UNP Q15276
F	788	SER	-	CLONING ARTIFACT	UNP Q15276
G	784	GLY	-	CLONING ARTIFACT	UNP Q15276
G	785	PRO	-	CLONING ARTIFACT	UNP Q15276
G	786	LEU	-	CLONING ARTIFACT	UNP Q15276
G	787	GLY	-	CLONING ARTIFACT	UNP Q15276
G	788	SER	-	CLONING ARTIFACT	UNP Q15276
H	784	GLY	-	CLONING ARTIFACT	UNP Q15276
H	785	PRO	-	CLONING ARTIFACT	UNP Q15276
H	786	LEU	-	CLONING ARTIFACT	UNP Q15276
H	787	GLY	-	CLONING ARTIFACT	UNP Q15276
H	788	SER	-	CLONING ARTIFACT	UNP Q15276
I	784	GLY	-	CLONING ARTIFACT	UNP Q15276
I	785	PRO	-	CLONING ARTIFACT	UNP Q15276
I	786	LEU	-	CLONING ARTIFACT	UNP Q15276
I	787	GLY	-	CLONING ARTIFACT	UNP Q15276
I	788	SER	-	CLONING ARTIFACT	UNP Q15276
J	784	GLY	-	CLONING ARTIFACT	UNP Q15276
J	785	PRO	-	CLONING ARTIFACT	UNP Q15276
J	786	LEU	-	CLONING ARTIFACT	UNP Q15276
J	787	GLY	-	CLONING ARTIFACT	UNP Q15276
J	788	SER	-	CLONING ARTIFACT	UNP Q15276

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	E	1	Total Mg 1 1	0	0

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	B	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	C	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	D	1	Total 32	C 10	N 6	O 13	P 3	0	0
4	E	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	62	Total O 62 62	0	0
5	B	24	Total O 24 24	0	0
5	C	17	Total O 17 17	0	0
5	D	20	Total O 20 20	0	0
5	E	61	Total O 61 61	0	0
5	F	9	Total O 9 9	0	0
5	G	13	Total O 13 13	0	0

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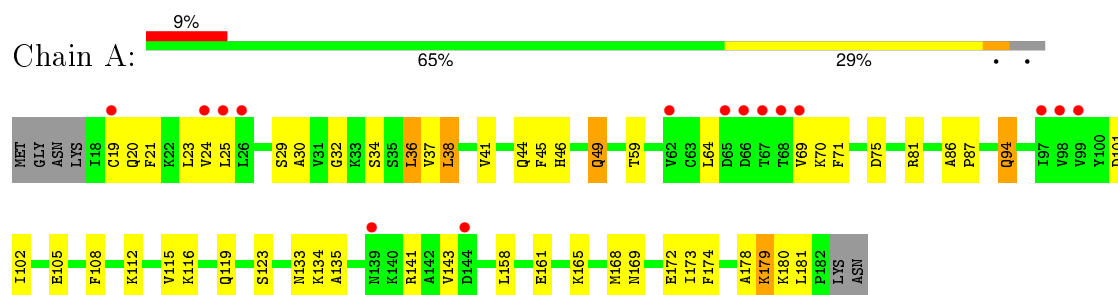
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	H	5	Total 5	O 5	0	0
5	I	2	Total 2	O 2	0	0
5	J	15	Total 15	O 15	0	0

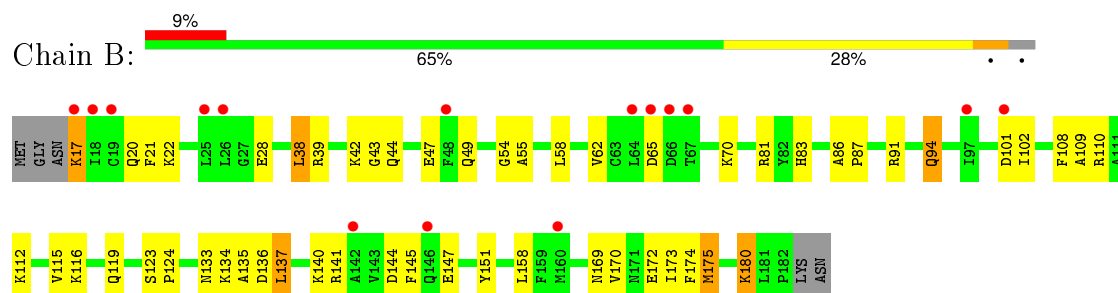
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

