Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:57 AM GMT

PDB ID	:	2VE9
Title	:	XRAY STRUCTURE OF KOPS BOUND GAMMA DOMAIN OF FTSK (P. AERUGINOSA)
Authors	:	Lowe, J.; Allen, M.D.; Sherratt, D.J.
Deposited on	:	2007-10-17
Resolution	:	1.90 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:

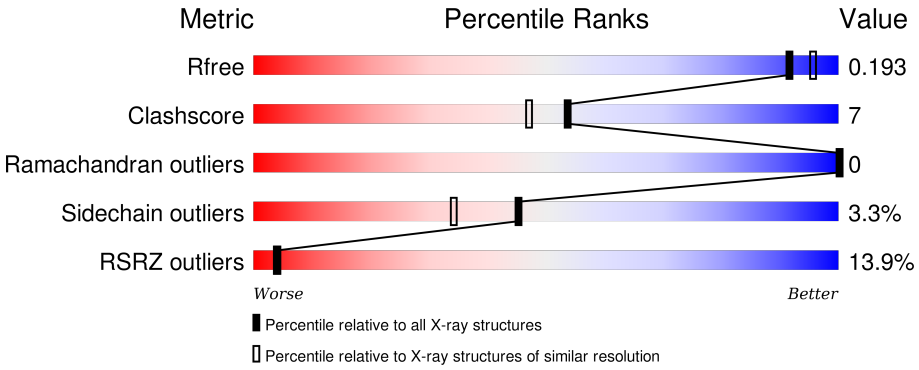
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	73	23% 78% 7% • 14%
1	B	73	14% 59% 23% • 15%
1	C	73	7% 78% 8% 14%
1	D	73	10% 77% 10% 14%
1	E	73	12% 73% 12% • 14%

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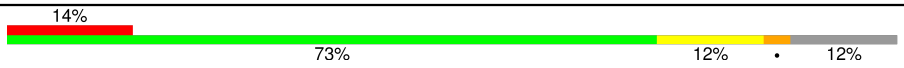
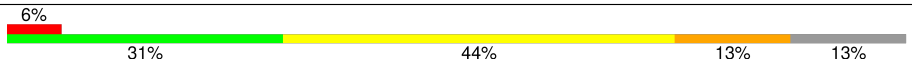
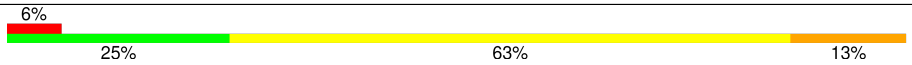
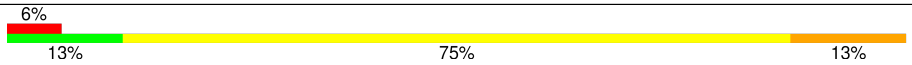
Mol	Chain	Length	Quality of chain
1	F	73	
2	I	16	
2	K	16	
3	J	16	
3	L	16	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4543 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 TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	63	Total	C	N	O	S	0	0	1
			478	293	90	91	4			
1	B	62	Total	C	N	O	S	0	0	1
			470	289	89	88	4			
1	C	63	Total	C	N	O	S	0	0	1
			478	293	90	91	4			
1	D	63	Total	C	N	O	S	0	0	1
			477	294	90	89	4			
1	E	63	Total	C	N	O	S	0	0	1
			477	294	90	89	4			
1	F	64	Total	C	N	O	S	0	0	1
			487	298	91	94	4			

- Molecule 2 is a DNA chain called 5'-D(*AP*CP*CP*AP*GP*GP*GP*CP*AP*GP *GP*GP*CP*GP*AP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	14	Total	C	N	O	P	0	0	0
			290	136	62	79	13			
2	K	14	Total	C	N	O	P	0	0	0
			290	136	62	79	13			

- Molecule 3 is a DNA chain called 5'-D(*GP*TP*CP*GP*CP*CP*CP*TP*GP*CP *CP*CP*TP*GP*GP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	16	Total	C	N	O	P	0	0	0
			320	153	54	98	15			
3	L	16	Total	C	N	O	P	0	0	0
			320	153	54	98	15			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total Mg 1 1	0	0

- Molecule 5 is water.

