



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 29, 2017 – 12:47 PM EST

PDB ID : 5O74
Title : Crystal structure of human Rab1b covalently bound to the GEF domain of DrrA/SidM from *Legionella pneumophila* in the presence of GDP
Authors : Cigler, M.; Mueller, T.; Horn-Ghetko, D.; von Wisberg, M.K.; Fottner, M.; Goody, R.S.; Itzen, A.; Mueller, M.P.; Lang, K.
Deposited on : unknown
Resolution : 2.50 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

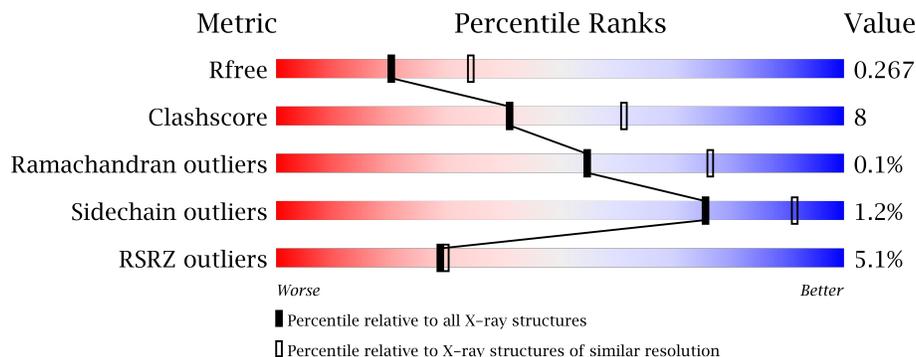
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	197	
1	C	197	
1	E	197	
1	G	197	
1	I	197	

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Mol	Chain	Length	Quality of chain
1	K	197	
2	B	180	
2	D	180	
2	F	180	
2	H	180	
2	J	180	
2	L	180	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 33987 atoms, of which 16983 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 Multifunctional virulence effector protein DrrA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	191	2998	939	1505	254	291	9	0	0	0
1	C	192	3012	943	1512	255	293	9	0	0	0
1	E	191	2998	939	1505	254	291	9	0	0	0
1	G	192	3012	943	1512	255	293	9	0	0	0
1	I	193	3024	944	1521	256	293	10	0	0	0
1	K	191	2987	934	1499	254	291	9	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	GLY	-	expression tag	UNP Q29ST3
A	338	HIS	-	expression tag	UNP Q29ST3
A	339	MET	-	expression tag	UNP Q29ST3
A	512	CYS	ASP	engineered mutation	UNP Q29ST3
C	337	GLY	-	expression tag	UNP Q29ST3
C	338	HIS	-	expression tag	UNP Q29ST3
C	339	MET	-	expression tag	UNP Q29ST3
C	512	CYS	ASP	engineered mutation	UNP Q29ST3
E	337	GLY	-	expression tag	UNP Q29ST3
E	338	HIS	-	expression tag	UNP Q29ST3
E	339	MET	-	expression tag	UNP Q29ST3
E	512	CYS	ASP	engineered mutation	UNP Q29ST3
G	337	GLY	-	expression tag	UNP Q29ST3
G	338	HIS	-	expression tag	UNP Q29ST3
G	339	MET	-	expression tag	UNP Q29ST3
G	512	CYS	ASP	engineered mutation	UNP Q29ST3
I	337	GLY	-	expression tag	UNP Q29ST3

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Chain	Residue	Modelled	Actual	Comment	Reference
I	338	HIS	-	expression tag	UNP Q29ST3
I	339	MET	-	expression tag	UNP Q29ST3
I	512	CYS	ASP	engineered mutation	UNP Q29ST3
K	337	GLY	-	expression tag	UNP Q29ST3
K	338	HIS	-	expression tag	UNP Q29ST3
K	339	MET	-	expression tag	UNP Q29ST3
K	512	CYS	ASP	engineered mutation	UNP Q29ST3

