wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:54 AM GMT

PDB ID	:	2J59
Title	:	CRYSTAL STRUCTURE OF THE ARF1:ARHGAP21-ARFBD COMPLEX
Authors	:	Menetrey, J.; Perderiset, M.; Cicolari, J.; Dubois, T.; El Khatib, N.; El Khadali, F.; Franco, M.; Chavrier, P.; Houdusse, A.
Deposited on	:	2006-09-13
Resolution	:	2.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

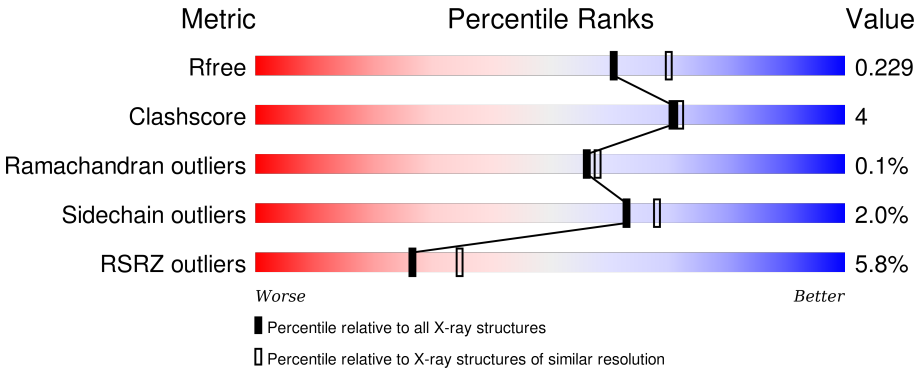
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 <=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	166	3% 87% 11%
1	B	166	2% 91% 8%
1	C	166	% 90% 9%
1	D	166	% 91% 8%
1	E	166	% 89% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	166	2% 89% 10%
2	M	168	5% 65% 33%
2	N	168	5% 63% 32%
2	O	168	11% 54% 11% 34%
2	P	168	8% 55% 10% 32%
2	Q	168	8% 61% 7% 32%
2	R	168	9% 55% 12% 33%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	DIO	F	1183	-	-	-	X
6	EDO	O	2063	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15535 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 ADP-RIBOSYLATION FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	165	Total	C	N	O	S	0	2	0
			1328	840	233	249	6			
1	B	165	Total	C	N	O	S	0	1	0
			1323	836	232	249	6			
1	C	165	Total	C	N	O	S	0	2	0
			1328	838	233	251	6			
1	D	165	Total	C	N	O	S	0	5	0
			1334	840	234	254	6			
1	E	165	Total	C	N	O	S	5	4	0
			1330	838	233	253	6			
1	F	165	Total	C	N	O	S	0	0	0
			1322	836	232	248	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078
B	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078
C	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078
D	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078
E	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078
F	71	LEU	GLN	ENGINEERED MUTATION	UNP P84078

- Molecule 2 is a protein called RHO-GTPASE ACTIVATING PROTEIN 10.

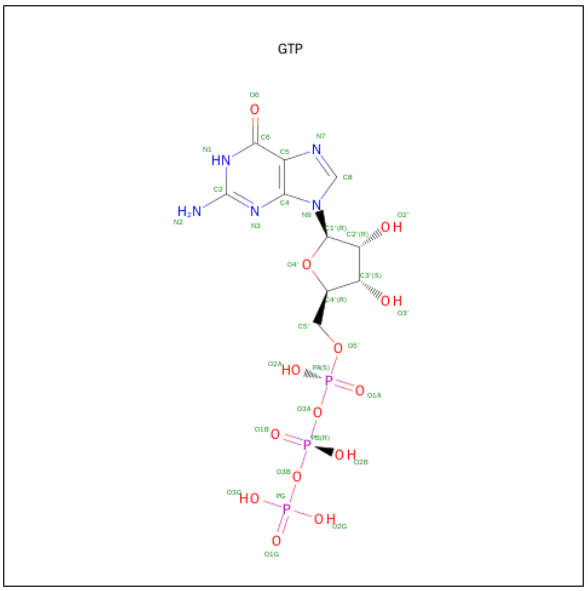
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	113	Total	C	N	O	S	0	1	0
			943	594	167	177	5			
2	N	114	Total	C	N	O	S	4	0	0
			948	596	168	179	5			
2	O	111	Total	C	N	O	S	6	0	0
			923	581	163	174	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	114	Total	C	N	O	S	8	1	0
			951	597	168	181	5			
2	Q	114	Total	C	N	O	S	7	2	0
			952	597	168	182	5			
2	R	113	Total	C	N	O	S	0	0	0
			939	591	166	177	5			