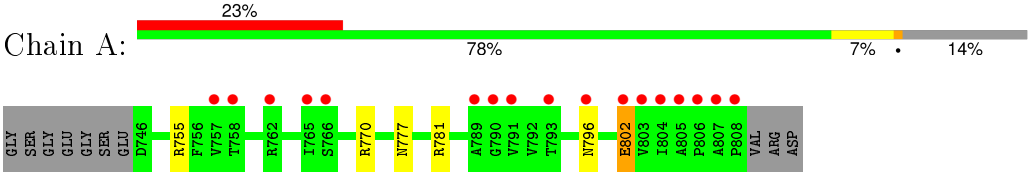
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	37	Total O 37 37	0	0
5	B	43	Total O 43 43	0	0
5	C	41	Total O 41 41	0	0
5	D	54	Total O 54 54	0	0
5	E	44	Total O 44 44	0	0
5	F	46	Total O 46 46	0	0
5	I	46	Total O 46 46	0	0
5	J	52	Total O 52 52	0	0
5	K	49	Total O 49 49	0	0
5	L	43	Total O 43 43	0	0

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.

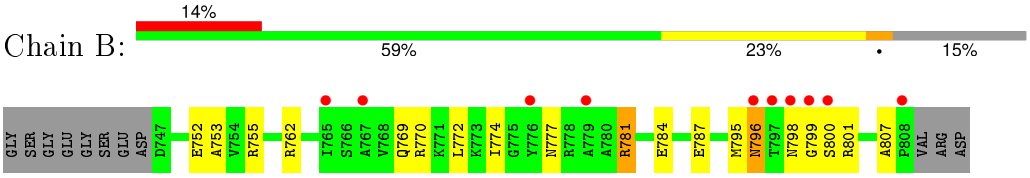
- Molecule 1: DNA TRANSLOCASE FTSK

Chain A:



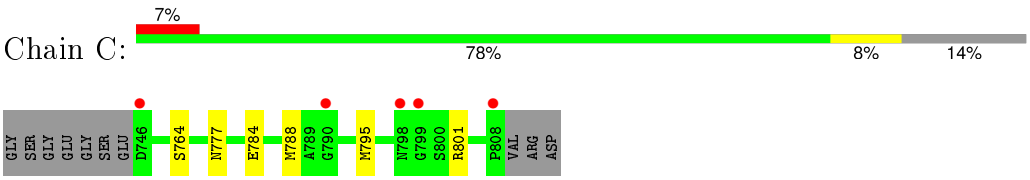
- Molecule 1: DNA TRANSLOCASE FTSK

Chain B:



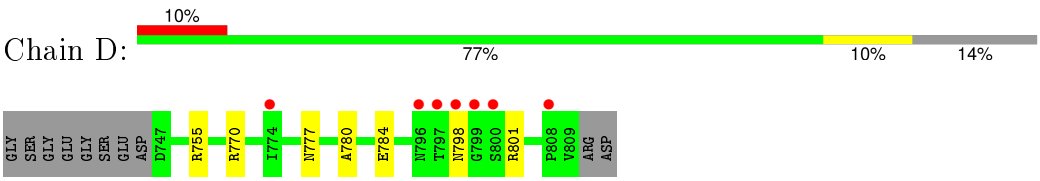
- Molecule 1: DNA TRANSLOCASE FTSK

Chain C:



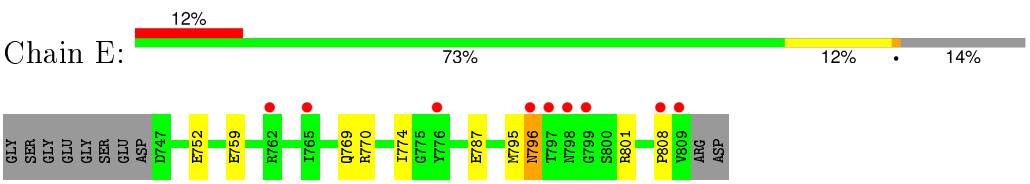
- Molecule 1: DNA TRANSLOCASE FTSK

Chain D:



- Molecule 1: DNA TRANSLOCASE FTSK

Chain E:

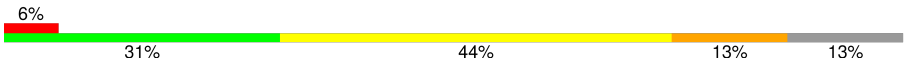


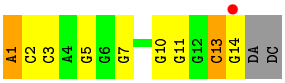
- Molecule 1: DNA TRANSLOCASE FTSK

Chain F:

• Molecule 2: 5'-D(*AP*CP*CP*AP*GP*GP*GP*CP*AP*GP *GP*GP*CP*GP*AP*C)-3
'

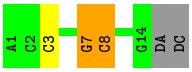
Chain I:





• Molecule 2: 5'-D(*AP*CP*CP*AP*GP*GP*GP*CP*AP*GP *GP*GP*CP*GP*AP*C)-3
'

Chain K:

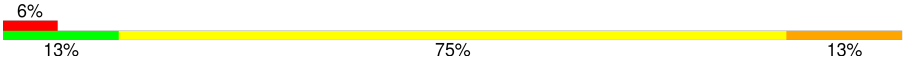


• Molecule 3: 5'-D(*GP*TP*CP*GP*CP*CP*CP*TP*GP*CP *CP*CP*TP*GP*GP*T)-3
'

Chain J:

• Molecule 3: 5'-D(*GP*TP*CP*GP*CP*CP*CP*TP*GP*CP *CP*CP*TP*GP*GP*T)-3
'

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	137.94Å 63.07Å 76.03Å 90.00° 118.76° 90.00°	Depositor
Resolution (Å)	66.67 – 1.90 31.92 – 1.90	Depositor EDS
% Data completeness (in resolution range)	91.4 (66.67-1.90) 90.4 (31.92-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.49 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.249 0.196 , 0.193	Depositor DCC
R_{free} test set	2052 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	33.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 36.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 40886 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4543	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.47% 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: 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	1.26	3/483 (0.6%)	0.74	1/651 (0.2%)
1	B	0.62	1/475 (0.2%)	0.70	1/640 (0.2%)
1	C	0.67	0/483	0.67	0/651
1	D	0.62	0/483	0.70	0/652
1	E	0.60	0/483	0.60	0/652
1	F	0.64	1/492 (0.2%)	0.74	1/663 (0.2%)
2	I	1.03	0/327	1.99	14/504 (2.8%)
2	K	1.10	0/327	1.61	4/504 (0.8%)
3	J	1.14	0/356	1.86	12/547 (2.2%)
3	L	1.13	0/356	1.84	10/547 (1.8%)
All	All	0.89	5/4265 (0.1%)	1.22	43/6011 (0.7%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	GLU	CD-OE2	19.75	1.47	1.25
1	A	802	GLU	CD-OE1	12.43	1.39	1.25
1	A	802	GLU	C-O	6.00	1.34	1.23
1	B	807	ALA	C-N	-5.35	1.24	1.34
1	F	807	ALA	C-N	-5.32	1.24	1.34

