Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 03:16 AM EST

PDB ID	:	4RIA
Title	:	FAN1 Nuclease bound to 5' phosphorylated nicked DNA
Authors	:	Pavletich, N.P.; Wang, R.
Deposited on	:	2014-10-05
Resolution	:	3.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

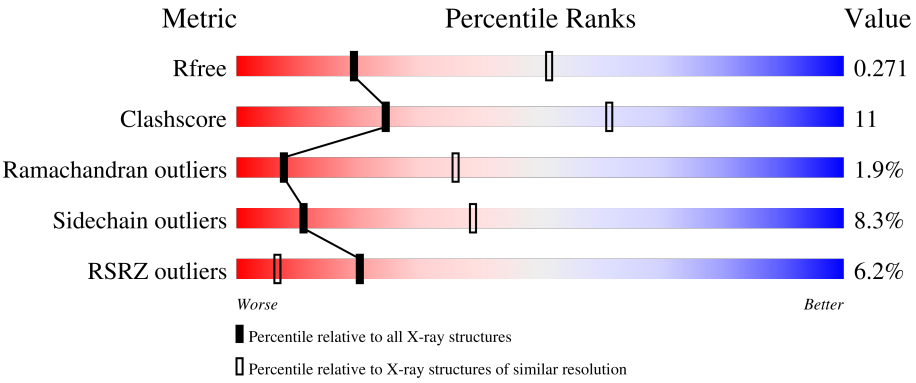
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	651	6% 69% 21% · 6%
1	B	651	6% 68% 23% · 6%
2	F	10	50% 50%
2	L	10	50% 50%
3	I	9	67% 33%

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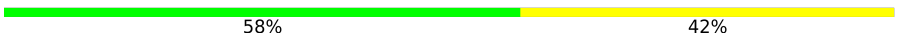
Mol	Chain	Length	Quality of chain
3	K	9	
4	G	14	
4	J	14	
5	E	12	
5	H	12	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11410 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 Fanconi-associated nuclease 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	613	Total	C	N	O	S	0	0	0
			4927	3136	877	887	27			
1	B	613	Total	C	N	O	S	0	0	0
			4927	3136	877	887	27			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	358	GLY	-	expression tag	UNP Q9Y2M0
A	359	ALA	-	expression tag	UNP Q9Y2M0
A	360	HIS	-	expression tag	UNP Q9Y2M0
A	361	MET	-	expression tag	UNP Q9Y2M0
A	362	THR	-	expression tag	UNP Q9Y2M0
A	363	ARG	-	expression tag	UNP Q9Y2M0
A	364	ASN	-	expression tag	UNP Q9Y2M0
A	365	GLY	-	expression tag	UNP Q9Y2M0
A	366	PRO	-	expression tag	UNP Q9Y2M0
A	367	GLY	-	expression tag	UNP Q9Y2M0
A	368	GLN	-	expression tag	UNP Q9Y2M0
A	369	THR	-	expression tag	UNP Q9Y2M0
A	487	ALA	VAL	engineered mutation	UNP Q9Y2M0
A	?	-	CYS	deletion	UNP Q9Y2M0
A	?	-	THR	deletion	UNP Q9Y2M0
A	?	-	TRP	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	ASN	deletion	UNP Q9Y2M0
A	?	-	LYS	deletion	UNP Q9Y2M0
A	?	-	PRO	deletion	UNP Q9Y2M0
A	?	-	GLY	deletion	UNP Q9Y2M0
B	358	GLY	-	expression tag	UNP Q9Y2M0
B	359	ALA	-	expression tag	UNP Q9Y2M0
B	360	HIS	-	expression tag	UNP Q9Y2M0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	361	MET	-	expression tag	UNP Q9Y2M0
B	362	THR	-	expression tag	UNP Q9Y2M0
B	363	ARG	-	expression tag	UNP Q9Y2M0
B	364	ASN	-	expression tag	UNP Q9Y2M0
B	365	GLY	-	expression tag	UNP Q9Y2M0
B	366	PRO	-	expression tag	UNP Q9Y2M0
B	367	GLY	-	expression tag	UNP Q9Y2M0
B	368	GLN	-	expression tag	UNP Q9Y2M0
B	369	THR	-	expression tag	UNP Q9Y2M0
B	487	ALA	VAL	engineered mutation	UNP Q9Y2M0
B	?	-	CYS	deletion	UNP Q9Y2M0
B	?	-	THR	deletion	UNP Q9Y2M0
B	?	-	TRP	deletion	UNP Q9Y2M0
B	?	-	GLY	deletion	UNP Q9Y2M0
B	?	-	LYS	deletion	UNP Q9Y2M0
B	?	-	ASN	deletion	UNP Q9Y2M0
B	?	-	LYS	deletion	UNP Q9Y2M0
B	?	-	PRO	deletion	UNP Q9Y2M0
B	?	-	GLY	deletion	UNP Q9Y2M0

