Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:01 PM GMT

PDB ID	:	4BA9
Title	:	The structural basis for the coordination of Y-family Translesion DNA Polymerases by Rev1
Authors	:	Grummitt, C.G.; Kilkenny, M.L.; Frey, A.; Roe, S.M.; Oliver, A.W.; Sale, J.E.; Pearl, L.H.
Deposited on	:	2012-09-12
Resolution	:	2.73 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
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:

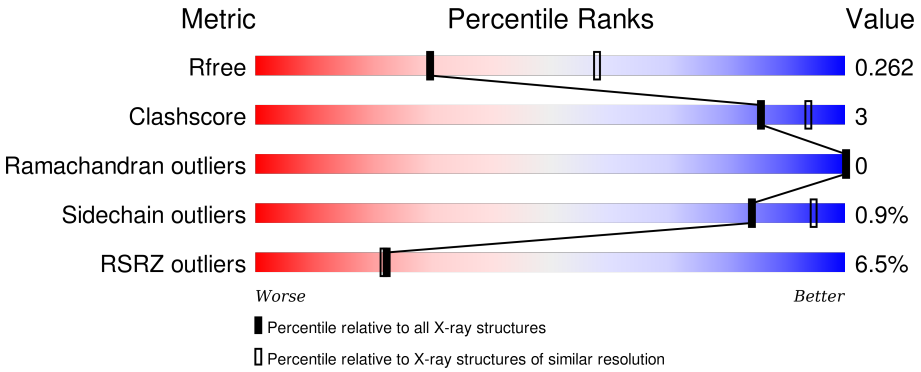
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.73 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	3050 (2.78-2.70)
Clashscore	102246	3424 (2.78-2.70)
Ramachandran outliers	100387	3367 (2.78-2.70)
Sidechain outliers	100360	3368 (2.78-2.70)
RSRZ outliers	91569	3055 (2.78-2.70)

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	114	4% 88% • 9%
1	B	114	3% 83% 8% 9%
1	C	114	12% 80% 12% • 6%
1	D	114	2% 85% 6% 9%
1	E	114	7% 87% • 9%

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Mol	Chain	Length	Quality of chain
1	F	114	9% 88% 9%