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	DA	P-O3'-C3'	10.78	132.63	119.70
3	L	15	DG	O4'-C1'-N9	-9.91	101.06	108.00
1	F	782	MET	CG-SD-CE	-9.77	84.57	100.20
2	I	1	DA	C1'-O4'-C4'	-9.66	100.44	110.10
3	L	13	DT	O4'-C1'-N1	-9.63	101.26	108.00
3	J	14	DG	O4'-C1'-N9	-9.17	101.58	108.00
3	L	2	DT	O4'-C4'-C3'	-9.12	100.53	106.00
2	I	10	DG	O4'-C1'-N9	9.07	114.35	108.00
3	L	6	DC	O4'-C1'-N1	-8.57	102.00	108.00
2	I	5	DG	O4'-C1'-N9	8.47	113.93	108.00
1	A	802	GLU	OE1-CD-OE2	-8.07	113.61	123.30
3	J	15	DG	O3'-P-O5'	-8.04	88.73	104.00
3	L	11	DC	O4'-C1'-N1	-7.55	102.72	108.00
3	J	6	DC	O4'-C1'-N1	-7.37	102.84	108.00
2	I	1	DA	O4'-C4'-C3'	-7.13	101.65	104.50
2	K	7	DG	N9-C1'-C2'	-6.84	99.60	112.60
3	J	16	DT	P-O5'-C5'	6.62	131.49	120.90
2	I	11	DG	O4'-C1'-N9	-6.52	103.43	108.00
2	K	8	DC	O4'-C4'-C3'	-6.46	101.92	104.50
3	J	15	DG	O4'-C1'-N9	6.45	112.51	108.00
3	J	13	DT	O4'-C1'-N1	-6.29	103.60	108.00
2	K	8	DC	O4'-C1'-N1	6.26	112.38	108.00
2	I	2	DC	O5'-P-OP2	-6.22	100.10	105.70
2	I	2	DC	O4'-C1'-N1	-6.20	103.66	108.00
3	J	11	DC	P-O3'-C3'	6.05	126.97	119.70
3	J	7	DC	P-O3'-C3'	5.84	126.71	119.70
2	K	3	DC	P-O3'-C3'	5.81	126.67	119.70
3	L	13	DT	C6-C5-C7	-5.79	119.42	122.90
2	I	7	DG	O4'-C4'-C3'	-5.74	102.20	104.50
3	J	13	DT	P-O5'-C5'	-5.60	111.94	120.90
2	I	3	DC	C5-C6-N1	-5.58	118.21	121.00
1	B	781	ARG	NE-CZ-NH2	-5.55	117.52	120.30
3	J	13	DT	N1-C1'-C2'	5.51	123.06	112.60
2	I	10	DG	C5'-C4'-C3'	-5.48	104.23	114.10
3	J	12	DC	O4'-C1'-N1	-5.39	104.23	108.00
3	J	13	DT	C5'-C4'-O4'	-5.36	99.13	109.30
3	L	16	DT	C4-C5-C7	5.32	122.19	119.00
2	I	13	DC	O4'-C4'-C3'	5.23	109.14	106.00
3	L	16	DT	C6-C5-C7	-5.19	119.78	122.90
3	L	12	DC	P-O3'-C3'	5.14	125.87	119.70
2	I	10	DG	C1'-O4'-C4'	-5.04	105.06	110.10
3	L	5	DC	O4'-C1'-N1	-5.00	104.50	108.00
2	I	13	DC	O4'-C1'-C2'	5.00	109.90	105.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	802	GLU	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	478	0	483	2	1
1	B	470	0	479	12	0
1	C	478	0	483	4	0
1	D	477	0	486	6	1
1	E	477	0	486	10	1
1	F	487	0	489	8	0
2	I	290	0	156	2	0
2	K	290	0	156	1	0
3	J	320	0	182	5	0
3	L	320	0	182	8	1
4	L	1	0	0	0	0
5	A	37	0	0	0	0
5	B	43	0	0	1	0
5	C	41	0	0	1	0
5	D	54	0	0	2	0
5	E	44	0	0	1	0
5	F	46	0	0	4	0
5	I	46	0	0	0	0
5	J	52	0	0	1	0
5	K	49	0	0	0	0
5	L	43	0	0	0	0
All	All	4543	0	3582	50	2

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 7.