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*AP*CP*GP*CP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	10	Total	C	N	O	P	0	0	0
			202	95	37	60	10			
2	L	10	Total	C	N	O	P	0	0	0
			202	95	37	60	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	9	Total	C	N	O	P	0	0	0
			180	86	31	54	9			
3	I	9	Total	C	N	O	P	0	0	0
			180	86	31	54	9			

- Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*G*AP*GP*GP*CP*GP*TP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	7	Total	C	N	O	P	0	0	0
			145	69	30	40	6			
4	J	7	Total	C	N	O	P	0	0	0
			145	69	30	40	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	12	Total	C	N	O	P	0	0	0
			250	118	47	73	12			
5	H	12	Total	C	N	O	P	0	0	0
			250	118	47	73	12			

- Molecule 6 is BARIUM ION (three-letter code: BA) (formula: Ba).

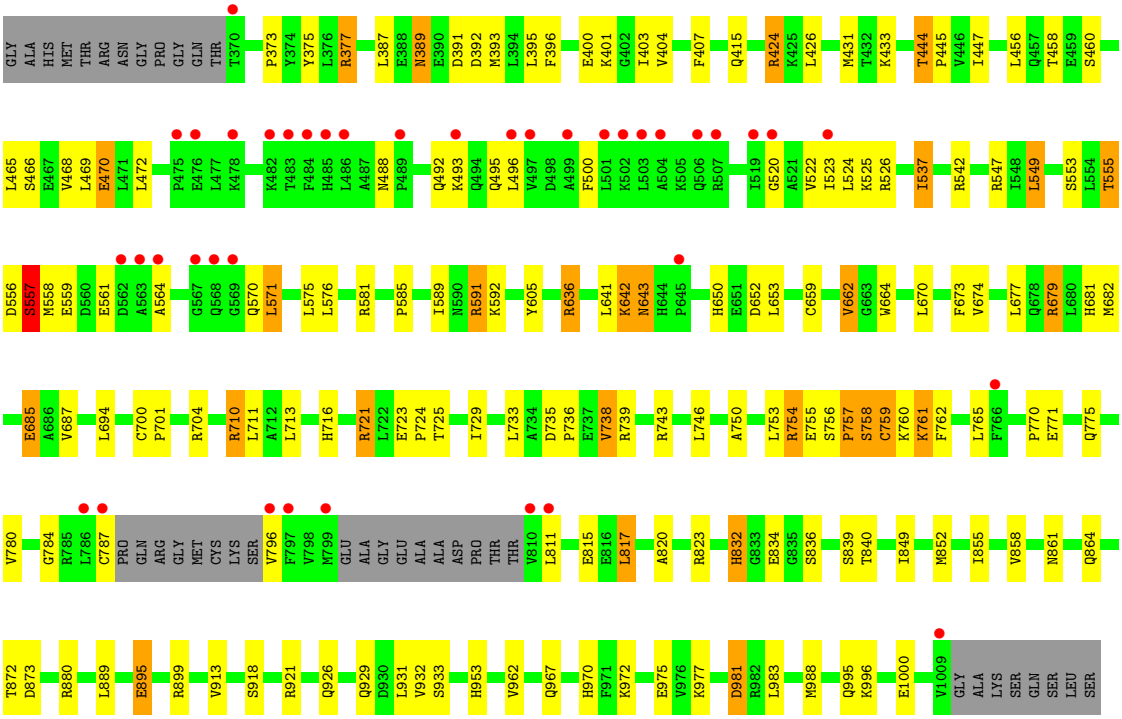
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Ba	0	0
			1	1		
6	B	1	Total	Ba	0	0
			1	1		

3 Residue-property plots (i)

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

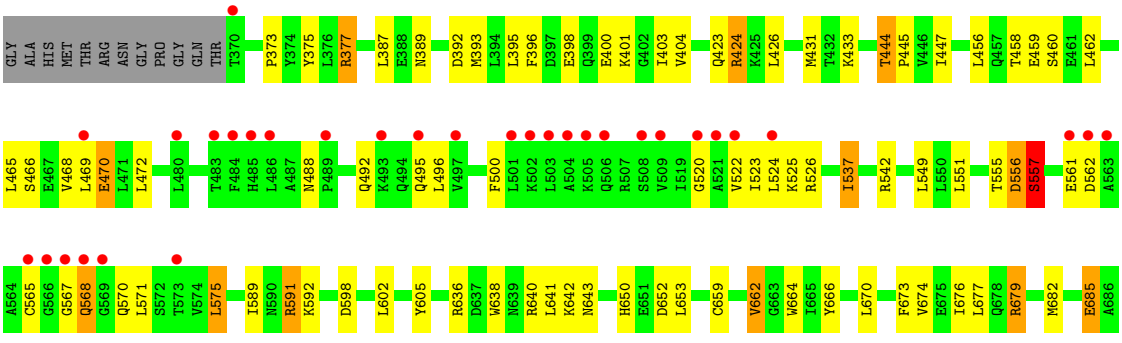
• Molecule 1: Fanconi-associated nuclease 1