- Molecule 3 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

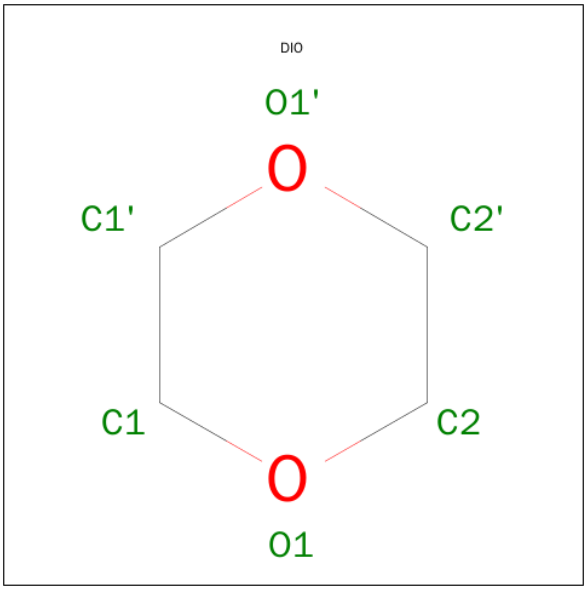


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	E	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
3	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

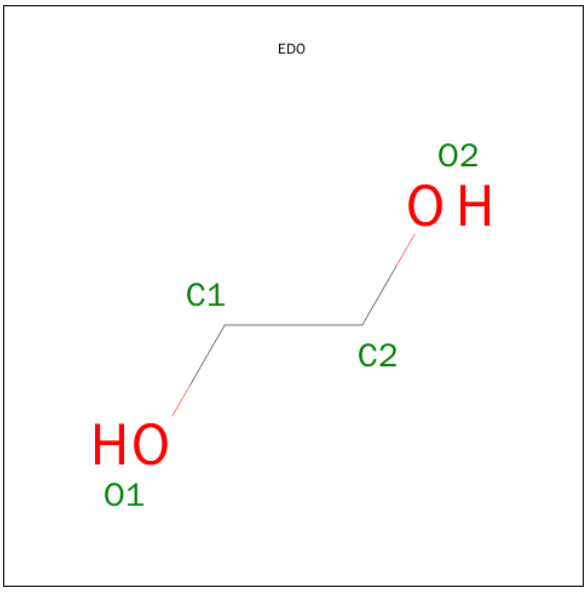
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	F	1	Total Mg 1 1	0	0

- Molecule 5 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: $C_4H_8O_2$).



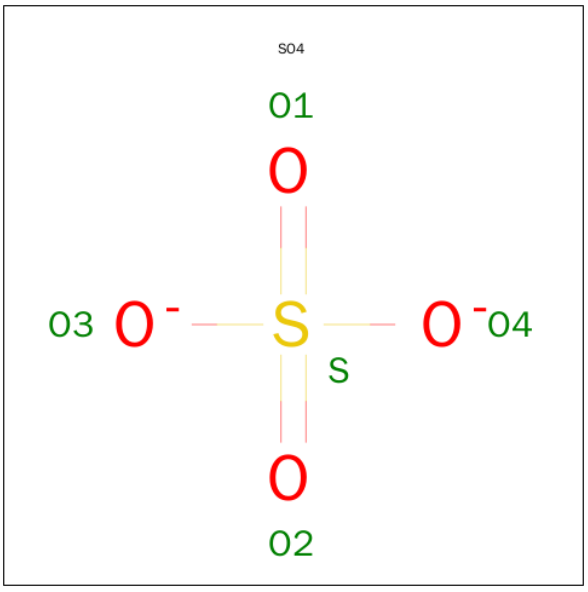
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 4 2	0	0
5	B	1	Total C O 6 4 2	0	0
5	F	1	Total C O 6 4 2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 4 2 2	0	0
6	E	1	Total C O 4 2 2	0	0
6	O	1	Total C O 4 2 2	0	0