All (50) 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:F:781:ARG:NH2	5:F:2033:HOH:O	1.78	1.10
1:C:784:GLU:HG3	5:C:2036:HOH:O	1.74	0.87
1:F:787:GLU:OE1	1:F:801:ARG:NH1	2.09	0.86
1:F:746:ASP:HB3	5:F:2002:HOH:O	1.86	0.74
1:F:778:ARG:O	1:F:782:MET:HG3	1.90	0.71
3:L:8:DT:H2'	3:L:9:DG:C8	2.29	0.67
3:J:12:DC:H2"	3:J:13:DT:H72	1.78	0.66
1:D:780:ALA:O	1:D:784:GLU:HG3	1.97	0.64
1:F:762:ARG:NH2	5:F:2013:HOH:O	2.30	0.64
3:J:8:DT:H2'	3:J:9:DG:C8	2.33	0.64
3:L:2:DT:OP2	3:L:2:DT:H6	1.83	0.60
1:D:777:ASN:HD22	1:E:770:ARG:HH11	1.50	0.60
1:B:770:ARG:HH11	1:C:777:ASN:HD22	1.51	0.57
1:B:770:ARG:HH11	1:C:777:ASN:ND2	2.03	0.55
1:E:769:GLN:HG3	1:E:774:ILE:O	2.06	0.55
1:E:787:GLU:OE1	1:E:801:ARG:NH1	2.32	0.54
1:A:777:ASN:O	1:A:781:ARG:HD3	2.08	0.53
1:B:752:GLU:HG2	1:B:755:ARG:HH12	1.73	0.52
2:I:13:DC:H2'	2:I:14:DG:C8	2.44	0.52
1:D:784:GLU:HG3	5:D:2036:HOH:O	2.10	0.51
1:B:787:GLU:OE1	1:B:801:ARG:NH1	2.43	0.50
1:E:752:GLU:HG2	5:E:2008:HOH:O	2.11	0.50
1:D:777:ASN:ND2	1:E:770:ARG:HH11	2.09	0.50
1:F:762:ARG:NH1	3:L:8:DT:OP1	2.44	0.50
2:I:1:DA:N1	3:L:15:DG:N7	2.59	0.49
2:K:7:DG:H2"	2:K:8:DC:O5'	2.11	0.49
1:D:784:GLU:CG	5:D:2036:HOH:O	2.59	0.49
1:F:750:TYR:HA	1:F:782:MET:HE2	1.95	0.48
3:L:2:DT:H2'	3:L:3:DC:C6	2.50	0.47
3:L:3:DC:H2'	3:L:4:DG:C8	2.50	0.47
3:J:3:DC:H2'	3:J:4:DG:C8	2.49	0.47
1:E:759:GLU:HG3	1:E:808:PRO:HD2	1.96	0.47
1:B:769:GLN:HG3	1:B:774:ILE:O	2.15	0.47
1:A:770:ARG:NH2	1:B:784:GLU:OE2	2.48	0.47
1:B:753:ALA:HB2	1:B:772:LEU:HD11	1.96	0.46
1:E:796:ASN:ND2	1:E:796:ASN:H	2.13	0.46
1:E:759:GLU:HG3	1:E:808:PRO:CD	2.46	0.46
1:E:759:GLU:CG	1:E:808:PRO:HD2	2.45	0.46
3:J:13:DT:H6	3:J:13:DT:H5"	1.81	0.46
1:B:796:ASN:ND2	1:B:800:SER:O	2.49	0.46
1:B:795:MET:HE3	1:B:799:GLY:HA2	1.98	0.46
3:L:1:DG:H8	3:L:1:DG:O5'	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:777:ASN:HD22	1:B:777:ASN:HA	1.68	0.43
1:B:781:ARG:NH2	5:B:2032:HOH:O	2.53	0.42
1:B:762:ARG:HD3	5:J:2049:HOH:O	2.19	0.42
1:F:770:ARG:HD3	5:F:2013:HOH:O	2.20	0.41
1:D:770:ARG:NH1	3:L:3:DC:OP2	2.46	0.41
3:J:13:DT:C6	3:J:13:DT:H5"	2.56	0.41
1:E:787:GLU:CD	1:E:801:ARG:HH12	2.19	0.41
1:C:795:MET:HG3	1:C:801:ARG:NH2	2.36	0.40

All (2) 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:755:ARG:NH2	1:E:795:MET:O[2_656]	1.98	0.22
1:D:755:ARG:NH2	3:L:10:DC:OP1[4_545]	2.02	0.18

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	61/73 (84%)	60 (98%)	1 (2%)	0	100	100
1	B	60/73 (82%)	60 (100%)	0	0	100	100
1	C	61/73 (84%)	61 (100%)	0	0	100	100
1	D	61/73 (84%)	61 (100%)	0	0	100	100
1	E	61/73 (84%)	61 (100%)	0	0	100	100
1	F	62/73 (85%)	62 (100%)	0	0	100	100
All	All	366/438 (84%)	365 (100%)	1 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	50/58 (86%)	49 (98%)	1 (2%)	63	57
1	B	49/58 (84%)	47 (96%)	2 (4%)	37	25
1	C	50/58 (86%)	48 (96%)	2 (4%)	38	26
1	D	50/58 (86%)	48 (96%)	2 (4%)	38	26
1	E	50/58 (86%)	49 (98%)	1 (2%)	63	57
1	F	51/58 (88%)	49 (96%)	2 (4%)	39	27
All	All	300/348 (86%)	290 (97%)	10 (3%)	45	34