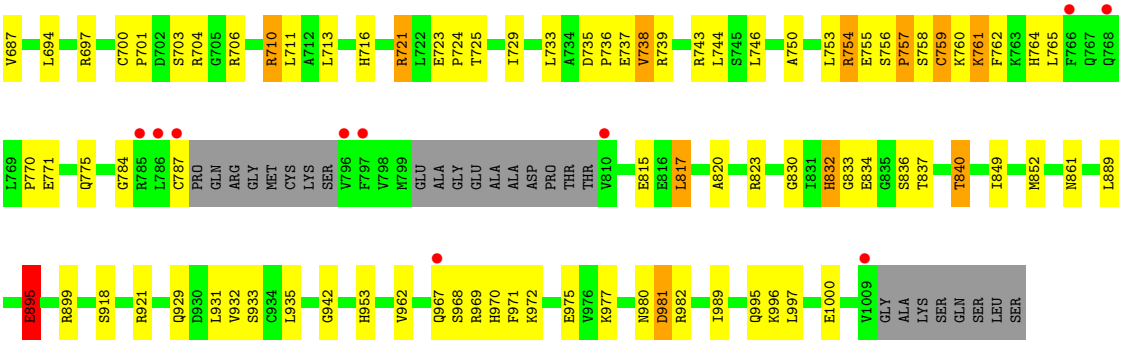
Chain A:



• Molecule 1: Fanconi-associated nuclease 1

Chain B:



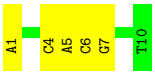


• Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*AP*CP*GP*CP*CP*T)-3')

Chain F:

• Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*AP*CP*GP*CP*CP*T)-3')

Chain L:

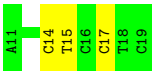


• Molecule 3: DNA (5'-D(P*AP*GP*AP*CP*TP*CP*CP*TP*C)-3')

Chain K:

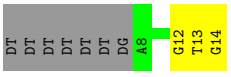
• Molecule 3: DNA (5'-D(P*AP*GP*AP*CP*TP*CP*CP*TP*C)-3')

Chain I:



• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*G*AP*GP*GP*CP*GP*TP*G)-3')

Chain G:

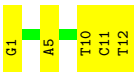


• Molecule 4: DNA (5'-D(*TP*TP*TP*TP*TP*TP*G*AP*GP*GP*CP*GP*TP*G)-3')

Chain J:

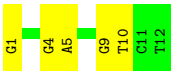
• Molecule 5: DNA (5'-D(P*GP*CP*TP*GP*AP*GP*GP*AP*GP*TP*CP*T)-3')

Chain E:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	87.81Å 100.32Å 212.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 48.82 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.6 (40.00-3.00) 93.3 (48.82-2.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.224 , 0.267 0.224 , 0.271	Depositor DCC
R_{free} test set	1512 reflections (4.02%)	wwPDB-VP
Wilson B-factor (Å^2)	55.4	Xtriage
Anisotropy	0.514	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11410	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.72 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.3913e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: BA

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	0.44	0/5029	0.65	0/6799
1	B	0.46	0/5029	0.65	0/6799
2	F	0.81	1/225 (0.4%)	0.89	0/342
2	L	0.78	1/225 (0.4%)	0.87	0/342
3	I	0.37	0/200	0.82	0/305
3	K	0.31	0/200	0.82	0/305
4	G	0.42	0/163	0.64	0/251
4	J	0.41	0/163	0.70	0/251
5	E	0.30	0/280	0.79	0/431
5	H	0.32	0/280	0.77	1/431 (0.2%)
All	All	0.46	2/11794 (0.0%)	0.68	1/16256 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1	DA	OP3-P	-10.59	1.48	1.61
2	L	1	DA	OP3-P	-10.04	1.49	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	9	DG	C1'-O4'-C4'	-5.13	104.97	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4927	0	4960	108	0
1	B	4927	0	4960	114	0
2	F	202	0	112	2	0
2	L	202	0	112	4	0
3	I	180	0	102	2	0
3	K	180	0	102	2	0
4	G	145	0	80	7	0
4	J	145	0	80	6	0
5	E	250	0	136	8	0
5	H	250	0	136	5	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	11410	0	10780	241	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 11.