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	M	1	Total O S 5 4 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	N	1	Total O S 5 4 1	0	0
7	O	1	Total O S 5 4 1	0	0
7	P	1	Total O S 5 4 1	0	0
7	Q	1	Total O S 5 4 1	0	0
7	R	1	Total O S 5 4 1	0	0

- Molecule 8 is water.

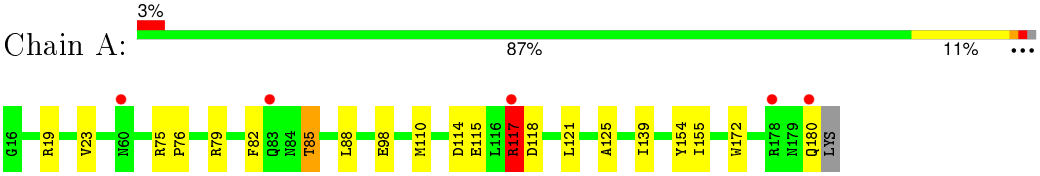
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	188	Total O 188 188	0	0
8	B	179	Total O 179 179	0	0
8	C	180	Total O 180 180	0	0
8	D	177	Total O 177 177	0	0
8	E	197	Total O 197 197	0	0
8	F	162	Total O 162 162	0	0
8	M	120	Total O 120 120	0	0
8	N	103	Total O 103 103	0	0
8	O	76	Total O 76 76	0	0
8	P	93	Total O 93 93	0	0
8	Q	104	Total O 104 104	0	0
8	R	77	Total O 77 77	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.

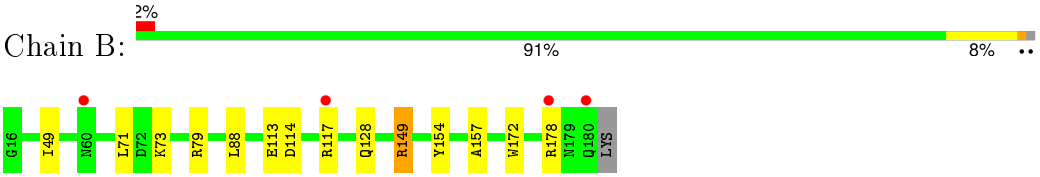
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain A:



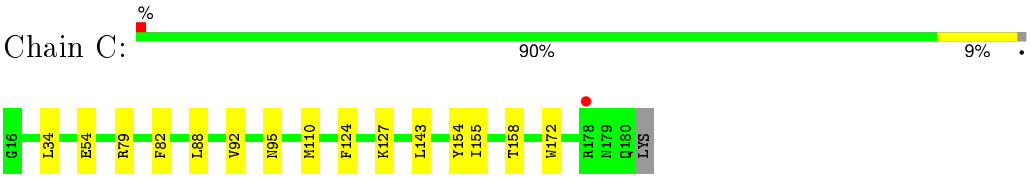
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain B:



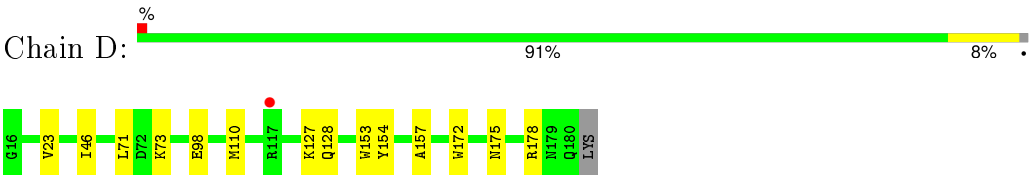
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain C:



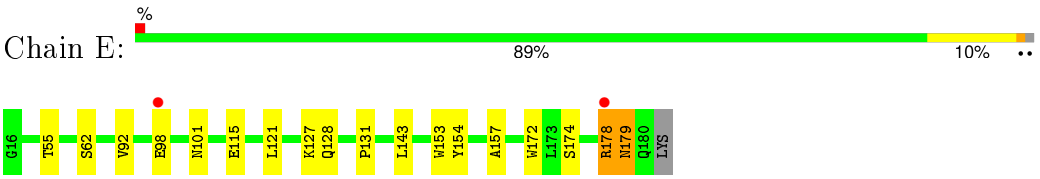
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain D:



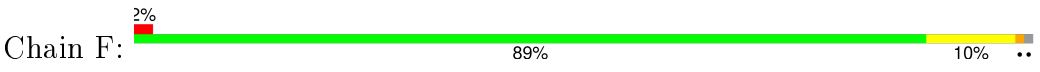
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain E:



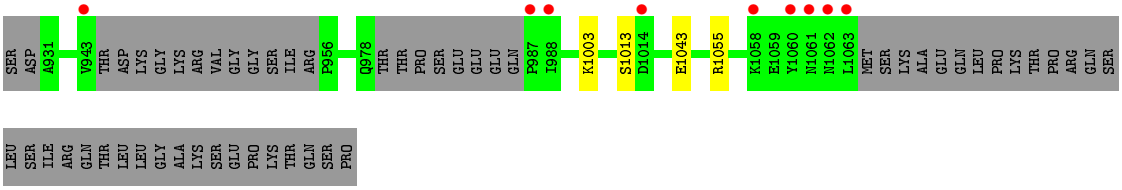
- Molecule 1: ADP-RIBOSYLATION FACTOR 1

Chain F:



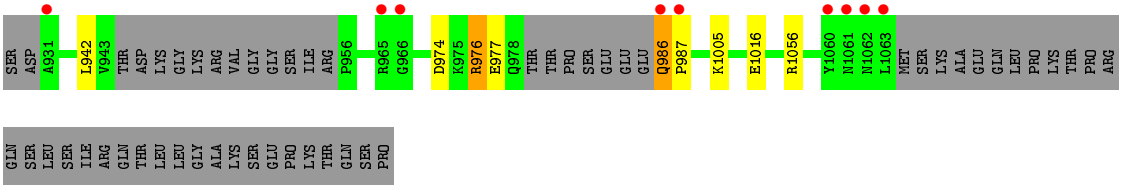
• Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10

Chain M:



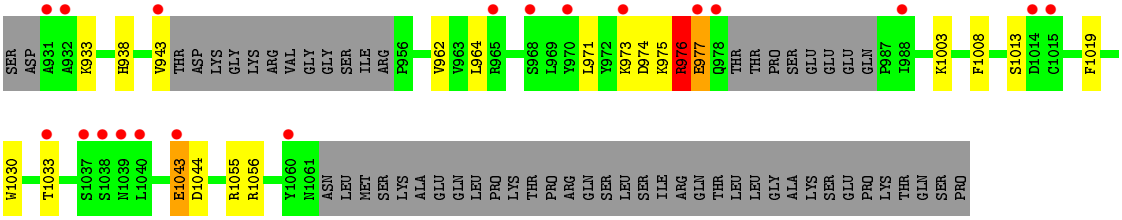
• Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10

Chain N:



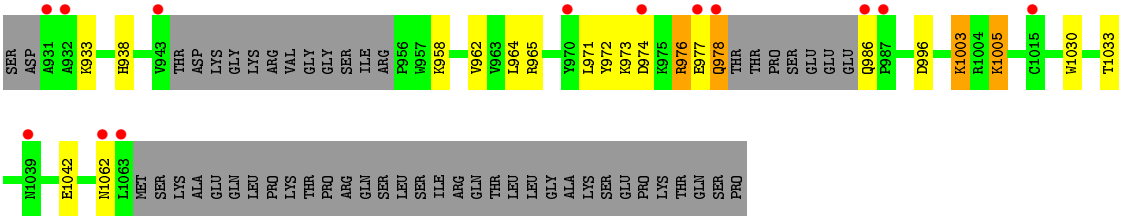
• Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10