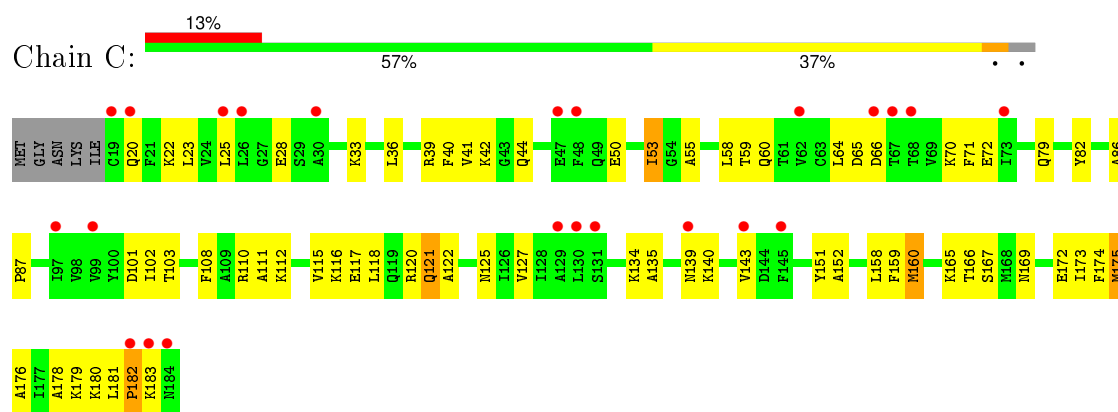
- Molecule 1: Ras-related protein Rab-5A



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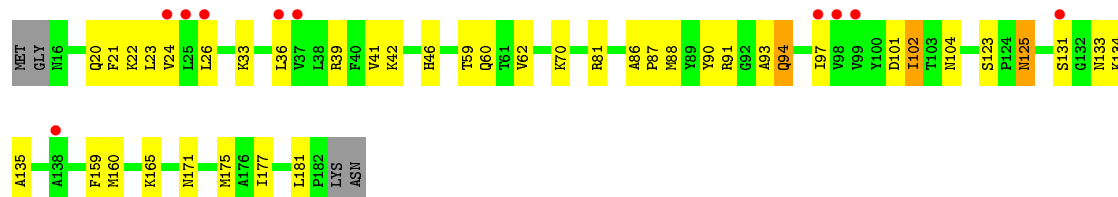
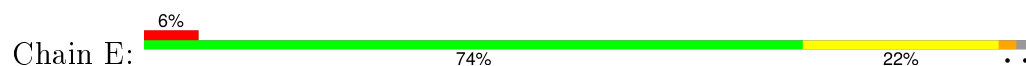
- Molecule 1: Ras-related protein Rab-5A



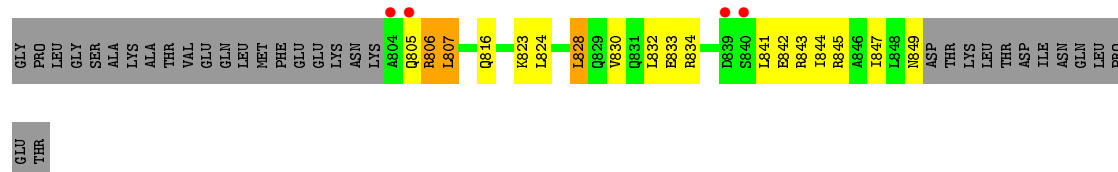
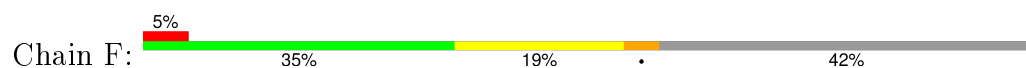
- Molecule 1: Ras-related protein Rab-5A