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
3	NI	B	2245	-	-	-	X
3	NI	D	2245	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5313 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 DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			845	540	138	161	6			
1	B	104	Total	C	N	O	S	0	0	0
			849	542	138	163	6			
1	C	107	Total	C	N	O	S	0	2	0
			881	560	144	169	8			
1	D	104	Total	C	N	O	S	0	0	0
			855	545	141	163	6			
1	E	104	Total	C	N	O	S	0	1	0
			846	540	136	163	7			
1	F	104	Total	C	N	O	S	0	1	0
			860	549	141	163	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
A	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
A	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
A	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
A	218	GLY	-	LINKER	UNP Q9UBZ9
A	219	SER	-	LINKER	UNP Q9UBZ9
A	220	ASP	-	LINKER	UNP Q9UBZ9
A	1149	ALA	-	LINKER	UNP Q9UBZ9
A	1150	GLY	-	LINKER	UNP Q9UBZ9
A	1151	SER	-	LINKER	UNP Q9UBZ9
A	1152	ALA	-	LINKER	UNP Q9UBZ9
A	1153	GLY	-	LINKER	UNP Q9UBZ9
A	1154	ASP	-	LINKER	UNP Q9UBZ9
A	1155	GLY	-	LINKER	UNP Q9UBZ9
A	1156	ALA	-	LINKER	UNP Q9UBZ9
A	1157	SER	-	LINKER	UNP Q9UBZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
B	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
B	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
B	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
B	218	GLY	-	LINKER	UNP Q9UBZ9
B	219	SER	-	LINKER	UNP Q9UBZ9
B	220	ASP	-	LINKER	UNP Q9UBZ9
B	1149	ALA	-	LINKER	UNP Q9UBZ9
B	1150	GLY	-	LINKER	UNP Q9UBZ9
B	1151	SER	-	LINKER	UNP Q9UBZ9
B	1152	ALA	-	LINKER	UNP Q9UBZ9
B	1153	GLY	-	LINKER	UNP Q9UBZ9
B	1154	ASP	-	LINKER	UNP Q9UBZ9
B	1155	GLY	-	LINKER	UNP Q9UBZ9
B	1156	ALA	-	LINKER	UNP Q9UBZ9
B	1157	SER	-	LINKER	UNP Q9UBZ9
C	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
C	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
C	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
C	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
C	218	GLY	-	LINKER	UNP Q9UBZ9
C	219	SER	-	LINKER	UNP Q9UBZ9
C	220	ASP	-	LINKER	UNP Q9UBZ9
C	1149	ALA	-	LINKER	UNP Q9UBZ9
C	1150	GLY	-	LINKER	UNP Q9UBZ9
C	1151	SER	-	LINKER	UNP Q9UBZ9
C	1152	ALA	-	LINKER	UNP Q9UBZ9
C	1153	GLY	-	LINKER	UNP Q9UBZ9
C	1154	ASP	-	LINKER	UNP Q9UBZ9
C	1155	GLY	-	LINKER	UNP Q9UBZ9
C	1156	ALA	-	LINKER	UNP Q9UBZ9
C	1157	SER	-	LINKER	UNP Q9UBZ9
D	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
D	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
D	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
D	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
D	218	GLY	-	LINKER	UNP Q9UBZ9
D	219	SER	-	LINKER	UNP Q9UBZ9
D	220	ASP	-	LINKER	UNP Q9UBZ9
D	1149	ALA	-	LINKER	UNP Q9UBZ9
D	1150	GLY	-	LINKER	UNP Q9UBZ9
D	1151	SER	-	LINKER	UNP Q9UBZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1152	ALA	-	LINKER	UNP Q9UBZ9
D	1153	GLY	-	LINKER	UNP Q9UBZ9
D	1154	ASP	-	LINKER	UNP Q9UBZ9
D	1155	GLY	-	LINKER	UNP Q9UBZ9
D	1156	ALA	-	LINKER	UNP Q9UBZ9
D	1157	SER	-	LINKER	UNP Q9UBZ9
E	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
E	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
E	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
E	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
E	218	GLY	-	LINKER	UNP Q9UBZ9
E	219	SER	-	LINKER	UNP Q9UBZ9
E	220	ASP	-	LINKER	UNP Q9UBZ9
E	1149	ALA	-	LINKER	UNP Q9UBZ9
E	1150	GLY	-	LINKER	UNP Q9UBZ9
E	1151	SER	-	LINKER	UNP Q9UBZ9
E	1152	ALA	-	LINKER	UNP Q9UBZ9
E	1153	GLY	-	LINKER	UNP Q9UBZ9
E	1154	ASP	-	LINKER	UNP Q9UBZ9
E	1155	GLY	-	LINKER	UNP Q9UBZ9
E	1156	ALA	-	LINKER	UNP Q9UBZ9
E	1157	SER	-	LINKER	UNP Q9UBZ9
F	201	GLY	-	EXPRESSION TAG	UNP Q9UBT6
F	202	PRO	-	EXPRESSION TAG	UNP Q9UBT6
F	203	HIS	-	EXPRESSION TAG	UNP Q9UBT6
F	204	MET	-	EXPRESSION TAG	UNP Q9UBT6
F	218	GLY	-	LINKER	UNP Q9UBZ9
F	219	SER	-	LINKER	UNP Q9UBZ9
F	220	ASP	-	LINKER	UNP Q9UBZ9
F	1149	ALA	-	LINKER	UNP Q9UBZ9
F	1150	GLY	-	LINKER	UNP Q9UBZ9
F	1151	SER	-	LINKER	UNP Q9UBZ9
F	1152	ALA	-	LINKER	UNP Q9UBZ9
F	1153	GLY	-	LINKER	UNP Q9UBZ9
F	1154	ASP	-	LINKER	UNP Q9UBZ9
F	1155	GLY	-	LINKER	UNP Q9UBZ9
F	1156	ALA	-	LINKER	UNP Q9UBZ9
F	1157	SER	-	LINKER	UNP Q9UBZ9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mg 1 1	0	0
2	E	2	Total Mg 2 2	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ni 2 2	0	0
3	A	2	Total Ni 2 2	0	0
3	D	2	Total Ni 2 2	0	0
3	F	2	Total Ni 2 2	0	0
3	E	2	Total Ni 2 2	0	0

- Molecule 4 is water.

