



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:43 PM GMT

PDB ID : 4UJ4
Title : Crystal structure of human Rab11-Rabin8-FIP3
Authors : Vetter, M.; Lorentzen, E.
Deposited on : 2015-04-08
Resolution : 4.20 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

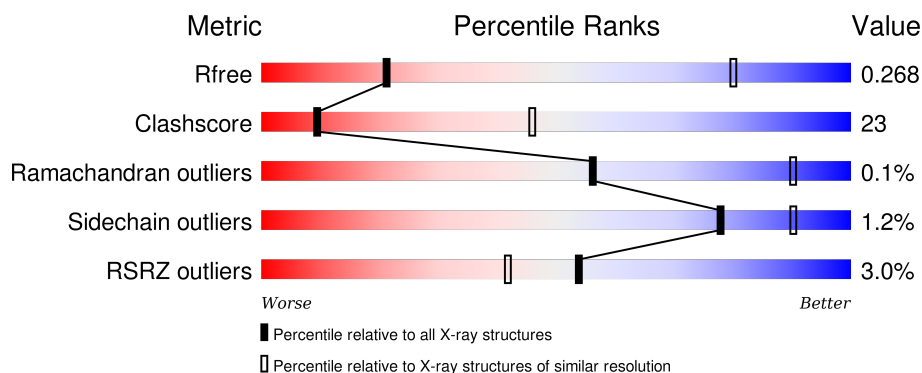
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.20 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	1039 (4.80-3.60)
Clashscore	102246	1140 (4.80-3.60)
Ramachandran outliers	100387	1083 (4.80-3.60)
Sidechain outliers	100360	1067 (4.80-3.60)
RSRZ outliers	91569	1042 (4.80-3.60)

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. 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	185	<div> <div>2%</div> <div>68%</div> <div>26%</div> <div>• 5%</div> </div>
1	D	185	<div> <div>4%</div> <div>68%</div> <div>26%</div> <div>5%</div> </div>
1	G	185	<div> <div>3%</div> <div>64%</div> <div>28%</div> <div>• 5%</div> </div>
1	J	185	<div> <div>%</div> <div>59%</div> <div>34%</div> <div>• 6%</div> </div>
2	B	195	<div> <div>3%</div> <div>52%</div> <div>30%</div> <div>• 17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	195	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>56%</div><div>26%</div><div>17%</div></div></div>
2	H	195	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>46%</div><div>33%</div><div>21%</div></div></div>
2	K	195	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>46%</div><div>35%</div><div>18%</div></div></div>
3	C	66	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>32%</div><div>23%</div><div>45%</div></div></div>
3	F	66	<div><div><div></div><div></div><div></div></div><div><div></div><div>27%</div><div>29%</div><div>44%</div></div></div>
3	I	66	<div><div><div></div><div></div><div></div></div><div><div>6%</div><div>33%</div><div>29%</div><div>38%</div></div></div>
3	L	66	<div><div><div></div><div></div><div></div></div><div><div>3%</div><div>44%</div><div>14%</div><div>42%</div></div></div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11717 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-11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	0	0	0
			1365	862	232	270	1			
1	D	175	Total	C	N	O	S	0	2	0
			1368	864	233	270	1			
1	G	175	Total	C	N	O	S	0	2	0
			1370	865	233	271	1			
1	J	174	Total	C	N	O	S	0	0	0
			1336	847	225	263	1			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	GLY	-	EXPRESSION TAG	UNP P62491
A	3	ALA	-	EXPRESSION TAG	UNP P62491
A	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
D	2	GLY	-	EXPRESSION TAG	UNP P62491
D	3	ALA	-	EXPRESSION TAG	UNP P62491
D	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
G	2	GLY	-	EXPRESSION TAG	UNP P62491
G	3	ALA	-	EXPRESSION TAG	UNP P62491
G	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491
J	2	GLY	-	EXPRESSION TAG	UNP P62491
J	3	ALA	-	EXPRESSION TAG	UNP P62491
J	4	ARG	-	EXPRESSION TAG	UNP P62491
J	5	ASP	-	EXPRESSION TAG	UNP P62491
J	70	LEU	GLN	ENGINEERED MUTATION	UNP P62491