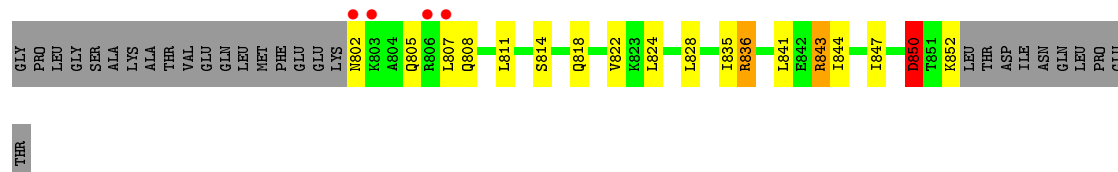
- Molecule 1: Ras-related protein Rab-5A



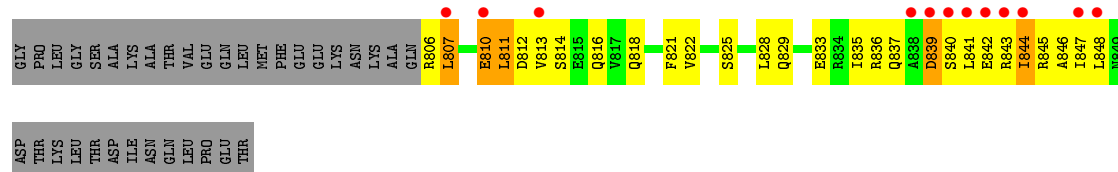
- Molecule 2: Rab GTPase binding effector protein 1



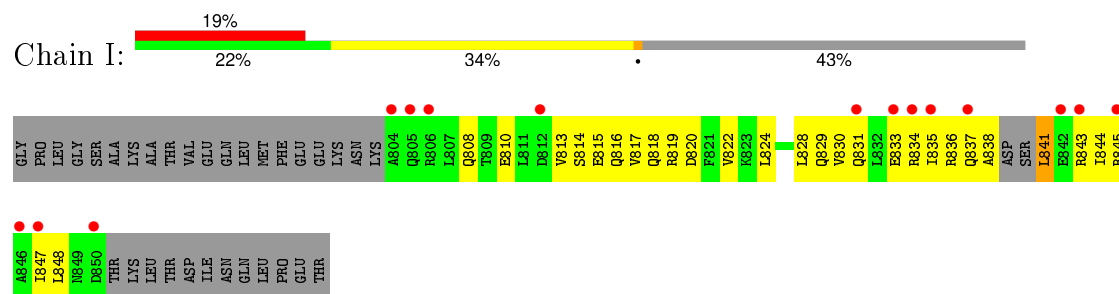
- Molecule 2: Rab GTPase binding effector protein 1



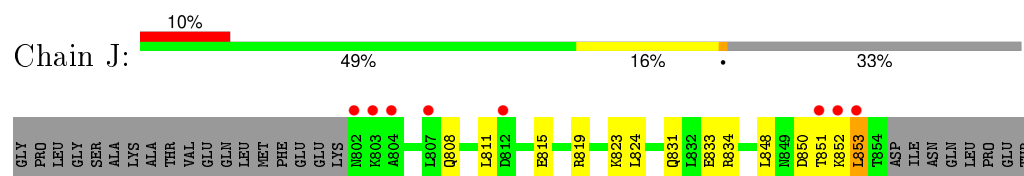
- Molecule 2: Rab GTPase binding effector protein 1



- Molecule 2: Rab GTPase binding effector protein 1



- Molecule 2: Rab GTPase binding effector protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.40Å 83.50Å 144.90Å 90.00° 102.20° 90.00°	Depositor
Resolution (Å)	29.72 – 2.31 29.71 – 2.32	Depositor EDS
% Data completeness (in resolution range)	90.6 (29.72-2.31) 90.8 (29.71-2.32)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.277 0.223 , 0.279	Depositor DCC
R_{free} test set	1035 reflections (1.99%)	DCC
Wilson B-factor (Å ²)	44.5	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 54048 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8735	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: GNP, 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	0.54	0/1319	0.64	0/1782
1	B	0.48	0/1328	0.56	0/1793
1	C	0.44	0/1328	0.52	0/1793
1	D	0.41	0/1155	0.53	0/1555
1	E	0.56	0/1336	0.64	0/1804
2	F	0.48	0/381	0.59	0/511
2	G	0.48	0/422	0.54	0/565
2	H	0.40	0/367	0.47	0/492
2	I	0.37	0/374	0.48	0/500
2	J	0.52	0/437	0.62	0/586
All	All	0.48	0/8447	0.57	0/11381