- Molecule 2 is a protein called Ras-related protein Rab-1B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	B	170	2716	868	1356	220	268	4	0	0	0
2	D	161	2593	828	1300	210	251	4	0	0	0
2	F	165	2641	843	1323	215	256	4	0	0	0
2	H	170	2721	868	1361	220	268	4	0	0	0
2	J	164	2628	841	1313	213	257	4	0	0	0
2	L	152	2429	775	1216	201	233	4	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q9H0U4
B	2	ALA	-	expression tag	UNP Q9H0U4
B	79	9MN	ARG	engineered mutation	UNP Q9H0U4
B	175	HIS	-	expression tag	UNP Q9H0U4
B	176	HIS	-	expression tag	UNP Q9H0U4
B	177	HIS	-	expression tag	UNP Q9H0U4
B	178	HIS	-	expression tag	UNP Q9H0U4
B	179	HIS	-	expression tag	UNP Q9H0U4
B	180	HIS	-	expression tag	UNP Q9H0U4
D	1	MET	-	initiating methionine	UNP Q9H0U4
D	2	ALA	-	expression tag	UNP Q9H0U4
D	79	9MN	ARG	engineered mutation	UNP Q9H0U4
D	175	HIS	-	expression tag	UNP Q9H0U4
D	176	HIS	-	expression tag	UNP Q9H0U4
D	177	HIS	-	expression tag	UNP Q9H0U4

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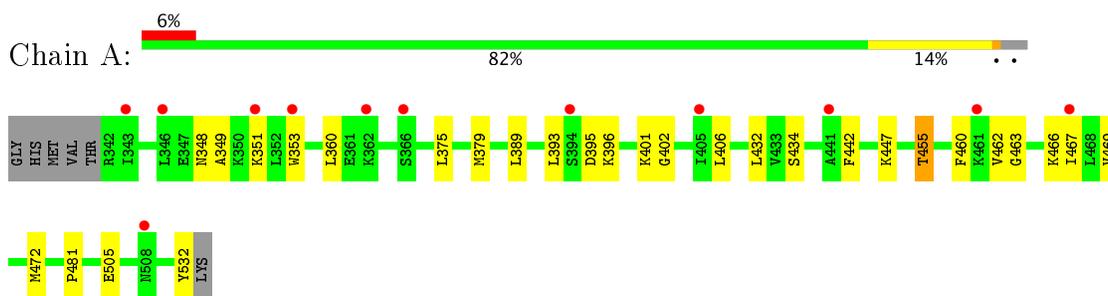
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D	178	HIS	-	expression tag	UNP Q9H0U4
D	179	HIS	-	expression tag	UNP Q9H0U4
D	180	HIS	-	expression tag	UNP Q9H0U4
F	1	MET	-	initiating methionine	UNP Q9H0U4
F	2	ALA	-	expression tag	UNP Q9H0U4
F	79	9MN	ARG	engineered mutation	UNP Q9H0U4
F	175	HIS	-	expression tag	UNP Q9H0U4
F	176	HIS	-	expression tag	UNP Q9H0U4
F	177	HIS	-	expression tag	UNP Q9H0U4
F	178	HIS	-	expression tag	UNP Q9H0U4
F	179	HIS	-	expression tag	UNP Q9H0U4
F	180	HIS	-	expression tag	UNP Q9H0U4
H	1	MET	-	initiating methionine	UNP Q9H0U4
H	2	ALA	-	expression tag	UNP Q9H0U4
H	79	9MN	ARG	engineered mutation	UNP Q9H0U4
H	175	HIS	-	expression tag	UNP Q9H0U4
H	176	HIS	-	expression tag	UNP Q9H0U4
H	177	HIS	-	expression tag	UNP Q9H0U4
H	178	HIS	-	expression tag	UNP Q9H0U4
H	179	HIS	-	expression tag	UNP Q9H0U4
H	180	HIS	-	expression tag	UNP Q9H0U4
J	1	MET	-	initiating methionine	UNP Q9H0U4
J	2	ALA	-	expression tag	UNP Q9H0U4
J	79	9MN	ARG	engineered mutation	UNP Q9H0U4
J	175	HIS	-	expression tag	UNP Q9H0U4
J	176	HIS	-	expression tag	UNP Q9H0U4
J	177	HIS	-	expression tag	UNP Q9H0U4
J	178	HIS	-	expression tag	UNP Q9H0U4
J	179	HIS	-	expression tag	UNP Q9H0U4
J	180	HIS	-	expression tag	UNP Q9H0U4
L	1	MET	-	initiating methionine	UNP Q9H0U4
L	2	ALA	-	expression tag	UNP Q9H0U4
L	79	9MN	ARG	engineered mutation	UNP Q9H0U4
L	175	HIS	-	expression tag	UNP Q9H0U4
L	176	HIS	-	expression tag	UNP Q9H0U4
L	177	HIS	-	expression tag	UNP Q9H0U4
L	178	HIS	-	expression tag	UNP Q9H0U4
L	179	HIS	-	expression tag	UNP Q9H0U4
L	180	HIS	-	expression tag	UNP Q9H0U4

- Molecule 3 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).

