



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:56 PM GMT

PDB ID : 1R8Q  
Title : FULL-LENGTH ARF1-GDP-MG IN COMPLEX WITH BREFELDIN A  
AND A SEC7 DOMAIN  
Authors : Renault, L.; Guibert, B.; Cherfils, J.  
Deposited on : 2003-10-28  
Resolution : 1.86 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

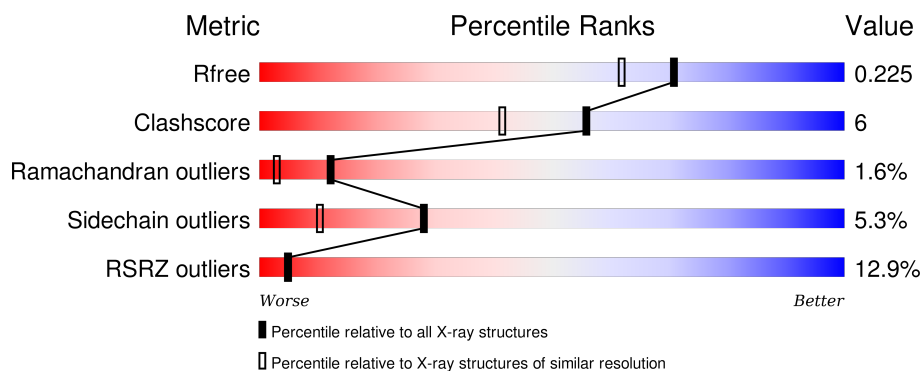
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.86 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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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  $\geq 3$ , 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	181	 16% 75% 21% ...
1	B	181	 20% 78% 14% . . .
2	E	203	 9% 81% 10% . 6%
2	F	203	 6% 80% 13% . .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6487 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	179	Total	C	N	O	S	0	2	0
			1445	920	252	267	6			
1	B	179	Total	C	N	O	S	0	1	0
			1442	918	252	266	6			

- Molecule 2 is a protein called Arno.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	191	Total	C	N	O	S	0	1	0
			1559	987	274	287	11			
2	F	194	Total	C	N	O	S	0	2	0
			1589	1003	280	295	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	190	TYR	PHE	ENGINEERED	UNP Q99418
E	191	SER	ALA	ENGINEERED	UNP Q99418
E	198	ASP	SER	ENGINEERED	UNP Q99418
E	208	MET	PRO	ENGINEERED	UNP Q99418
F	190	TYR	PHE	ENGINEERED	UNP Q99418
F	191	SER	ALA	ENGINEERED	UNP Q99418
F	198	ASP	SER	ENGINEERED	UNP Q99418
F	208	MET	PRO	ENGINEERED	UNP Q99418

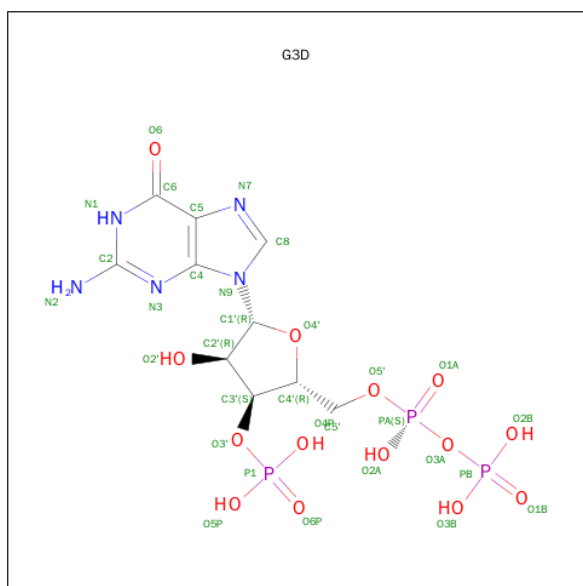
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