- Molecule 2 is a protein called RAB-3A-INTERACTING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	161	Total	C	N	O	S	0	0	0
			1288	822	211	243	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	162	Total	C	N	O	S	0	0	0
			1268	811	207	238	12			
2	H	155	Total	C	N	O	S	0	2	0
			1263	810	208	233	12			
2	K	159	Total	C	N	O	S	0	1	0
			1259	804	204	239	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	266	GLY	-	EXPRESSION TAG	UNP Q96QF0
B	267	ALA	-	EXPRESSION TAG	UNP Q96QF0
B	268	ALA	-	EXPRESSION TAG	UNP Q96QF0
B	269	SER	-	EXPRESSION TAG	UNP Q96QF0
E	266	GLY	-	EXPRESSION TAG	UNP Q96QF0
E	267	ALA	-	EXPRESSION TAG	UNP Q96QF0
E	268	ALA	-	EXPRESSION TAG	UNP Q96QF0
E	269	SER	-	EXPRESSION TAG	UNP Q96QF0
H	266	GLY	-	EXPRESSION TAG	UNP Q96QF0
H	267	ALA	-	EXPRESSION TAG	UNP Q96QF0
H	268	ALA	-	EXPRESSION TAG	UNP Q96QF0
H	269	SER	-	EXPRESSION TAG	UNP Q96QF0
K	266	GLY	-	EXPRESSION TAG	UNP Q96QF0
K	267	ALA	-	EXPRESSION TAG	UNP Q96QF0
K	268	ALA	-	EXPRESSION TAG	UNP Q96QF0
K	269	SER	-	EXPRESSION TAG	UNP Q96QF0

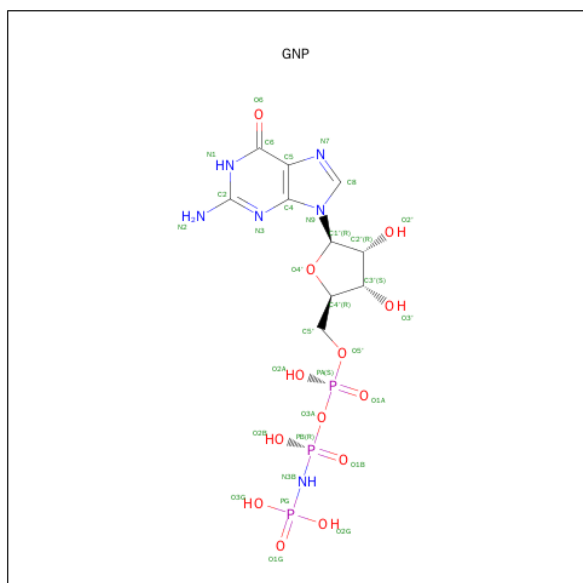
- Molecule 3 is a protein called RAB11 FAMILY-INTERACTING PROTEIN 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	36	Total	C	N	O	S	0	0	0
			265	169	46	48	2			
3	F	37	Total	C	N	O	S	0	0	0
			251	163	40	46	2			
3	I	41	Total	C	N	O	S	0	0	0
			287	184	47	54	2			
3	L	38	Total	C	N	O	S	0	0	0
			265	172	44	47	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	691	GLY	-	EXPRESSION TAG	UNP O75154
C	692	ALA	-	EXPRESSION TAG	UNP O75154
C	693	ALA	-	EXPRESSION TAG	UNP O75154
C	694	SER	-	EXPRESSION TAG	UNP O75154
F	691	GLY	-	EXPRESSION TAG	UNP O75154
F	692	ALA	-	EXPRESSION TAG	UNP O75154
F	693	ALA	-	EXPRESSION TAG	UNP O75154
F	694	SER	-	EXPRESSION TAG	UNP O75154
I	691	GLY	-	EXPRESSION TAG	UNP O75154
I	692	ALA	-	EXPRESSION TAG	UNP O75154
I	693	ALA	-	EXPRESSION TAG	UNP O75154
I	694	SER	-	EXPRESSION TAG	UNP O75154
L	691	GLY	-	EXPRESSION TAG	UNP O75154
L	692	ALA	-	EXPRESSION TAG	UNP O75154
L	693	ALA	-	EXPRESSION TAG	UNP O75154
L	694	SER	-	EXPRESSION TAG	UNP O75154