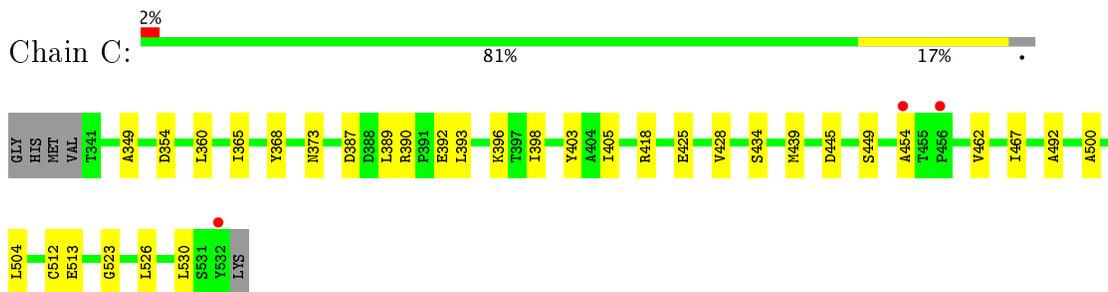
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

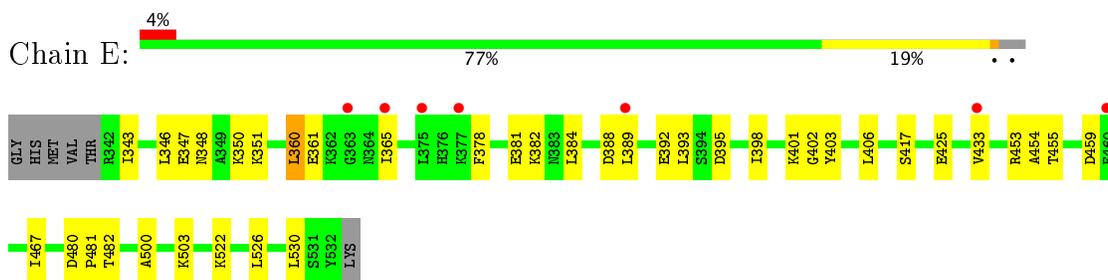
- Molecule 1: Multifunctional virulence effector protein DrrA



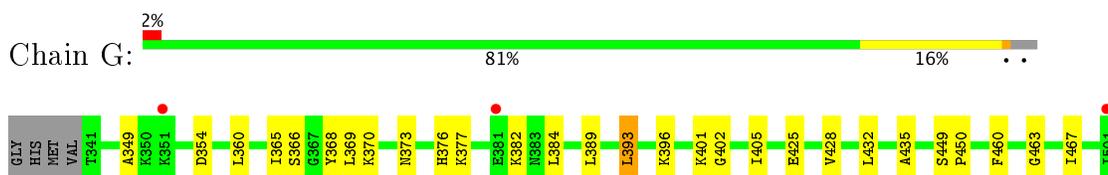
- Molecule 1: Multifunctional virulence effector protein DrrA