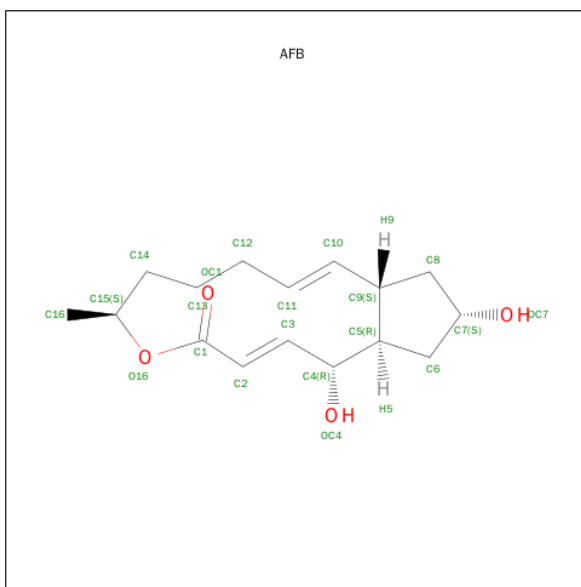
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Zn	0	0
			1	1		

- Molecule 5 is GUANOSINE-3'-MONOPHOSPHATE-5'-DIPHOSPHATE (three-letter code: G3D) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>14</sub>P<sub>3</sub>).



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

- Molecule 6 is 1,6,7,8,9,11A,12,13,14,14A-DECAHYDRO-1,13-DIHYDROXY-6-METHYL-4H-CYCLOPENT[F]OXACYCLOTRIDECIN-4-ONE (three-letter code: AFB) (formula: C<sub>16</sub>H<sub>24</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			20	16	4		
6	B	1	Total	C	O	0	0
			20	16	4		

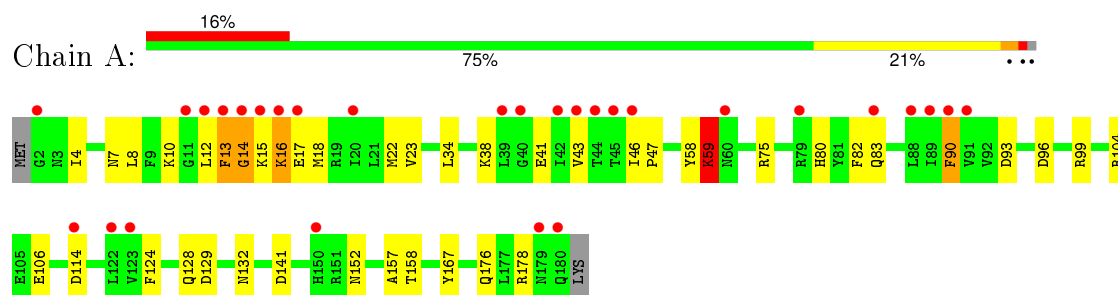
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	108	Total	O	0	0
			108	108		
7	B	73	Total	O	0	0
			73	73		
7	E	71	Total	O	0	0
			71	71		
7	F	93	Total	O	0	0
			93	93		

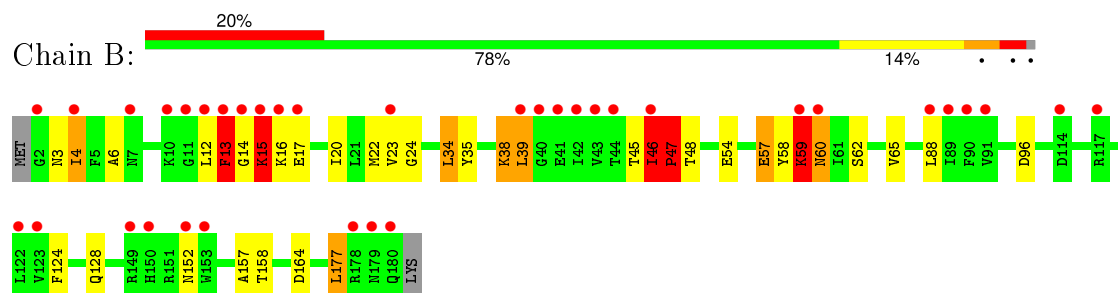
### 3 Residue-property plots [i](#)

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.