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	90	TYR	Sidechain

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	1296	0	1285	39	0
1	B	1305	0	1298	50	0
1	C	1305	0	1293	41	0
1	D	1141	0	1138	74	0
1	E	1313	0	1304	30	0
2	F	381	0	395	20	0
2	G	422	0	438	19	0
2	H	367	0	382	39	0
2	I	375	0	389	33	0
2	J	437	0	456	12	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	32	0	13	0	0
4	B	32	0	13	0	0
4	C	32	0	13	0	0
4	D	32	0	13	1	0
4	E	32	0	13	0	0
5	A	62	0	0	1	0
5	B	24	0	0	1	0
5	C	17	0	0	1	0
5	D	20	0	0	2	0
5	E	61	0	0	0	0
5	F	9	0	0	0	0
5	G	13	0	0	1	0
5	H	5	0	0	0	0
5	I	2	0	0	0	0
5	J	15	0	0	2	0
All	All	8735	0	8443	317	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 317 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:HB2	1:A:94:GLN:HG3	1.40	1.00
1:B:38:LEU:HD22	1:B:44:GLN:HB2	1.48	0.94
1:A:38:LEU:HD12	1:A:44:GLN:HB2	1.54	0.90
2:H:843:ARG:HH21	2:H:846:ALA:HB3	1.38	0.89
1:B:158:LEU:HD11	1:B:180:LYS:HZ3	1.38	0.89

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	163/171 (95%)	147 (90%)	15 (9%)	1 (1%)	30	35
1	B	164/171 (96%)	155 (94%)	8 (5%)	1 (1%)	30	35
1	C	164/171 (96%)	147 (90%)	13 (8%)	4 (2%)	7	5
1	D	137/171 (80%)	118 (86%)	16 (12%)	3 (2%)	8	6
1	E	165/171 (96%)	156 (94%)	8 (5%)	1 (1%)	30	35
2	F	44/79 (56%)	42 (96%)	2 (4%)	0	100	100
2	G	49/79 (62%)	45 (92%)	3 (6%)	1 (2%)	9	7
2	H	42/79 (53%)	37 (88%)	3 (7%)	2 (5%)	3	1
2	I	41/79 (52%)	35 (85%)	6 (15%)	0	100	100
2	J	51/79 (65%)	48 (94%)	2 (4%)	1 (2%)	9	7
All	All	1020/1250 (82%)	930 (91%)	76 (8%)	14 (1%)	14	13

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	182	PRO
1	A	64	LEU
1	B	65	ASP

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Mol	Chain	Res	Type
1	D	165	LYS
2	G	850	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	138/143 (96%)	131 (95%)	7 (5%)	29	39
1	B	139/143 (97%)	130 (94%)	9 (6%)	21	27
1	C	139/143 (97%)	131 (94%)	8 (6%)	25	33
1	D	121/143 (85%)	114 (94%)	7 (6%)	25	33
1	E	140/143 (98%)	135 (96%)	5 (4%)	42	57
2	F	43/72 (60%)	38 (88%)	5 (12%)	7	7
2	G	48/72 (67%)	44 (92%)	4 (8%)	14	16
2	H	42/72 (58%)	38 (90%)	4 (10%)	11	12
2	I	42/72 (58%)	40 (95%)	2 (5%)	31	42
2	J	50/72 (69%)	47 (94%)	3 (6%)	24	31
All	All	902/1075 (84%)	848 (94%)	54 (6%)	24	31

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	29	SER
1	D	140	LYS
2	I	808	GLN
1	D	60	GLN
1	D	103	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	146	GLN