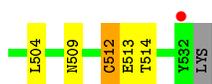


- Molecule 1: Multifunctional virulence effector protein DrrA

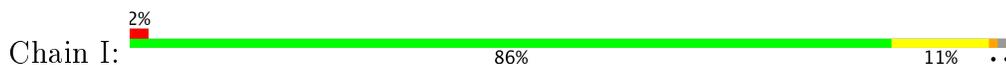


- Molecule 1: Multifunctional virulence effector protein DrrA

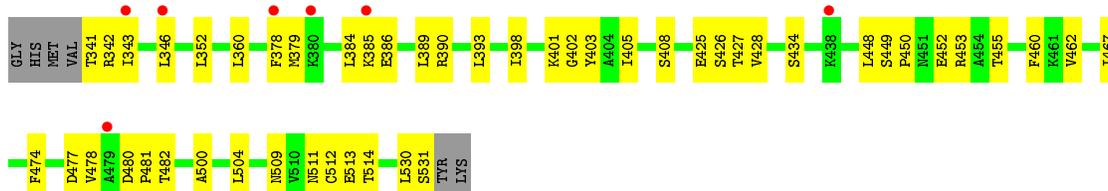




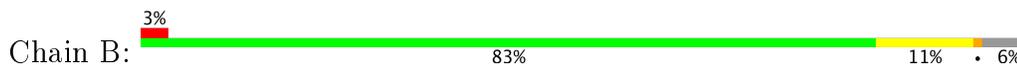
- Molecule 1: Multifunctional virulence effector protein DrrA



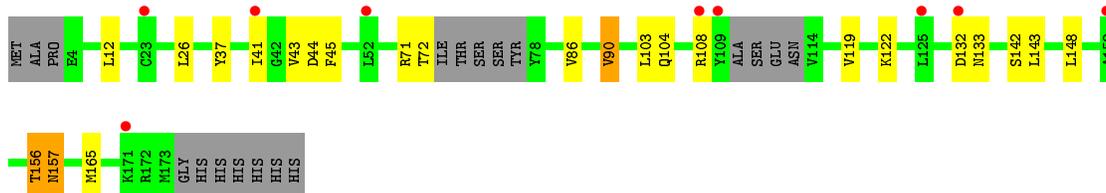
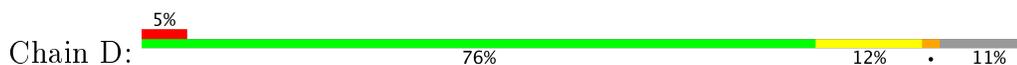
- Molecule 1: Multifunctional virulence effector protein DrrA



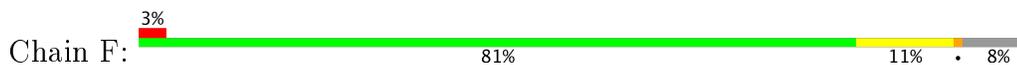
- Molecule 2: Ras-related protein Rab-1B



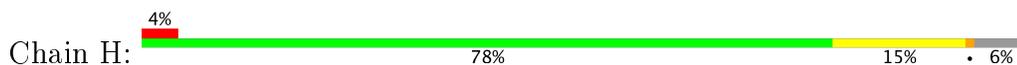
- Molecule 2: Ras-related protein Rab-1B