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	J	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

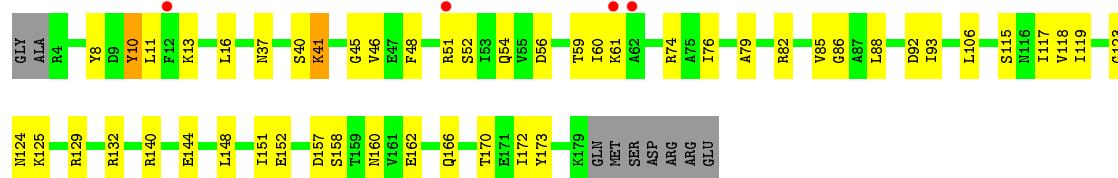
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Mg	0	0
			1	1		
5	J	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

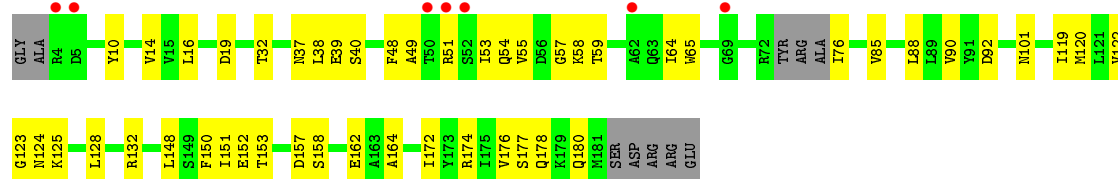
3 Residue-property plots

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.

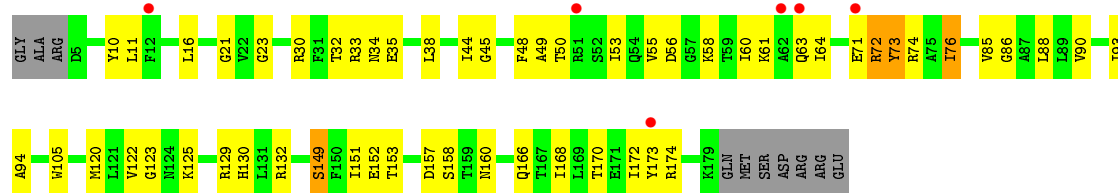
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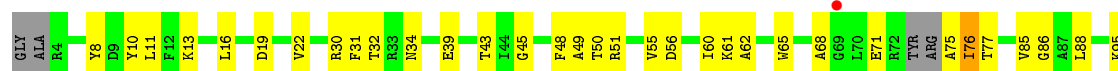
• Molecule 1: RAS-RELATED PROTEIN RAB-11A



• Molecule 1: RAS-RELATED PROTEIN RAB-11A

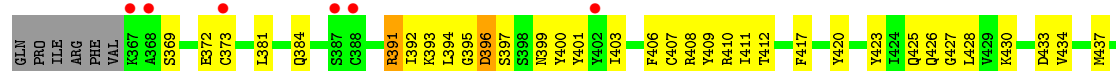


• Molecule 1: RAS-RELATED PROTEIN RAB-11A

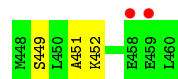
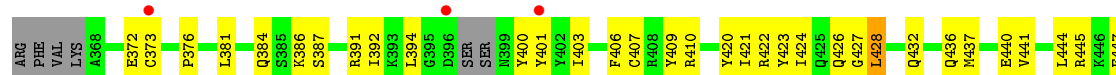