Chain O:



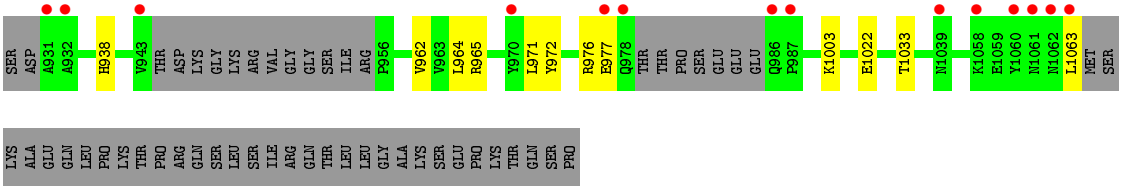
• Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10

Chain P:

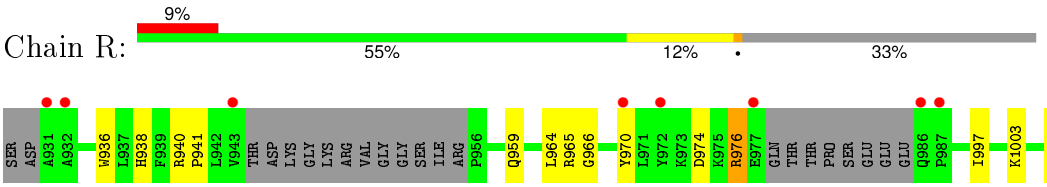


• Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10

Chain Q:



- Molecule 2: RHO-GTPASE ACTIVATING PROTEIN 10



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.64Å 132.14Å 146.28Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 49.03 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.3 (40.00-2.10) 98.2 (49.03-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.19 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.243 0.196 , 0.229	Depositor DCC
R_{free} test set	16193 reflections (11.09%)	DCC
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.4	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 162200 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15535	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, MG, DIO, EDO, SO4

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	0.47	0/1361	0.59	0/1843
1	B	0.48	0/1351	0.64	1/1829 (0.1%)
1	C	0.48	0/1361	0.61	0/1843
1	D	0.46	0/1382	0.58	0/1871
1	E	0.49	0/1373	0.61	0/1859
1	F	0.46	0/1345	0.58	0/1821
2	M	0.42	0/964	0.57	0/1295
2	N	0.44	0/964	0.59	0/1297
2	O	0.65	3/939 (0.3%)	0.72	3/1262 (0.2%)
2	P	0.44	0/972	0.70	3/1308 (0.2%)
2	Q	0.52	1/978 (0.1%)	0.64	1/1316 (0.1%)
2	R	0.42	0/955	0.58	0/1285
All	All	0.48	4/13945 (0.0%)	0.62	8/18829 (0.0%)

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	A	0	1
2	O	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	943	VAL	CB-CG2	-9.58	1.32	1.52
2	Q	1063	LEU	CB-CG	-9.02	1.26	1.52
2	O	975	LYS	C-N	7.86	1.52	1.34
2	O	943	VAL	CB-CG1	5.56	1.64	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	986	GLN	CA-CB-CG	11.14	137.91	113.40
2	O	943	VAL	CA-CB-CG2	8.28	123.33	110.90
2	O	976	ARG	NE-CZ-NH2	7.26	123.93	120.30
2	O	975	LYS	C-N-CA	-6.55	105.33	121.70
2	Q	1063	LEU	CB-CG-CD2	6.53	122.09	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	117	ARG	Sidechain
2	O	1056	ARG	Sidechain