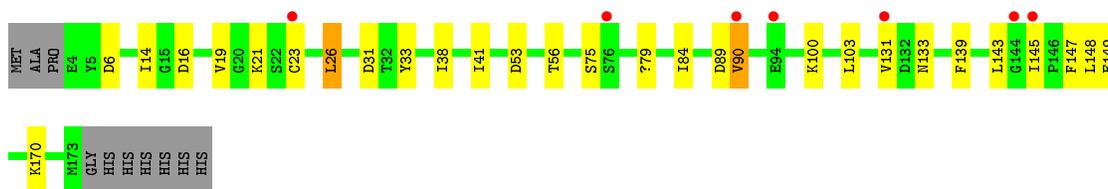


- Molecule 2: Ras-related protein Rab-1B

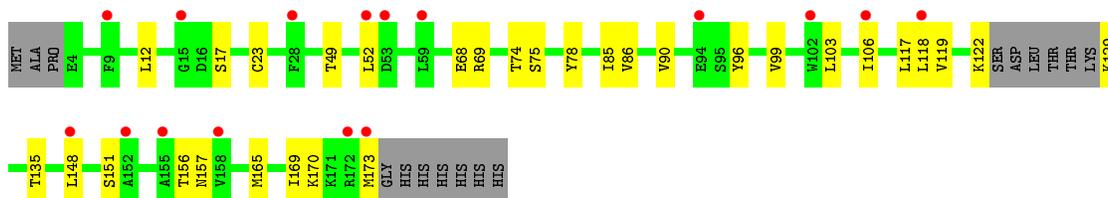


- Molecule 2: Ras-related protein Rab-1B

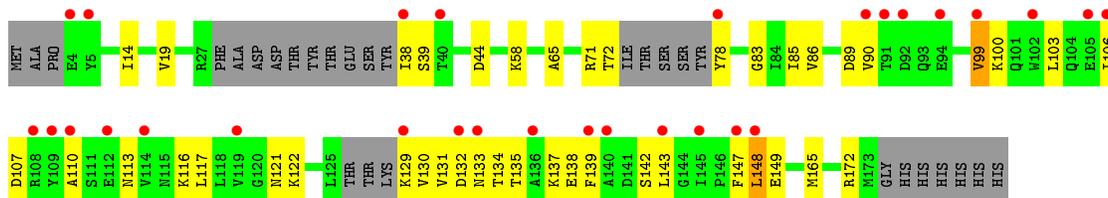




- Molecule 2: Ras-related protein Rab-1B



- Molecule 2: Ras-related protein Rab-1B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	77.91Å 87.45Å 93.17Å 114.61° 97.69° 100.74°	Depositor
Resolution (Å)	46.52 – 2.50 46.52 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.0 (46.52-2.50) 81.9 (46.52-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 2.51Å)	Xtrriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.229 , 0.266 0.230 , 0.267	Depositor DCC
R_{free} test set	3617 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	49.8	Xtrriage
Anisotropy	0.333	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	33987	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: GDP, 9MN

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	0.30	0/1518	0.54	0/2044
1	C	0.30	0/1525	0.51	0/2054
1	E	0.35	0/1518	0.57	1/2044 (0.0%)
1	G	0.31	0/1525	0.53	1/2054 (0.0%)
1	I	0.29	0/1527	0.51	0/2056
1	K	0.31	0/1512	0.55	0/2036
2	B	0.31	0/1364	0.58	1/1841 (0.1%)
2	D	0.31	0/1294	0.53	1/1742 (0.1%)
2	F	0.29	0/1320	0.57	1/1778 (0.1%)
2	H	0.32	0/1364	0.59	1/1841 (0.1%)
2	J	0.32	0/1318	0.54	0/1777
2	L	0.34	0/1210	0.62	1/1625 (0.1%)
All	All	0.31	0/16995	0.55	7/22892 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	99	VAL	CG1-CB-CG2	8.36	124.28	110.90
2	F	90	VAL	CG1-CB-CG2	8.06	123.79	110.90
2	B	90	VAL	CG1-CB-CG2	8.05	123.78	110.90
2	H	90	VAL	CG1-CB-CG2	7.81	123.40	110.90
2	D	90	VAL	CA-CB-CG1	7.55	122.22	110.90

There are no chirality outliers.

There are no planarity outliers.

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	1493	1505	1505	21	0
1	C	1500	1512	1512	32	0
1	E	1493	1505	1505	36	2
1	G	1500	1512	1512	23	0
1	I	1503	1521	1521	17	2
1	K	1488	1499	1503	39	0
2	B	1360	1356	1341	15	1
2	D	1293	1300	1280	20	0
2	F	1318	1323	1309	10	1
2	H	1360	1361	1341	22	0
2	J	1315	1313	1293	18	0
2	L	1213	1216	1209	42	0
3	B	28	10	12	0	0
3	D	28	10	12	0	0
3	F	28	10	12	0	0
3	H	28	10	12	1	0
3	J	28	10	12	1	0
3	L	28	10	12	0	0
All	All	17004	16983	16903	275	3

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 8.

The worst 5 of 275 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:I:425:GLU:OE2	1:I:428:VAL:N	2.13	0.81
2:L:129:LYS:NZ	2:L:149:GLU:OE2	2.13	0.80
1:G:512:CYS:SG	1:G:513:GLU:N	2.54	0.80
1:C:390:ARG:NH1	1:C:445:ASP:O	2.16	0.77
2:B:132:ASP:OD2	2:B:134:THR:OG1	2.02	0.77

All (3) 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:B:157:ASN:H	2:F:159:GLU:OE2[1_455]	1.53	0.07
1:E:459:ASP:OD2	1:I:464:LYS:H[1_565]	1.56	0.04
1:E:459:ASP:OD2	1:I:464:LYS:N[1_565]	2.17	0.03