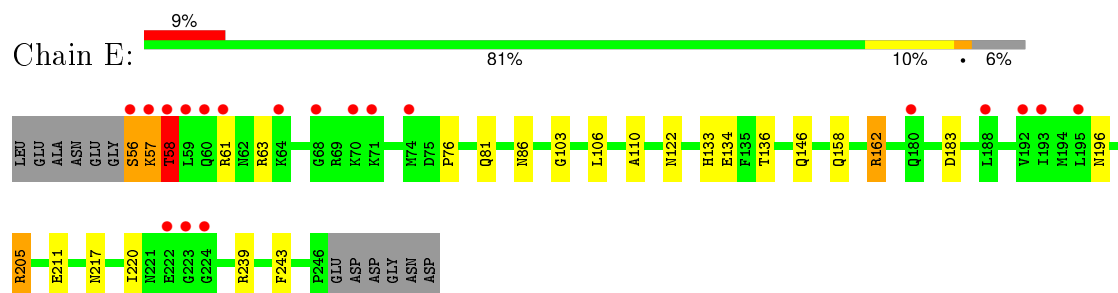
- Molecule 1: ADP-ribosylation factor 1



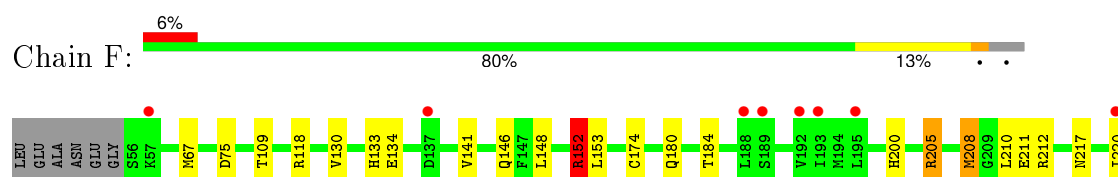
- Molecule 1: ADP-ribosylation factor 1

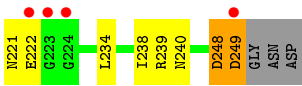


- Molecule 2: Arno



- Molecule 2: Arno





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.08Å 109.77Å 118.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.88 – 1.86 23.49 – 1.86	Depositor EDS
% Data completeness (in resolution range)	98.3 (29.88-1.86) 98.3 (23.49-1.86)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.179 , 0.220 0.189 , 0.225	Depositor DCC
$R_{free}$ test set	3692 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.7	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 51.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 74905 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6487	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, AFB, G3D

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	1.16	4/1479 (0.3%)	1.05	7/1999 (0.4%)
1	B	1.06	6/1472 (0.4%)	1.01	3/1989 (0.2%)
2	E	1.05	1/1592 (0.1%)	1.06	7/2142 (0.3%)
2	F	1.05	1/1626 (0.1%)	1.13	10/2188 (0.5%)
All	All	1.08	12/6169 (0.2%)	1.07	27/8318 (0.3%)

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
1	B	0	1
All	All	0	2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	PRO	CA-C	8.41	1.69	1.52
1	B	22	MET	SD-CE	-7.22	1.37	1.77
1	A	106	GLU	CD-OE1	6.98	1.33	1.25
1	B	152	ASN	CG-ND2	6.80	1.49	1.32
1	B	152	ASN	CA-C	5.90	1.68	1.52
1	B	62	SER	CB-OG	-5.62	1.34	1.42
1	B	48	THR	N-CA	5.41	1.57	1.46
1	A	90	PHE	CG-CD2	-5.36	1.30	1.38
1	A	22	MET	SD-CE	-5.24	1.48	1.77
2	E	162	ARG	CG-CD	5.21	1.65	1.51
2	F	130	VAL	CB-CG1	-5.16	1.42	1.52
1	A	82	PHE	CE1-CZ	-5.04	1.27	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	152	ARG	NE-CZ-NH2	-14.73	112.94	120.30
2	F	205	ARG	NE-CZ-NH2	-14.16	113.22	120.30
2	E	162	ARG	NE-CZ-NH2	-13.42	113.59	120.30
2	F	205	ARG	NE-CZ-NH1	11.59	126.10	120.30
2	E	162	ARG	NE-CZ-NH1	11.59	126.09	120.30
1	B	47	PRO	N-CA-C	9.27	136.21	112.10
1	A	104	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	F	152	ARG	NE-CZ-NH1	7.42	124.01	120.30
2	E	183	ASP	CB-CG-OD2	6.78	124.40	118.30
2	E	63	ARG	NE-CZ-NH2	-6.73	116.93	120.30
2	E	239	ARG	NE-CZ-NH1	6.68	123.64	120.30
2	E	205	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	83	GLN	C-N-CA	-6.24	106.09	121.70
2	F	75	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	114	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	104	ARG	CG-CD-NE	-5.79	99.65	111.80
1	A	75	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	E	162	ARG	CD-NE-CZ	5.70	131.57	123.60
2	F	208	MET	CG-SD-CE	5.68	109.29	100.20
1	B	164	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	96	ASP	CB-CG-OD2	5.41	123.17	118.30
2	F	205	ARG	CG-CD-NE	-5.41	100.45	111.80
2	F	152	ARG	CG-CD-NE	-5.31	100.65	111.80
2	F	205	ARG	CD-NE-CZ	5.18	130.85	123.60
2	F	248	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	93	ASP	CB-CG-OD2	5.06	122.86	118.30
1	A	129	ASP	CB-CG-OD2	5.02	122.82	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	GLY	Peptide
1	B	46	ILE	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	1445	0	1444	25	1
1	B	1442	0	1441	20	1
2	E	1559	0	1552	14	0
2	F	1589	0	1576	24	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	E	1	0	0	0	0
5	A	32	0	11	0	0
5	B	32	0	11	0	0
6	A	20	0	24	0	0
6	B	20	0	24	0	0
7	A	108	0	0	0	0
7	B	73	0	0	0	0
7	E	71	0	0	3	0
7	F	93	0	0	4	0
All	All	6487	0	6083	76	1