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	1328	0	1324	19	0
1	B	1323	0	1316	8	0
1	C	1328	0	1317	12	0
1	D	1334	0	1323	10	0
1	E	1330	0	1319	13	0
1	F	1322	0	1315	11	0
2	M	943	0	938	3	0
2	N	948	0	936	5	0
2	O	923	0	912	11	0
2	P	951	0	936	14	0
2	Q	952	0	937	5	0
2	R	939	0	928	13	0
3	A	32	0	12	0	0
3	B	32	0	12	0	0
3	C	32	0	12	1	0
3	D	32	0	12	1	0
3	E	32	0	12	1	0
3	F	32	0	12	0	0
4	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	6	0	8	3	0
5	B	6	0	8	0	0
5	F	6	0	8	3	0
6	C	4	0	6	0	0
6	E	4	0	6	0	0
6	O	4	0	6	1	0
7	M	5	0	0	1	0
7	N	5	0	0	0	0
7	O	5	0	0	1	0
7	P	5	0	0	1	0
7	Q	5	0	0	1	0
7	R	5	0	0	0	0
8	A	188	0	0	2	0
8	B	179	0	0	4	0
8	C	180	0	0	1	0
8	D	177	0	0	2	0
8	E	197	0	0	3	0
8	F	162	0	0	0	0
8	M	120	0	0	0	0
8	N	103	0	0	1	0
8	O	76	0	0	2	0
8	P	93	0	0	2	0
8	Q	104	0	0	1	0
8	R	77	0	0	2	0
All	All	15535	0	13615	120	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 4.

The worst 5 of 120 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:B:73:LYS:HG2	8:B:3068:HOH:O	1.72	0.90
1:A:23:VAL:HG21	1:A:110:MET:HE1	1.61	0.83
1:B:149:ARG:HD3	2:M:1043:GLU:OE1	1.79	0.80
1:A:19:ARG:HH11	1:A:19:ARG:HG2	1.51	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HG22	5:A:1183:DIO:H2'2	1.67	0.75

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	165/166 (99%)	162 (98%)	3 (2%)	0	100	100
1	B	164/166 (99%)	162 (99%)	2 (1%)	0	100	100
1	C	165/166 (99%)	165 (100%)	0	0	100	100
1	D	168/166 (101%)	167 (99%)	1 (1%)	0	100	100
1	E	167/166 (101%)	165 (99%)	2 (1%)	0	100	100
1	F	163/166 (98%)	162 (99%)	1 (1%)	0	100	100
2	M	108/168 (64%)	108 (100%)	0	0	100	100
2	N	108/168 (64%)	107 (99%)	1 (1%)	0	100	100
2	O	105/168 (62%)	103 (98%)	1 (1%)	1 (1%)	19	13
2	P	109/168 (65%)	107 (98%)	2 (2%)	0	100	100
2	Q	110/168 (66%)	108 (98%)	2 (2%)	0	100	100
2	R	107/168 (64%)	107 (100%)	0	0	100	100
All	All	1639/2004 (82%)	1623 (99%)	15 (1%)	1 (0%)	56	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	977	GLU

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	144/143 (101%)	141 (98%)	3 (2%)	61	66
1	B	143/143 (100%)	139 (97%)	4 (3%)	51	55
1	C	144/143 (101%)	143 (99%)	1 (1%)	88	92
1	D	147/143 (103%)	147 (100%)	0	100	100
1	E	146/143 (102%)	144 (99%)	2 (1%)	74	80
1	F	142/143 (99%)	140 (99%)	2 (1%)	74	80
2	M	106/154 (69%)	106 (100%)	0	100	100
2	N	106/154 (69%)	103 (97%)	3 (3%)	51	55
2	O	103/154 (67%)	100 (97%)	3 (3%)	50	53
2	P	107/154 (70%)	102 (95%)	5 (5%)	32	30
2	Q	108/154 (70%)	105 (97%)	3 (3%)	51	55
2	R	105/154 (68%)	102 (97%)	3 (3%)	50	53
All	All	1501/1782 (84%)	1472 (98%)	29 (2%)	63	70

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	986	GLN
2	O	976	ARG
2	R	976	ARG
2	N	1005	LYS
2	O	1043	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	152	ASN
2	M	1035	GLN
2	R	938	HIS
1	F	176	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	152	ASN