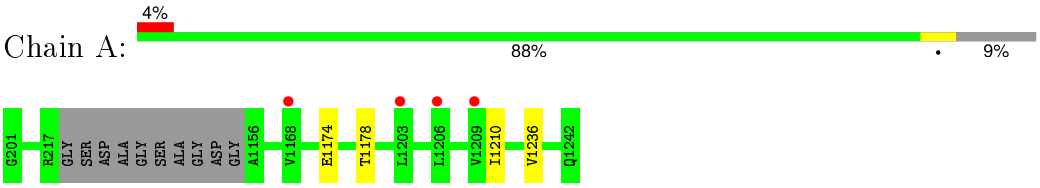
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	29	Total O 29 29	0	0
4	B	47	Total O 47 47	0	0
4	C	21	Total O 21 21	0	0
4	D	34	Total O 34 34	0	0
4	E	12	Total O 12 12	0	0
4	F	16	Total O 16 16	0	0

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.

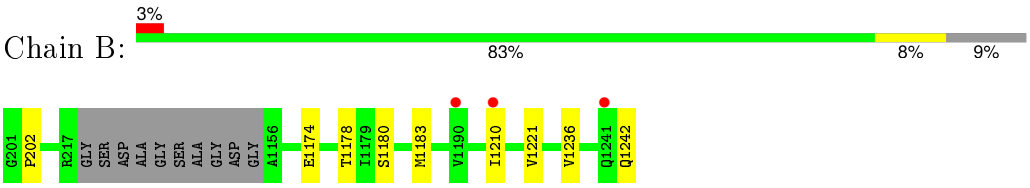
- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain A:



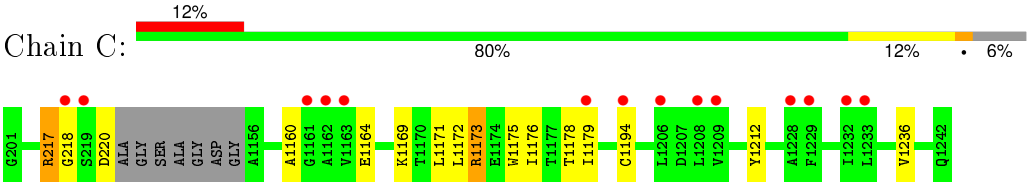
- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain B:



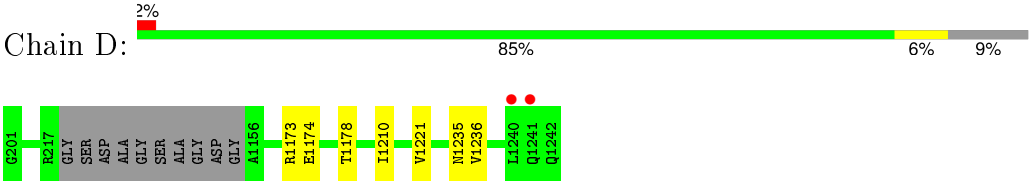
- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain C:



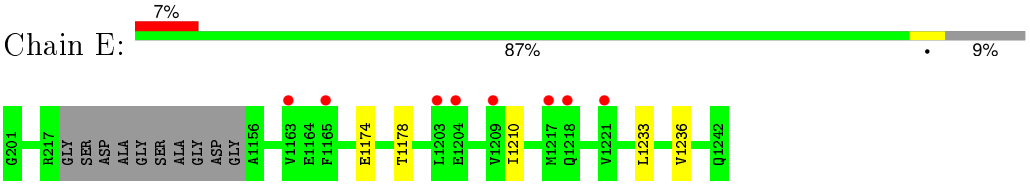
- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain D:



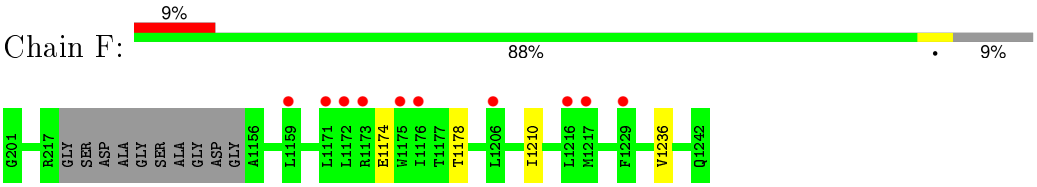
- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain E:



- Molecule 1: DNA POLYMERASE KAPPA, DNA REPAIR PROTEIN REV1

Chain F:


9%
88%
9%
G201
R217
GLY
SER
ASP
ALA
GLY
SER
ALA
GLY
ASP
GLY
A1156
L1159
L1171
L1172
R1173
E1174
W1175
I1176
T1177
T1178
L1206
I1210
L1216
M1217
F1229
V1236
Q1242