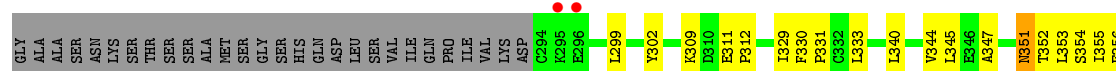
• Molecule 2: RAB-3A-INTERACTING PROTEIN



• Molecule 2: RAB-3A-INTERACTING PROTEIN

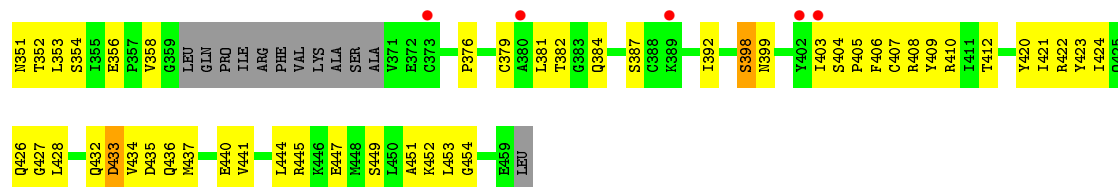


• Molecule 2: RAB-3A-INTERACTING PROTEIN

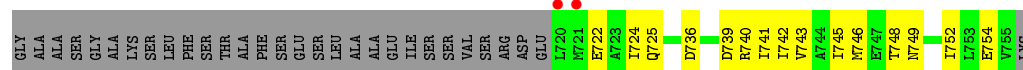
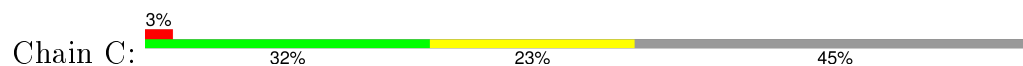


• Molecule 2: RAB-3A-INTERACTING PROTEIN

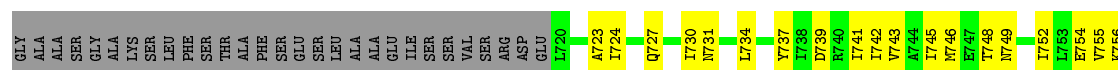
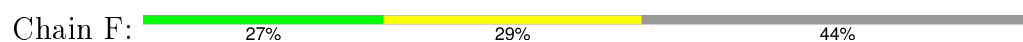




• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



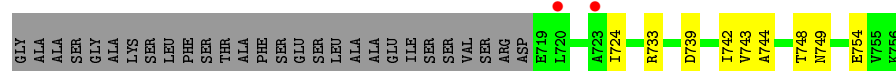
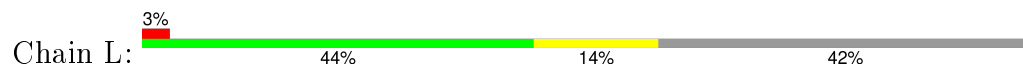
• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



• Molecule 3: RAB11 FAMILY-INTERACTING PROTEIN 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	66.12Å 161.70Å 192.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 4.20 49.47 – 4.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.47-4.20) 87.6 (49.47-4.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 4.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.252 , 0.266 0.243 , 0.268	Depositor DCC
R_{free} test set	751 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	127.6	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 121.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	1 of 18023 reflections (0.006%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11717	wwPDB-VP
Average B, all atoms (Å ²)	161.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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	0.37	0/1386	0.56	0/1878
1	D	0.37	0/1394	0.58	0/1889
1	G	0.41	0/1397	0.63	0/1893
1	J	0.36	0/1356	0.56	0/1839
2	B	0.37	0/1315	0.57	0/1772
2	E	0.32	0/1294	0.53	0/1748
2	H	0.40	0/1296	0.63	0/1746
2	K	0.32	0/1289	0.57	0/1742
3	C	0.33	0/266	0.52	0/362
3	F	0.33	0/252	0.53	0/346
3	I	0.31	0/288	0.53	0/394
3	L	0.33	0/266	0.56	0/364
All	All	0.36	0/11799	0.58	0/15973