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 6.

All (76) 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:152:ASN:ND2	1:A:176:GLN:OE1	1.78	1.17
2:F:148:LEU:HD22	7:F:305:HOH:O	1.55	1.06
2:F:109[B]:THR:HG23	2:F:152:ARG:NH1	1.72	1.02
1:A:58:TYR:O	1:A:59:LYS:HB2	1.81	0.81
2:F:174:CYS:SG	7:F:317:HOH:O	2.40	0.80
1:A:58:TYR:O	1:A:59:LYS:CB	2.33	0.71
2:F:148:LEU:CD2	7:F:305:HOH:O	2.28	0.67
1:B:13:PHE:O	1:B:15:LYS:N	2.29	0.66
1:A:12:LEU:HD13	1:A:18:MET:HE2	1.78	0.65
1:A:13:PHE:CG	1:A:13:PHE:O	2.50	0.65
2:F:133:HIS:HD2	2:F:146:GLN:HE21	1.46	0.64
2:F:200:HIS:HE1	2:F:238:ILE:O	1.82	0.62
1:B:57:GLU:OE2	2:F:205:ARG:HD3	2.00	0.60
1:A:59:LYS:HB3	2:F:211:GLU:CG	2.31	0.60
2:F:153:LEU:HB2	7:F:305:HOH:O	2.01	0.59
2:E:133:HIS:HD2	2:E:146:GLN:HE21	1.50	0.58
2:F:239[B]:ARG:NH1	2:F:240:ASN:HD21	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ASN:O	1:B:4:ILE:CG1	2.53	0.57
1:B:58:TYR:O	1:B:59:LYS:C	2.44	0.56
1:A:124:PHE:CD1	1:A:158:THR:HG21	2.42	0.54
1:A:7:ASN:O	1:A:10:LYS:HE2	2.08	0.54
1:A:59:LYS:HE3	2:F:210:LEU:HD23	1.90	0.53
1:B:17:GLU:HA	1:B:60:ASN:ND2	2.24	0.53
1:B:128:GLN:HG3	1:B:157:ALA:HB1	1.90	0.52
1:A:59:LYS:HB3	2:F:211:GLU:HG3	1.90	0.52
1:A:59:LYS:HD3	2:F:210:LEU:HD23	1.92	0.52
2:F:248:ASP:O	2:F:249:ASP:HB2	2.09	0.51
2:E:122:ASN:HD22	2:E:122:ASN:H	1.59	0.51
1:A:128:GLN:HG3	1:A:157:ALA:HB1	1.94	0.50
1:A:15:LYS:O	1:A:16:LYS:HB3	2.11	0.50
1:B:58:TYR:O	1:B:59:LYS:O	2.30	0.49
1:A:59:LYS:CE	2:F:210:LEU:HD23	2.43	0.48
2:F:141:VAL:HG23	2:F:234:LEU:HD22	1.94	0.48
1:B:34:LEU:HD23	1:B:38:LYS:HD3	1.96	0.47
2:E:133:HIS:CD2	2:E:146:GLN:HE21	2.32	0.47
2:E:103:GLY:HA2	2:E:106:LEU:HD12	1.95	0.47
2:E:162:ARG:HD2	7:E:602:HOH:O	2.13	0.47
2:F:180:GLN:NE2	2:F:221:ASN:HD21	2.14	0.46
1:A:13:PHE:O	1:A:13:PHE:CD1	2.68	0.46
2:E:76:PRO:HG3	2:E:110:ALA:HB1	1.96	0.46
2:F:109[B]:THR:HG23	2:F:152:ARG:HH12	1.70	0.46
1:A:152:ASN:HD21	1:A:176:GLN:CD	1.99	0.45
2:E:196:ASN:ND2	2:E:243:PHE:H	2.14	0.45
1:B:46:ILE:HG13	1:B:47:PRO:N	2.32	0.45