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 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	$\#\|Z\| > 2$
3	GTP	A	1181	4	25,34,34	0.94	2 (8%)	34,54,54	1.71	8 (23%)
5	DIO	A	1183	-	6,6,6	0.44	0	6,6,6	1.19	1 (16%)
3	GTP	B	1181	4	25,34,34	1.01	1 (4%)	34,54,54	1.76	9 (26%)
5	DIO	B	1183	-	6,6,6	0.56	0	6,6,6	0.62	0
3	GTP	C	1181	4	25,34,34	0.96	2 (8%)	34,54,54	1.74	10 (29%)
6	EDO	C	1183	-	3,3,3	0.43	0	2,2,2	0.63	0
3	GTP	D	1181	4	25,34,34	1.00	2 (8%)	34,54,54	1.74	9 (26%)
3	GTP	E	1181	4	25,34,34	1.00	2 (8%)	34,54,54	1.80	8 (23%)
6	EDO	E	1183	-	3,3,3	0.58	0	2,2,2	0.28	0
3	GTP	F	1181	4	25,34,34	0.88	1 (4%)	34,54,54	1.74	7 (20%)
5	DIO	F	1183	-	6,6,6	0.57	0	6,6,6	1.06	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	SO4	M	2064	-	4,4,4	0.42	0	6,6,6	0.20	0
7	SO4	N	2064	-	4,4,4	0.32	0	6,6,6	0.17	0
7	SO4	O	2062	-	4,4,4	0.24	0	6,6,6	0.11	0
6	EDO	O	2063	-	3,3,3	0.54	0	2,2,2	0.26	0
7	SO4	P	2064	-	4,4,4	0.36	0	6,6,6	0.21	0
7	SO4	Q	2064	-	4,4,4	0.36	0	6,6,6	0.17	0
7	SO4	R	2064	-	4,4,4	0.29	0	6,6,6	0.25	0

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	GTP	A	1181	4	-	0/18/38/38	0/3/3/3
5	DIO	A	1183	-	-	0/0/6/6	0/1/1/1
3	GTP	B	1181	4	-	0/18/38/38	0/3/3/3
5	DIO	B	1183	-	-	0/0/6/6	0/1/1/1
3	GTP	C	1181	4	-	0/18/38/38	0/3/3/3
6	EDO	C	1183	-	-	0/1/1/1	0/0/0/0
3	GTP	D	1181	4	-	0/18/38/38	0/3/3/3
3	GTP	E	1181	4	-	0/18/38/38	0/3/3/3
6	EDO	E	1183	-	-	0/1/1/1	0/0/0/0
3	GTP	F	1181	4	-	0/18/38/38	0/3/3/3
5	DIO	F	1183	-	-	0/0/6/6	0/1/1/1
7	SO4	M	2064	-	-	0/0/0/0	0/0/0/0
7	SO4	N	2064	-	-	0/0/0/0	0/0/0/0
7	SO4	O	2062	-	-	0/0/0/0	0/0/0/0
6	EDO	O	2063	-	-	0/1/1/1	0/0/0/0
7	SO4	P	2064	-	-	0/0/0/0	0/0/0/0
7	SO4	Q	2064	-	-	0/0/0/0	0/0/0/0
7	SO4	R	2064	-	-	0/0/0/0	0/0/0/0

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1181	GTP	C2-N1	2.15	1.39	1.35
3	C	1181	GTP	C2-N1	2.17	1.39	1.35
3	D	1181	GTP	C2-N1	2.28	1.39	1.35
3	E	1181	GTP	C2-N1	2.30	1.39	1.35
3	F	1181	GTP	C6-N1	2.66	1.38	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	1181	GTP	N3-C2-N1	-5.38	119.25	127.44
3	D	1181	GTP	N3-C2-N1	-5.20	119.53	127.44
3	B	1181	GTP	N3-C2-N1	-5.01	119.81	127.44
3	F	1181	GTP	N3-C2-N1	-4.95	119.90	127.44
3	C	1181	GTP	N3-C2-N1	-4.89	119.99	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1183	DIO	3	0
3	C	1181	GTP	1	0
3	D	1181	GTP	1	0
3	E	1181	GTP	1	0
5	F	1183	DIO	3	0
7	M	2064	SO4	1	0
7	O	2062	SO4	1	0
6	O	2063	EDO	1	0
7	P	2064	SO4	1	0
7	Q	2064	SO4	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