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	G	0	3
2	B	0	1
2	K	0	1
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	396	ASP	Peptide
1	G	72	ARG	Peptide
1	G	73	TYR	Peptide
1	G	74	ARG	Peptide
2	K	398	SER	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	1365	0	1322	62	1
1	D	1368	0	1322	51	2
1	G	1370	0	1328	54	0
1	J	1336	0	1290	77	3
2	B	1288	0	1249	69	0
2	E	1268	0	1197	57	1
2	H	1263	0	1244	68	3
2	K	1259	0	1185	68	1
3	C	265	0	255	31	0
3	F	251	0	227	46	0
3	I	287	0	261	35	0
3	L	265	0	249	21	1
4	A	32	0	13	1	0
4	D	32	0	13	1	0
4	G	32	0	13	6	0
4	J	32	0	13	2	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
5	J	1	0	0	0	0
All	All	11717	0	11181	518	6

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 23.

The worst 5 of 518 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:J:76:ILE:CG2	3:L:743:VAL:HG22	1.60	1.29
1:J:76:ILE:CG2	3:L:743:VAL:CG2	2.25	1.15
1:J:76:ILE:HG21	3:L:743:VAL:CG2	1.78	1.12
1:A:76:ILE:HD11	3:C:742:ILE:HG22	1.31	1.12
1:J:48:PHE:CZ	3:L:754:GLU:HB2	1.87	1.10

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:371:VAL:CG1	1:J:160:ASN:OD1[3_554]	1.06	1.14
1:D:150:PHE:O	2:E:311:GLU:OE2[4_545]	1.66	0.54
1:D:57:GLY:CA	2:K:336:SER:O[4_545]	1.81	0.39
2:H:371:VAL:CG1	1:J:160:ASN:CG[3_554]	2.07	0.13
2:H:371:VAL:CB	1:J:160:ASN:OD1[3_554]	2.15	0.05

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	174/185 (94%)	169 (97%)	5 (3%)	0	100	100
1	D	173/185 (94%)	169 (98%)	4 (2%)	0	100	100
1	G	175/185 (95%)	168 (96%)	5 (3%)	2 (1%)	17	64
1	J	170/185 (92%)	165 (97%)	5 (3%)	0	100	100
2	B	157/195 (80%)	152 (97%)	5 (3%)	0	100	100
2	E	156/195 (80%)	152 (97%)	4 (3%)	0	100	100
2	H	153/195 (78%)	150 (98%)	3 (2%)	0	100	100
2	K	156/195 (80%)	149 (96%)	7 (4%)	0	100	100
3	C	34/66 (52%)	33 (97%)	1 (3%)	0	100	100
3	F	35/66 (53%)	33 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	I	39/66 (59%)	36 (92%)	3 (8%)	0	100	100
3	L	36/66 (54%)	35 (97%)	1 (3%)	0	100	100
All	All	1458/1784 (82%)	1411 (97%)	45 (3%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	76	ILE
1	G	73	TYR

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	142/157 (90%)	140 (99%)	2 (1%)	74	89
1	D	143/157 (91%)	143 (100%)	0	100	100
1	G	143/157 (91%)	142 (99%)	1 (1%)	88	94
1	J	138/157 (88%)	136 (99%)	2 (1%)	74	89
2	B	141/175 (81%)	138 (98%)	3 (2%)	61	85
2	E	133/175 (76%)	131 (98%)	2 (2%)	72	89
2	H	140/175 (80%)	139 (99%)	1 (1%)	88	94
2	K	134/175 (77%)	131 (98%)	3 (2%)	60	84
3	C	25/56 (45%)	25 (100%)	0	100	100
3	F	21/56 (38%)	21 (100%)	0	100	100
3	I	25/56 (45%)	24 (96%)	1 (4%)	38	73
3	L	23/56 (41%)	22 (96%)	1 (4%)	35	72
All	All	1208/1552 (78%)	1192 (99%)	16 (1%)	78	90

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	149	SER
2	H	351	ASN
2	K	332	CYS
2	E	428	LEU
2	K	433[A]	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	54	GLN
2	E	384	GLN
3	F	727	GLN
2	H	351	ASN
3	I	727	GLN