2:F:109[B]:THR:HG23	2:F:152:ARG:CZ	2.42	0.45
2:E:86:ASN:ND2	7:E:644:HOH:O	2.50	0.44
1:B:39:LEU:HA	1:B:39:LEU:HD22	1.91	0.44
1:B:3:ASN:O	1:B:4:ILE:HG13	2.18	0.44
2:E:217:ASN:O	2:E:220:ILE:HG12	2.18	0.44
2:F:217:ASN:O	2:F:220:ILE:HG12	2.18	0.44
1:A:59:LYS:HB3	2:F:211:GLU:HG2	1.99	0.44
1:A:12:LEU:HD13	1:A:18:MET:CE	2.48	0.43
1:B:23[A]:VAL:HG22	1:B:88:LEU:HD11	2.00	0.43
1:A:96:ASP:OD2	1:A:99:ARG:HD3	2.17	0.43
2:F:133:HIS:CD2	2:F:146:GLN:HE21	2.31	0.43
2:E:56:SER:O	2:E:58:THR:N	2.51	0.43
2:E:162:ARG:CD	7:E:602:HOH:O	2.65	0.43
1:B:23[B]:VAL:HG12	1:B:24:GLY:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23[A]:VAL:HG23	1:A:90:PHE:CD1	2.54	0.42
2:E:158:GLN:OE1	2:E:162:ARG:NH2	2.49	0.42
1:B:34:LEU:HD22	1:B:54:GLU:HB3	2.01	0.42
1:A:13:PHE:O	1:A:14:GLY:C	2.57	0.42
1:A:46:ILE:HA	1:A:47:PRO:HD3	1.92	0.42
1:B:3:ASN:HD22	1:B:6:ALA:H	1.67	0.42
1:B:20:ILE:HD11	1:B:177:LEU:HD21	2.02	0.42
2:E:134[A]:GLU:OE1	2:E:136:THR:HB	2.18	0.42
1:B:34:LEU:HD13	1:B:65:VAL:HG23	2.01	0.42
1:B:34:LEU:O	1:B:38:LYS:HG3	2.20	0.42
2:F:184:THR:OG1	2:F:221:ASN:HA	2.19	0.41
2:E:196:ASN:HD21	2:E:243:PHE:H	1.68	0.41
1:A:8:LEU:HD21	1:A:167:TYR:CZ	2.56	0.40
1:A:13:PHE:C	1:A:15:LYS:N	2.72	0.40
1:B:12:LEU:O	1:B:13:PHE:C	2.59	0.40
1:B:124:PHE:CD1	1:B:158:THR:HG21	2.56	0.40
2:F:208:MET:HG3	2:F:212:ARG:HB2	2.03	0.40

All (1) 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)
1:A:141:ASP:OD2	1:B:35:TYR:OH[3_555]	2.13	0.07

## 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	179/181 (99%)	170 (95%)	6 (3%)	3 (2%)	11	2
1	B	178/181 (98%)	167 (94%)	5 (3%)	6 (3%)	5	0
2	E	190/203 (94%)	187 (98%)	1 (0%)	2 (1%)	17	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	194/203 (96%)	192 (99%)	1 (0%)	1 (0%)	34	17
All	All	741/768 (96%)	716 (97%)	13 (2%)	12 (2%)	12	3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	PHE
1	A	16	LYS
2	E	57	LYS
2	E	58	THR
1	B	4	ILE
1	B	13	PHE
1	B	14	GLY
1	B	47	PRO
1	B	59	LYS
2	F	222	GLU
1	B	15	LYS
1	A	59	LYS