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	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
1	C	190/197 (96%)	188 (99%)	2 (1%)	0	100	100
1	E	189/197 (96%)	188 (100%)	1 (0%)	0	100	100
1	G	190/197 (96%)	188 (99%)	2 (1%)	0	100	100
1	I	191/197 (97%)	189 (99%)	2 (1%)	0	100	100
1	K	189/197 (96%)	187 (99%)	2 (1%)	0	100	100
2	B	167/180 (93%)	164 (98%)	3 (2%)	0	100	100
2	D	154/180 (86%)	150 (97%)	2 (1%)	2 (1%)	14	25
2	F	160/180 (89%)	154 (96%)	6 (4%)	0	100	100
2	H	167/180 (93%)	163 (98%)	4 (2%)	0	100	100
2	J	159/180 (88%)	156 (98%)	3 (2%)	0	100	100
2	L	143/180 (79%)	139 (97%)	3 (2%)	1 (1%)	25	43
All	All	2088/2262 (92%)	2053 (98%)	32 (2%)	3 (0%)	55	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	157	ASN
2	D	122	LYS
2	L	122	LYS

5.3.2 Protein sidechains [i](#)

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	166/171 (97%)	164 (99%)	2 (1%)	75	91
1	C	167/171 (98%)	166 (99%)	1 (1%)	89	97
1	E	166/171 (97%)	165 (99%)	1 (1%)	89	97
1	G	167/171 (98%)	166 (99%)	1 (1%)	89	97
1	I	168/171 (98%)	167 (99%)	1 (1%)	89	97
1	K	166/171 (97%)	165 (99%)	1 (1%)	89	97
2	B	147/155 (95%)	144 (98%)	3 (2%)	60	84
2	D	139/155 (90%)	136 (98%)	3 (2%)	57	82
2	F	142/155 (92%)	139 (98%)	3 (2%)	59	83
2	H	147/155 (95%)	145 (99%)	2 (1%)	71	90
2	J	141/155 (91%)	139 (99%)	2 (1%)	71	90
2	L	130/155 (84%)	128 (98%)	2 (2%)	70	89
All	All	1846/1956 (94%)	1824 (99%)	22 (1%)	75	91

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	455	THR
2	F	125	LEU
2	L	99	VAL
2	F	28	PHE
2	F	90	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	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](#)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	9MN	B	79	1,2	15,15,17	1.56	2 (13%)	13,16,19	1.39	2 (15%)
2	9MN	D	79	1,2	15,15,17	1.75	3 (20%)	13,16,19	3.13	5 (38%)
2	9MN	F	79	1,2	15,15,17	1.63	3 (20%)	13,16,19	1.37	2 (15%)
2	9MN	H	79	1,2	15,15,17	1.53	2 (13%)	13,16,19	2.18	3 (23%)
2	9MN	J	79	1,2	15,15,17	1.66	2 (13%)	13,16,19	2.72	5 (38%)
2	9MN	L	79	1,2	15,15,17	1.56	2 (13%)	13,16,19	1.19	1 (7%)

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
2	9MN	B	79	1,2	-	0/13/15/18	0/0/0/0
2	9MN	D	79	1,2	-	0/13/15/18	0/0/0/0
2	9MN	F	79	1,2	-	0/13/15/18	0/0/0/0
2	9MN	H	79	1,2	-	0/13/15/18	0/0/0/0
2	9MN	J	79	1,2	-	0/13/15/18	0/0/0/0
2	9MN	L	79	1,2	-	0/13/15/18	0/0/0/0

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	79	9MN	O11-C10	-2.30	1.18	1.23
2	F	79	9MN	O11-C10	-2.15	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	79	9MN	O11-C10	-2.08	1.18	1.23
2	H	79	9MN	O11-C10	-2.08	1.18	1.23
2	J	79	9MN	O11-C10	-2.05	1.19	1.23

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	79	9MN	CB-CA-C	-6.45	101.02	111.65
2	D	79	9MN	O11-C10-NZ	-4.63	114.13	122.97
2	J	79	9MN	O11-C10-C12	-3.67	115.11	122.01
2	D	79	9MN	O11-C10-C12	-3.55	115.34	122.01
2	J	79	9MN	O11-C10-NZ	-3.27	116.74	122.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	79	9MN	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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
3	GDP	B	500	-	25,30,30	1.33	3 (12%)	23,47,47	1.75	6 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GDP	D	500	-	25,30,30	1.36	3 (12%)	23,47,47	1.35	2 (8%)
3	GDP	F	500	-	25,30,30	1.39	4 (16%)	23,47,47	1.53	4 (17%)
3	GDP	H	500	-	25,30,30	1.31	2 (8%)	23,47,47	1.69	5 (21%)
3	GDP	J	500	-	25,30,30	1.41	5 (20%)	23,47,47	1.42	3 (13%)
3	GDP	L	500	-	25,30,30	1.40	4 (16%)	23,47,47	1.53	3 (13%)