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	105.75Å 105.75Å 424.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.82 – 2.73 84.08 – 2.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.82-2.73) 98.8 (84.08-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.214 , 0.250 0.225 , 0.262	Depositor DCC
R_{free} test set	1256 reflections (5.39%)	DCC
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.297	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 24571 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5313	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: NI, 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	0.47	0/858	0.58	0/1154
1	B	0.49	0/862	0.58	0/1159
1	C	0.58	0/900	0.68	0/1208
1	D	0.51	0/868	0.61	0/1166
1	E	0.48	0/862	0.58	0/1161
1	F	0.46	0/876	0.58	0/1176
All	All	0.50	0/5226	0.60	0/7024

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	845	0	838	2	0
1	B	849	0	842	9	0
1	C	881	0	879	11	0
1	D	855	0	853	4	0
1	E	846	0	829	5	0
1	F	860	0	862	2	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	29	0	0	0	0
4	B	47	0	0	4	0
4	C	21	0	0	1	0
4	D	34	0	0	0	0
4	E	12	0	0	0	0
4	F	16	0	0	0	0
All	All	5313	0	5103	29	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 3.

All (29) 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:C:1194[B]:CYS:SG	1:C:1236:VAL:HG22	1.71	1.29
1:C:217:ARG:HB2	1:C:218:GLY:HA2	1.44	0.99
1:C:1194[B]:CYS:SG	1:C:1236:VAL:CG2	2.52	0.97
1:B:1242:GLN:OXT	1:E:1233:LEU:HD21	1.80	0.81
1:C:217:ARG:HB2	1:C:218:GLY:CA	2.13	0.79
1:B:1174:GLU:O	1:B:1178:THR:HB	1.93	0.69
1:A:1174:GLU:O	1:A:1178:THR:HB	1.95	0.67
1:E:1174:GLU:O	1:E:1178:THR:HB	1.95	0.66
1:D:1174:GLU:O	1:D:1178:THR:HB	1.96	0.65
1:F:1174:GLU:O	1:F:1178:THR:HB	1.98	0.62
1:B:1180:SER:HA	4:B:2016:HOH:O	2.03	0.58
1:B:1210:ILE:HD11	1:B:1236:VAL:HG11	1.88	0.54
1:C:1173:ARG:HG3	1:C:1212:TYR:OH	2.08	0.53
1:C:1160:ALA:HB3	1:C:1171:LEU:HD13	1.90	0.53
1:C:1178:THR:HB	1:C:1179:ILE:HD12	1.94	0.50
1:F:1210:ILE:HD11	1:F:1236:VAL:HG11	1.94	0.49
1:B:1221:VAL:HG22	4:B:2035:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:ILE:HD11	1:A:1236:VAL:HG11	1.96	0.48
1:B:1242:GLN:OXT	1:E:1233:LEU:CD2	2.58	0.47
1:C:1175:TRP:HD1	1:C:1179:ILE:HD13	1.79	0.47
1:B:1242:GLN:HA	1:E:1233:LEU:HD11	1.97	0.47
1:C:1194[B]:CYS:HG	1:C:1236:VAL:HG22	1.68	0.46
1:B:202:PRO:HB3	1:D:1235:ASN:OD1	2.15	0.46
1:D:1210:ILE:HD11	1:D:1236:VAL:HG11	1.97	0.46
4:B:2037:HOH:O	1:D:1221:VAL:HG12	2.16	0.46
1:E:1210:ILE:HD11	1:E:1236:VAL:HG11	1.98	0.45
1:C:1172:LEU:O	1:C:1176:ILE:HD12	2.20	0.42
1:C:1164:GLU:HB3	4:C:2008:HOH:O	2.22	0.40
1:B:1183:MET:HB3	4:B:2020:HOH:O	2.21	0.40