### 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	155/155 (100%)	146 (94%)	9 (6%)	25	8
1	B	154/155 (99%)	141 (92%)	13 (8%)	14	2
2	E	170/178 (96%)	163 (96%)	7 (4%)	37	17
2	F	174/178 (98%)	169 (97%)	5 (3%)	50	31
All	All	653/666 (98%)	619 (95%)	34 (5%)	28	11

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	17	GLU

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Mol	Chain	Res	Type
1	A	34	LEU
1	A	41	GLU
1	A	43	VAL
1	A	59	LYS
1	A	80	HIS
1	A	132	ASN
1	A	178	ARG
2	E	56	SER
2	E	57	LYS
2	E	58	THR
2	E	61	ARG
2	E	81	GLN
2	E	205	ARG
2	E	211	GLU
1	B	13	PHE
1	B	15	LYS
1	B	16	LYS
1	B	34	LEU
1	B	38	LYS
1	B	39	LEU
1	B	45	THR
1	B	46	ILE
1	B	47	PRO
1	B	57	GLU
1	B	59	LYS
1	B	60	ASN
1	B	177	LEU
2	F	67	MET
2	F	118	ARG
2	F	134	GLU
2	F	152	ARG
2	F	249	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	71	GLN
1	A	84	ASN
2	E	62	ASN
2	E	86	ASN
2	E	91	ASN

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Mol	Chain	Res	Type
2	E	122	ASN
2	E	133	HIS
2	E	175	ASN
2	E	196	ASN
1	B	3	ASN
1	B	60	ASN
1	B	179	ASN
2	F	81	GLN
2	F	122	ASN
2	F	127	HIS
2	F	133	HIS
2	F	175	ASN
2	F	180	GLN
2	F	196	ASN
2	F	200	HIS
2	F	240	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 7 ligands modelled in this entry, 3 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
5	G3D	A	401	3	27,34,34	1.64	6 (22%)	36,54,54	2.26	13 (36%)
6	AFB	A	403	-	20,21,21	1.78	5 (25%)	21,28,28	2.34	9 (42%)
5	G3D	B	501	3	27,34,34	2.00	9 (33%)	36,54,54	2.12	9 (25%)
6	AFB	B	503	-	20,21,21	2.05	7 (35%)	21,28,28	2.15	9 (42%)