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	ASN
1	B	796	ASN
1	B	798	ASN
1	C	764	SER
1	C	788	MET
1	D	798	ASN
1	D	801	ARG
1	E	796	ASN
1	F	746	ASP
1	F	796	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	ASN
1	A	796	ASN
1	B	777	ASN
1	B	796	ASN
1	B	798	ASN
1	C	777	ASN
1	D	777	ASN

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Mol	Chain	Res	Type
1	E	777	ASN
1	E	796	ASN
1	F	796	ASN

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 1 ligands modelled in this entry, 1 is 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	63/73 (86%)	1.48	17 (26%) 1 1	36, 39, 43, 48	0
1	B	62/73 (84%)	1.19	10 (16%) 3 3	32, 40, 51, 54	0
1	C	63/73 (86%)	0.77	5 (7%) 15 17	32, 39, 50, 52	0
1	D	63/73 (86%)	0.72	7 (11%) 7 8	33, 39, 51, 56	0
1	E	63/73 (86%)	1.16	9 (14%) 4 4	34, 40, 53, 55	0
1	F	64/73 (87%)	1.01	10 (15%) 3 3	34, 39, 47, 49	0
2	I	14/16 (87%)	0.28	1 (7%) 19 21	36, 38, 44, 56	0
2	K	14/16 (87%)	0.40	0 100 100	36, 39, 43, 51	0
3	J	16/16 (100%)	0.23	1 (6%) 23 26	37, 38, 46, 47	0
3	L	16/16 (100%)	0.37	1 (6%) 23 26	36, 38, 43, 49	0
All	All	438/502 (87%)	0.95	61 (13%) 4 4	32, 39, 51, 56	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	808	PRO	13.8
1	B	798	ASN	5.9
1	B	797	THR	5.8
1	C	799	GLY	5.7
1	E	809	VAL	5.3
1	D	808	PRO	5.0
1	F	808	PRO	5.0
1	E	799	GLY	4.8
1	B	796	ASN	4.7
1	A	807	ALA	4.5
1	A	803	VAL	4.2
1	D	800	SER	3.8
1	B	808	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	805	ALA	3.3
1	E	765	ILE	3.3
1	E	796	ASN	3.3
1	E	808	PRO	3.2
1	F	765	ILE	3.1
1	B	776	TYR	3.1
1	D	799	GLY	3.0
1	A	802	GLU	3.0
1	E	797	THR	2.9
1	A	793	THR	2.9
1	F	807	ALA	2.8
2	I	14	DG	2.8
1	C	746	ASP	2.7
1	B	800	SER	2.6
1	F	805	ALA	2.6
1	E	798	ASN	2.6
1	A	804	ILE	2.6
1	F	803	VAL	2.6
1	F	776	TYR	2.6
1	C	808	PRO	2.5
3	L	1	DG	2.5
1	A	806	PRO	2.5
1	B	765	ILE	2.5
1	D	798	ASN	2.4
1	C	790	GLY	2.4
1	B	779	ALA	2.4
1	F	766	SER	2.4
1	C	798	ASN	2.4
1	A	762	ARG	2.3
1	B	767	ALA	2.3
1	A	757	VAL	2.3
3	J	1	DG	2.3
1	D	796	ASN	2.3
1	A	765	ILE	2.3
1	F	772	LEU	2.2
1	A	789	ALA	2.2
1	A	758	THR	2.2
1	A	791	VAL	2.2
1	A	790	GLY	2.2
1	E	776	TYR	2.2
1	A	766	SER	2.1
1	F	798	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	774	ILE	2.1
1	D	797	THR	2.1
1	B	799	GLY	2.1
1	E	762	ARG	2.0
1	A	796	ASN	2.0
1	F	767	ALA	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
4	MG	L	1017	1/1	0.99	0.15	-	26,26,26,26	0

6.5 Other polymers (i)

There are no such residues in this entry.