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, 95^{th} 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	165/166 (99%)	0.14	5 (3%) 54 62	12, 17, 29, 45	0
1	B	165/166 (99%)	0.09	4 (2%) 62 68	11, 17, 27, 40	0
1	C	165/166 (99%)	0.10	1 (0%) 90 92	12, 18, 27, 36	0
1	D	165/166 (99%)	0.09	1 (0%) 90 92	12, 18, 27, 40	0
1	E	165/166 (99%)	0.06	2 (1%) 81 85	11, 17, 28, 43	1 (0%)
1	F	165/166 (99%)	0.21	4 (2%) 62 68	13, 20, 31, 42	0
2	M	113/168 (67%)	0.36	9 (7%) 15 21	16, 24, 35, 50	0
2	N	114/168 (67%)	0.32	9 (7%) 15 21	16, 25, 37, 52	1 (0%)
2	O	111/168 (66%)	0.93	19 (17%) 2 3	18, 30, 46, 56	2 (1%)
2	P	114/168 (67%)	0.58	13 (11%) 7 9	18, 28, 40, 48	2 (1%)
2	Q	114/168 (67%)	0.44	14 (12%) 5 7	15, 23, 38, 48	2 (1%)
2	R	113/168 (67%)	0.90	15 (13%) 4 6	19, 30, 44, 59	0
All	All	1669/2004 (83%)	0.31	96 (5%) 26 34	11, 21, 37, 59	8 (0%)

The worst 5 of 96 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	1063	LEU	7.1
2	R	1060	TYR	6.5
2	M	1063	LEU	5.6
2	N	1063	LEU	5.3
2	O	931	ALA	5.1

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, 95^{th} 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
6	EDO	O	2063	4/4	0.63	0.27	4.61	34,35,35,35	0
5	DIO	F	1183	6/6	0.89	0.21	2.08	18,20,21,22	0
5	DIO	A	1183	6/6	0.96	0.18	0.85	17,18,18,19	0
6	EDO	E	1183	4/4	0.90	0.14	0.36	37,38,38,38	0
7	SO4	N	2064	5/5	0.96	0.12	-0.13	37,38,39,39	0
3	GTP	B	1181	32/32	0.98	0.11	-0.17	11,14,18,19	0
7	SO4	Q	2064	5/5	0.98	0.11	-0.47	38,38,39,40	0
4	MG	A	1182	1/1	0.98	0.10	-0.51	16,16,16,16	0
3	GTP	C	1181	32/32	0.98	0.10	-0.54	13,18,19,21	0
5	DIO	B	1183	6/6	0.97	0.13	-0.62	13,13,14,15	0
7	SO4	M	2064	5/5	0.98	0.10	-0.69	33,34,34,36	0
7	SO4	R	2064	5/5	0.98	0.12	-0.70	43,44,44,44	0
3	GTP	F	1181	32/32	0.98	0.10	-0.72	14,16,18,20	0
4	MG	C	1182	1/1	0.98	0.09	-0.91	17,17,17,17	0
7	SO4	P	2064	5/5	0.98	0.11	-0.93	34,34,35,37	0
3	GTP	A	1181	32/32	0.99	0.09	-0.97	12,15,19,21	0
3	GTP	E	1181	32/32	0.99	0.09	-1.04	11,16,17,22	0
4	MG	B	1182	1/1	0.96	0.10	-1.07	14,14,14,14	0
3	GTP	D	1181	32/32	0.99	0.09	-1.20	12,17,18,20	0
7	SO4	O	2062	5/5	0.99	0.08	-1.35	35,35,36,37	0
4	MG	F	1182	1/1	0.93	0.09	-1.72	20,20,20,20	0
4	MG	D	1182	1/1	0.98	0.08	-1.76	15,15,15,15	0
4	MG	E	1182	1/1	0.95	0.06	-2.78	14,14,14,14	0
6	EDO	C	1183	4/4	0.95	0.15	-	29,29,29,29	0

6.5 Other polymers (i)

There are no such residues in this entry.