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
5	G3D	A	401	3	-	0/17/37/37	0/3/3/3
6	AFB	A	403	-	-	0/21/33/33	0/1/2/2
5	G3D	B	501	3	-	0/17/37/37	0/3/3/3
6	AFB	B	503	-	-	0/21/33/33	0/1/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	501	G3D	O4'-C1'	-3.41	1.36	1.41
5	B	501	G3D	PB-O3B	-3.17	1.43	1.54
6	B	503	AFB	C2-C1	-3.07	1.41	1.48
5	A	401	G3D	PA-O5'	-2.74	1.46	1.59
6	B	503	AFB	C6-C7	-2.60	1.47	1.52
5	B	501	G3D	C6-C5	-2.17	1.36	1.41
5	A	401	G3D	C6-C5	-2.06	1.37	1.41
6	A	403	AFB	C2-C1	-2.04	1.43	1.48
5	B	501	G3D	P1-O4P	-2.02	1.47	1.54
5	A	401	G3D	C8-N7	2.05	1.38	1.34
6	A	403	AFB	C13-C12	2.18	1.60	1.52
5	B	501	G3D	C5'-C4'	2.20	1.58	1.51
5	A	401	G3D	P1-O6P	2.25	1.58	1.51
6	B	503	AFB	C9-C5	2.51	1.61	1.55
5	B	501	G3D	O6-C6	2.55	1.30	1.24
6	A	403	AFB	C6-C5	2.61	1.60	1.52
6	B	503	AFB	C9-C10	2.88	1.57	1.49
6	B	503	AFB	O16-C15	2.89	1.52	1.47
6	A	403	AFB	C2-C3	2.92	1.40	1.32
5	B	501	G3D	C6-N1	2.94	1.38	1.33
5	B	501	G3D	C8-N7	3.20	1.40	1.34
6	A	403	AFB	C4-C3	3.40	1.56	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	503	AFB	C2-C3	3.44	1.41	1.32
5	A	401	G3D	O6-C6	3.46	1.33	1.24
5	A	401	G3D	C5'-C4'	3.61	1.63	1.51
6	B	503	AFB	C4-C3	4.33	1.58	1.49
5	B	501	G3D	P1-O6P	4.55	1.66	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	401	G3D	N3-C2-N1	-5.82	118.57	127.44
5	B	501	G3D	C5-C6-N1	-4.89	116.90	123.59
5	A	401	G3D	C2'-C1'-N9	-4.88	106.84	114.29
6	A	403	AFB	C16-C15-C14	-4.87	100.92	114.04
5	B	501	G3D	C2'-C1'-N9	-4.59	107.27	114.29
6	A	403	AFB	O16-C15-C14	-3.94	98.91	107.00
5	B	501	G3D	N3-C2-N1	-3.92	121.48	127.44
5	B	501	G3D	O4'-C1'-N9	-3.60	100.57	108.10
6	A	403	AFB	O16-C1-OC1	-3.59	117.70	123.30
6	A	403	AFB	C3-C2-C1	-3.50	114.06	122.71
6	B	503	AFB	C8-C9-C10	-3.49	106.46	113.38
5	A	401	G3D	C5-C6-N1	-3.42	118.91	123.59
6	B	503	AFB	O16-C15-C14	-3.33	100.15	107.00
6	B	503	AFB	C9-C10-C11	-3.30	118.41	125.82
6	B	503	AFB	C3-C2-C1	-3.23	114.73	122.71
5	A	401	G3D	O3'-P1-O6P	-3.17	99.19	107.11
6	B	503	AFB	C4-C3-C2	-3.16	119.06	125.33
5	A	401	G3D	O3A-PA-O5'	-3.15	94.57	102.94
5	B	501	G3D	C4'-O4'-C1'	-2.87	106.57	109.72
5	A	401	G3D	C6-C5-C4	-2.81	117.54	120.90
6	A	403	AFB	C9-C10-C11	-2.56	120.08	125.82
5	B	501	G3D	O5P-P1-O6P	-2.53	102.45	110.58
6	B	503	AFB	O16-C1-OC1	-2.49	119.43	123.30
6	B	503	AFB	C14-C13-C12	-2.45	110.44	114.53
6	B	503	AFB	O16-C15-C16	-2.40	102.46	107.88
6	A	403	AFB	C12-C11-C10	-2.38	118.01	125.14
6	A	403	AFB	C8-C9-C10	-2.36	108.70	113.38
5	A	401	G3D	C4'-O4'-C1'	-2.22	107.28	109.72
5	A	401	G3D	O3'-C3'-C4'	-2.13	101.64	109.99
5	A	401	G3D	O5'-PA-O1A	-2.00	101.84	109.62
5	A	401	G3D	O5P-P1-O4P	2.19	115.72	107.38
6	A	403	AFB	C8-C9-C5	2.41	105.61	100.48
5	A	401	G3D	O2A-PA-O1A	2.48	125.96	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	501	G3D	O4P-P1-O6P	2.90	119.93	110.58