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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	200	5	29,34,34	1.82	7 (24%)	29,54,54	2.68	6 (20%)
4	GNP	D	200	5	29,34,34	1.91	7 (24%)	29,54,54	2.62	7 (24%)
4	GNP	G	200	5	29,34,34	1.84	6 (20%)	29,54,54	2.74	7 (24%)
4	GNP	J	200	5	29,34,34	1.80	5 (17%)	29,54,54	2.77	8 (27%)

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	200	5	-	0/13/38/38	0/3/3/3
4	GNP	D	200	5	-	0/13/38/38	0/3/3/3
4	GNP	G	200	5	-	1/13/38/38	0/3/3/3
4	GNP	J	200	5	-	0/13/38/38	0/3/3/3

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	200	GNP	PB-O3A	-4.81	1.53	1.59
4	G	200	GNP	PB-O3A	-4.54	1.53	1.59
4	J	200	GNP	PB-O3A	-4.28	1.53	1.59
4	A	200	GNP	PB-O3A	-3.83	1.54	1.59
4	A	200	GNP	PB-O2B	-3.03	1.48	1.56

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	200	GNP	C5-C6-N1	-9.37	111.27	123.52
4	A	200	GNP	C5-C6-N1	-9.37	111.27	123.52
4	J	200	GNP	C5-C6-N1	-8.88	111.91	123.52
4	D	200	GNP	C5-C6-N1	-8.74	112.10	123.52
4	G	200	GNP	O2G-PG-O1G	-4.27	102.34	113.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	200	GNP	O1B-PB-N3B-PG

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	GNP	1	0
4	D	200	GNP	1	0
4	G	200	GNP	6	0
4	J	200	GNP	2	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	176/185 (95%)	-0.06	4 (2%) 64 53	144, 166, 205, 258	0
1	D	175/185 (94%)	0.23	7 (4%) 42 32	129, 159, 214, 253	0
1	G	175/185 (94%)	0.22	6 (3%) 49 38	114, 141, 188, 226	0
1	J	174/185 (94%)	0.01	1 (0%) 90 86	121, 149, 200, 235	0
2	B	161/195 (82%)	0.36	6 (3%) 45 35	131, 166, 225, 273	0
2	E	162/195 (83%)	0.18	6 (3%) 45 35	120, 169, 205, 238	0
2	H	155/195 (79%)	0.01	2 (1%) 79 71	129, 149, 174, 201	0
2	K	159/195 (81%)	0.09	5 (3%) 52 41	124, 162, 208, 218	0
3	C	36/66 (54%)	0.14	2 (5%) 28 21	139, 164, 221, 224	0
3	F	37/66 (56%)	-0.00	0 100 100	122, 143, 197, 209	0
3	I	41/66 (62%)	0.24	4 (9%) 10 8	133, 153, 227, 236	0
3	L	38/66 (57%)	0.20	2 (5%) 30 23	141, 168, 219, 231	0
All	All	1489/1784 (83%)	0.13	45 (3%) 54 42	114, 159, 210, 273	0

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	720	LEU	4.7
2	B	368	ALA	4.6
1	D	51	ARG	4.5
1	D	5	ASP	4.4
2	E	360	LEU	4.3

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

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(Å ²)	Q<0.9
4	GNP	D	200	32/32	0.91	0.22	-0.63	130,143,153,161	0
4	GNP	A	200	32/32	0.93	0.19	-0.69	140,150,162,164	0
4	GNP	J	200	32/32	0.93	0.20	-0.72	117,129,146,148	0
5	MG	J	201	1/1	0.90	0.13	-0.88	131,131,131,131	0
4	GNP	G	200	32/32	0.95	0.18	-1.02	113,129,142,149	0
5	MG	A	201	1/1	0.93	0.17	-1.64	145,145,145,145	0
5	MG	G	201	1/1	0.96	0.11	-1.87	111,111,111,111	0
5	MG	D	201	1/1	0.89	0.12	-	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.