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
3	GDP	B	500	-	-	0/12/32/32	0/3/3/3
3	GDP	D	500	-	-	0/12/32/32	0/3/3/3
3	GDP	F	500	-	-	0/12/32/32	0/3/3/3
3	GDP	H	500	-	-	0/12/32/32	0/3/3/3
3	GDP	J	500	-	-	0/12/32/32	0/3/3/3
3	GDP	L	500	-	-	0/12/32/32	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	500	GDP	C6-N1	-2.20	1.33	1.36
3	J	500	GDP	C6-N1	-2.08	1.33	1.36
3	J	500	GDP	C2-N2	2.05	1.35	1.32
3	L	500	GDP	C2-N3	2.23	1.36	1.33
3	B	500	GDP	C2-N2	2.33	1.35	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	500	GDP	C1'-N9-C4	-3.61	120.40	126.64
3	H	500	GDP	C4-C5-N7	-3.41	106.11	109.41
3	H	500	GDP	C1'-N9-C4	-3.41	120.75	126.64
3	B	500	GDP	C4-C5-N7	-3.21	106.31	109.41
3	H	500	GDP	N2-C2-N3	-3.03	116.54	120.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	500	GDP	1	0
3	J	500	GDP	1	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 [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	191/197 (96%)	0.53	12 (6%) 21 21	38, 64, 102, 131	0
1	C	192/197 (97%)	0.46	3 (1%) 72 73	39, 61, 96, 113	0
1	E	191/197 (96%)	0.48	7 (3%) 42 44	37, 67, 113, 138	0
1	G	192/197 (97%)	0.43	4 (2%) 64 66	36, 63, 103, 138	0
1	I	193/197 (97%)	0.52	4 (2%) 64 66	45, 61, 87, 101	0
1	K	191/197 (96%)	0.51	7 (3%) 42 44	43, 68, 106, 151	0
2	B	169/180 (93%)	0.51	5 (2%) 51 53	44, 65, 96, 135	0
2	D	160/180 (88%)	0.45	9 (5%) 25 26	45, 71, 107, 144	0
2	F	164/180 (91%)	0.47	5 (3%) 51 53	37, 60, 89, 106	0
2	H	169/180 (93%)	0.49	7 (4%) 38 40	35, 63, 106, 132	0
2	J	163/180 (90%)	0.79	16 (9%) 8 7	52, 79, 114, 134	0
2	L	151/180 (83%)	1.15	29 (19%) 1 1	46, 82, 125, 158	0
All	All	2126/2262 (93%)	0.56	108 (5%) 29 30	35, 67, 108, 158	0

The worst 5 of 108 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	52	LEU	6.6
2	L	129	LYS	5.6
2	J	158	VAL	5.0
2	L	94	GLU	4.5
2	L	143	LEU	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	9MN	B	79	16/18	0.80	0.44	-	82,146,181,186	0
2	9MN	D	79	16/18	0.73	0.41	-	93,140,168,169	0
2	9MN	F	79	16/18	0.80	0.30	-	73,133,159,160	0
2	9MN	H	79	16/18	0.81	0.38	-	68,157,192,195	0
2	9MN	J	79	16/18	0.76	0.31	-	76,137,185,188	0
2	9MN	L	79	16/18	0.83	0.51	-	95,182,236,241	0

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
3	GDP	F	500	28/28	0.82	0.23	0.61	44,82,117,131	0
3	GDP	J	500	28/28	0.80	0.23	0.39	82,124,178,189	0
3	GDP	B	500	28/28	0.93	0.19	0.31	54,80,124,148	0
3	GDP	H	500	28/28	0.93	0.19	0.06	40,84,127,131	0
3	GDP	L	500	28/28	0.89	0.18	-0.25	67,91,140,141	0
3	GDP	D	500	28/28	0.79	0.18	-0.38	79,97,153,176	0

6.5 Other polymers [i](#)

There are no such residues in this entry.