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Mol	Chain	Res	Type
1	D	94	GLN
2	I	816	GLN
1	D	44	GLN
1	B	46	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 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	GNP	A	1202	3	28,34,34	2.23	11 (39%)	33,54,54	2.58	8 (24%)
4	GNP	B	2202	3	28,34,34	2.16	11 (39%)	33,54,54	2.43	7 (21%)
4	GNP	C	3202	3	28,34,34	2.27	9 (32%)	33,54,54	2.69	9 (27%)
4	GNP	D	4202	3	28,34,34	2.54	12 (42%)	33,54,54	2.52	8 (24%)
4	GNP	E	5202	3	28,34,34	2.17	10 (35%)	33,54,54	2.46	8 (24%)

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	GNP	A	1202	3	-	0/12/38/38	0/3/3/3
4	GNP	B	2202	3	-	0/12/38/38	0/3/3/3
4	GNP	C	3202	3	-	0/12/38/38	0/3/3/3
4	GNP	D	4202	3	-	0/12/38/38	0/3/3/3
4	GNP	E	5202	3	-	1/12/38/38	0/3/3/3

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	4202	GNP	O6-C6	-3.04	1.17	1.24
4	A	1202	GNP	O6-C6	-3.00	1.17	1.24
4	E	5202	GNP	O6-C6	-2.98	1.17	1.24
4	B	2202	GNP	O6-C6	-2.93	1.17	1.24
4	B	2202	GNP	PG-O3G	-2.92	1.48	1.56

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1202	GNP	C5-C6-N1	-9.26	110.93	123.59
4	E	5202	GNP	C5-C6-N1	-9.12	111.13	123.59
4	C	3202	GNP	C5-C6-N1	-9.11	111.13	123.59
4	D	4202	GNP	C5-C6-N1	-9.03	111.25	123.59
4	B	2202	GNP	C5-C6-N1	-8.94	111.37	123.59

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	5202	GNP	O1B-PB-N3B-PG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	4202	GNP	1	0

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	165/171 (96%)	0.52	15 (9%) 11 17	26, 47, 84, 117	0
1	B	166/171 (97%)	0.61	15 (9%) 12 17	35, 61, 94, 117	0
1	C	166/171 (97%)	0.87	23 (13%) 4 6	40, 70, 107, 121	0
1	D	147/171 (85%)	1.34	37 (25%) 1 1	48, 84, 111, 118	0
1	E	167/171 (97%)	0.47	10 (5%) 25 33	26, 46, 76, 88	0
2	F	46/79 (58%)	0.29	4 (8%) 13 18	27, 55, 99, 101	0
2	G	51/79 (64%)	0.40	4 (7%) 16 22	32, 60, 108, 118	0
2	H	44/79 (55%)	1.13	12 (27%) 1 1	45, 79, 119, 127	0
2	I	45/79 (56%)	1.29	15 (33%) 0 1	55, 92, 115, 123	0
2	J	53/79 (67%)	0.50	8 (15%) 3 5	26, 56, 108, 117	0
All	All	1050/1250 (84%)	0.74	143 (13%) 4 6	26, 62, 111, 127	0

The worst 5 of 143 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	181	LEU	6.3
1	C	183	LYS	5.3
2	G	803	LYS	5.1
1	D	62	VAL	5.0
1	C	182	PRO	4.9

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	MG	B	2201	1/1	0.98	0.13	-0.44	40,40,40,40	0
4	GNP	D	4202	32/32	0.94	0.15	-0.70	42,97,116,120	0
4	GNP	C	3202	32/32	0.96	0.11	-1.00	29,75,81,82	0
4	GNP	A	1202	32/32	0.99	0.12	-1.12	20,46,57,69	0
4	GNP	E	5202	32/32	0.98	0.12	-1.13	26,53,73,77	0
4	GNP	B	2202	32/32	0.97	0.11	-1.18	39,50,64,64	0
3	MG	E	5201	1/1	0.98	0.10	-1.36	39,39,39,39	0
3	MG	D	4201	1/1	0.99	0.07	-1.97	51,51,51,51	0
3	MG	A	1201	1/1	0.98	0.09	-2.11	28,28,28,28	0
3	MG	C	3201	1/1	0.93	0.09	-2.99	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.