6	B	503	AFB	O16-C1-C2	3.47	120.02	111.42
6	A	403	AFB	O16-C1-C2	3.60	120.36	111.42
5	A	401	G3D	N2-C2-N3	3.65	124.81	117.80
5	B	501	G3D	O5P-P1-O4P	4.12	123.06	107.38
5	B	501	G3D	C6-N1-C2	4.40	122.05	115.94
5	A	401	G3D	C6-N1-C2	4.40	122.05	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	179/181 (98%)	0.78	29 (16%) <b>3</b> <b>3</b>	16, 24, 57, 74	0
1	B	179/181 (98%)	1.03	36 (20%) <b>1</b> <b>1</b>	17, 29, 61, 75	0
2	E	191/203 (94%)	0.57	19 (9%) <b>9</b> <b>9</b>	19, 29, 43, 61	0
2	F	194/203 (95%)	0.30	12 (6%) <b>24</b> <b>22</b>	15, 24, 45, 60	0
All	All	743/768 (96%)	0.66	96 (12%) <b>5</b> <b>5</b>	15, 27, 54, 75	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	PHE	12.2
1	B	40	GLY	11.7
1	B	13	PHE	11.2
1	B	2	GLY	9.6
1	A	2	GLY	9.1
1	B	42	ILE	8.7
1	B	15	LYS	7.2
1	B	39	LEU	7.1
1	B	14	GLY	6.5
1	A	44	THR	6.2
1	A	40	GLY	6.1
1	A	43	VAL	6.1
1	A	42	ILE	6.1
1	A	179	ASN	5.3
2	F	249	ASP	5.0
1	A	12	LEU	4.7
1	B	12	LEU	4.7
1	B	43	VAL	4.6
2	F	222	GLU	4.6
2	F	220	ILE	4.5
1	B	10	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
2	E	57	LYS	4.4
1	B	89	ILE	4.4
2	F	224	GLY	4.4
1	A	89	ILE	4.3
1	B	41	GLU	4.2
1	B	150	HIS	4.2
1	A	180	GLN	3.8
2	E	59	LEU	3.8
1	A	15	LYS	3.8
1	B	178	ARG	3.8
2	E	56	SER	3.7
1	A	16	LYS	3.7
2	F	223	GLY	3.6
1	A	14	GLY	3.6
1	A	46	ILE	3.5
2	E	192	VAL	3.5
1	B	180	GLN	3.5
1	B	152	ASN	3.3
1	B	179	ASN	3.2
1	B	60	ASN	3.2
1	B	91	VAL	3.1
2	E	70	LYS	3.1
2	F	193	ILE	3.1
1	B	88	LEU	3.0
1	A	91	VAL	3.0
2	F	57	LYS	2.9
1	B	11	GLY	2.8
2	E	222	GLU	2.8
1	B	117	ARG	2.7
2	E	68	GLY	2.7
1	A	123	VAL	2.7
1	A	60	ASN	2.7
1	B	7	ASN	2.7
1	A	11	GLY	2.7
2	E	74	MET	2.7
2	E	61	ARG	2.7
1	A	39	LEU	2.7
1	A	88	LEU	2.7
2	E	193	ILE	2.6
2	E	64	LYS	2.6
1	A	114	ASP	2.6
1	B	123	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	122	LEU	2.6
1	B	17	GLU	2.5
2	E	223	GLY	2.5
1	A	122	LEU	2.5
1	B	4	ILE	2.5
1	A	90	PHE	2.4
1	B	59	LYS	2.4
1	B	90	PHE	2.4
1	A	20	ILE	2.4
1	B	23[A]	VAL	2.4
2	E	60	GLN	2.4
2	E	180	GLN	2.4
2	F	188	LEU	2.4
1	B	44	THR	2.3
2	E	58	THR	2.3
2	E	195	LEU	2.3
2	F	192	VAL	2.3
1	A	83	GLN	2.3
2	E	188	LEU	2.3
1	B	16	LYS	2.3
2	F	195	LEU	2.2
1	B	153	TRP	2.2
1	B	149	ARG	2.2
1	A	17	GLU	2.1
1	A	45	THR	2.1
1	B	114	ASP	2.1
2	F	189	SER	2.1
2	E	224	GLY	2.1
1	A	79	ARG	2.0
1	A	150	HIS	2.0
2	E	71	LYS	2.0
2	F	137	ASP	2.0
1	B	46	ILE	2.0

## 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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	G3D	A	401	32/32	0.95	0.12	0.70	22,26,47,50	0
5	G3D	B	501	32/32	0.97	0.10	-0.32	23,27,51,56	0
6	AFB	A	403	20/20	0.97	0.09	-0.57	21,26,30,33	0
6	AFB	B	503	20/20	0.97	0.08	-0.67	20,24,28,29	0
4	ZN	E	601	1/1	0.99	0.03	-	34,34,34,34	0
3	MG	B	502	1/1	0.99	0.23	-	6,6,6,6	0
3	MG	A	402	1/1	0.99	0.32	-	8,8,8,8	0

## 6.5 Other polymers

There are no such residues in this entry.