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	100/114 (88%)	99 (99%)	1 (1%)	0	100	100
1	B	100/114 (88%)	99 (99%)	1 (1%)	0	100	100
1	C	105/114 (92%)	100 (95%)	5 (5%)	0	100	100
1	D	100/114 (88%)	99 (99%)	1 (1%)	0	100	100
1	E	101/114 (89%)	100 (99%)	1 (1%)	0	100	100
1	F	101/114 (89%)	99 (98%)	2 (2%)	0	100	100
All	All	607/684 (89%)	596 (98%)	11 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	95/102 (93%)	95 (100%)	0	100 100
1	B	96/102 (94%)	96 (100%)	0	100 100
1	C	101/102 (99%)	97 (96%)	4 (4%)	38 68
1	D	97/102 (95%)	96 (99%)	1 (1%)	82 94
1	E	95/102 (93%)	95 (100%)	0	100 100
1	F	98/102 (96%)	98 (100%)	0	100 100
All	All	582/612 (95%)	577 (99%)	5 (1%)	84 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	217	ARG
1	C	220	ASP
1	C	1169	LYS
1	C	1173	ARG
1	D	1173	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1237	GLN
1	E	1241	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 18 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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	104/114 (91%)	0.49	4 (3%) 44 46	38, 76, 100, 109	0
1	B	104/114 (91%)	0.37	3 (2%) 55 57	34, 56, 90, 107	0
1	C	107/114 (93%)	0.80	14 (13%) 5 4	41, 69, 91, 104	0
1	D	104/114 (91%)	0.33	2 (1%) 70 72	39, 53, 82, 105	0
1	E	104/114 (91%)	0.58	8 (7%) 16 15	42, 68, 94, 118	0
1	F	104/114 (91%)	0.76	10 (9%) 10 9	41, 80, 109, 114	0
All	All	627/684 (91%)	0.55	41 (6%) 22 22	34, 67, 99, 118	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1241	GLN	5.7
1	F	1216	LEU	5.1
1	F	1217	MET	5.0
1	E	1221	VAL	4.6
1	F	1173	ARG	4.4
1	C	1209	VAL	4.2
1	C	1229	PHE	4.0
1	C	1161	GLY	3.8
1	E	1217	MET	3.6
1	C	1233	LEU	3.4
1	C	1163	VAL	3.4
1	F	1229	PHE	3.2
1	F	1176	ILE	3.2
1	E	1218	GLN	3.2
1	C	1162	ALA	3.0
1	C	1228	ALA	3.0
1	B	1241	GLN	2.8
1	F	1171	LEU	2.6
1	F	1159	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	1232	ILE	2.5
1	B	1190	VAL	2.5
1	C	1179	ILE	2.4
1	E	1209	VAL	2.4
1	E	1203	LEU	2.4
1	A	1209	VAL	2.3
1	E	1163	VAL	2.3
1	F	1175	TRP	2.3
1	C	218	GLY	2.3
1	E	1204	GLU	2.3
1	C	219	SER	2.2
1	A	1168	VAL	2.2
1	F	1206	LEU	2.2
1	A	1206	LEU	2.2
1	C	1206	LEU	2.1
1	F	1172	LEU	2.1
1	E	1165	PHE	2.1
1	B	1210	ILE	2.1
1	C	1194[A]	CYS	2.1
1	C	1208	LEU	2.0
1	A	1203	LEU	2.0
1	D	1240	LEU	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	NI	D	2245	1/1	0.99	0.22	3.76	52,52,52,52	0
3	NI	B	2245	1/1	0.99	0.23	2.13	47,47,47,47	0
3	NI	E	2245	1/1	0.99	0.22	1.48	53,53,53,53	0
3	NI	A	2245	1/1	1.00	0.16	0.62	57,57,57,57	0
2	MG	E	2243	1/1	0.88	0.20	0.46	74,74,74,74	0
3	NI	B	2246	1/1	0.99	0.17	0.03	44,44,44,44	0
2	MG	B	2243	1/1	0.98	0.17	-	59,59,59,59	0
3	NI	F	2244	1/1	0.99	0.19	-	59,59,59,59	0
2	MG	F	2243	1/1	0.95	0.20	-	61,61,61,61	0
3	NI	E	2246	1/1	0.99	0.14	-	37,37,37,37	1
3	NI	F	2245	1/1	0.99	0.16	-	40,40,40,40	1
3	NI	D	2244	1/1	1.00	0.20	-	57,57,57,57	0
2	MG	C	2243	1/1	0.98	0.21	-	63,63,63,63	0
2	MG	D	2243	1/1	0.94	0.27	-	79,79,79,79	0
3	NI	A	2244	1/1	1.00	0.24	-	48,48,48,48	0
2	MG	E	2244	1/1	0.94	0.28	-	64,64,64,64	0
2	MG	B	2244	1/1	0.96	0.27	-	57,57,57,57	0
2	MG	A	2243	1/1	0.97	0.17	-	67,67,67,67	0

6.5 Other polymers (i)

There are no such residues in this entry.