All (241) 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:389:ASN:HB3	1:A:591:ARG:HH21	1.07	1.09
1:A:682:MET:HB3	1:A:685:GLU:HG3	1.34	1.09
1:B:682:MET:HB3	1:B:685:GLU:HG3	1.39	1.05
1:B:836:SER:O	1:B:840:THR:HG23	1.66	0.95
1:A:836:SER:O	1:A:840:THR:HG23	1.67	0.93
1:A:389:ASN:HB3	1:A:591:ARG:NH2	1.84	0.93
4:G:14:DG:O3'	5:E:1:DG:P	2.28	0.92
1:A:555:THR:HG21	1:A:861:ASN:ND2	1.90	0.87
1:A:377:ARG:HH11	1:A:377:ARG:HB3	1.42	0.83
1:A:555:THR:HG21	1:A:861:ASN:HD21	1.46	0.80
1:B:377:ARG:HH11	1:B:377:ARG:HB3	1.46	0.80
1:B:551:LEU:HD21	1:B:602:LEU:HD13	1.67	0.77
1:B:520:GLY:HA2	1:B:523:ILE:HD12	1.66	0.76
1:A:520:GLY:HA2	1:A:523:ILE:HD12	1.68	0.76
1:A:549:LEU:HD23	1:A:570:GLN:HA	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:GLN:HB2	1:A:495:GLN:HG2	1.70	0.73
1:A:557:SER:O	1:A:559:GLU:N	2.20	0.73
1:A:738:VAL:O	1:A:743:ARG:NH1	2.24	0.71
1:B:840:THR:CG2	1:B:918:SER:H	2.06	0.69
1:A:729:ILE:HG21	1:A:750:ALA:HB2	1.75	0.69
1:B:423:GLN:HE22	1:B:570:GLN:HG2	1.58	0.68
1:B:738:VAL:O	1:B:743:ARG:NH1	2.27	0.68
4:J:14:DG:O3'	5:H:1:DG:P	2.52	0.67
1:B:729:ILE:HG21	1:B:750:ALA:HB2	1.75	0.67
1:B:982:ARG:NH2	4:J:12:DG:N7	2.40	0.66
1:B:492:GLN:HB2	1:B:495:GLN:HG2	1.77	0.65
4:G:13:DT:H2"	4:G:14:DG:C8	2.32	0.65
1:B:555:THR:HG21	1:B:861:ASN:HD21	1.62	0.65
1:A:642:LYS:O	1:A:643:ASN:HB2	1.98	0.64
1:A:377:ARG:HH11	1:A:377:ARG:CB	2.11	0.64
1:A:377:ARG:HB3	1:A:377:ARG:NH1	2.13	0.64
1:B:567:GLY:O	1:B:568:GLN:HB2	1.98	0.63
1:A:537:ILE:HG21	1:A:542:ARG:HH11	1.64	0.63
1:A:571:LEU:HD13	1:A:576:LEU:HB2	1.81	0.63
1:A:549:LEU:CD2	1:A:570:GLN:HA	2.29	0.63
1:B:759:CYS:O	1:B:762:PHE:CD1	2.52	0.63
3:K:14:DC:H2"	3:K:15:DT:OP2	1.99	0.62
1:A:659:CYS:HA	1:A:664:TRP:CD2	2.34	0.62
1:A:849:ILE:HG23	1:A:852:MET:CE	2.29	0.62
1:B:377:ARG:HH11	1:B:377:ARG:CB	2.11	0.62
1:A:426:LEU:HD13	1:A:537:ILE:HG22	1.81	0.62
1:B:423:GLN:NE2	1:B:570:GLN:HG2	2.15	0.62
3:I:14:DC:H2"	3:I:15:DT:OP2	2.00	0.61
1:B:759:CYS:O	1:B:762:PHE:HD1	1.84	0.61
1:B:400:GLU:HA	1:B:403:ILE:HD12	1.82	0.61
1:B:377:ARG:HB3	1:B:377:ARG:NH1	2.14	0.60
1:B:642:LYS:O	1:B:643:ASN:HB2	2.00	0.60
1:A:723:GLU:HB3	1:A:724:PRO:HD3	1.83	0.60
1:B:931:LEU:HD11	1:B:962:VAL:HG11	1.84	0.60
1:A:757:PRO:HG2	1:A:758:SER:H	1.67	0.60
1:A:840:THR:CG2	1:A:918:SER:H	2.15	0.59
1:A:759:CYS:O	1:A:762:PHE:CD1	2.56	0.59
1:B:784:GLY:HA3	1:B:817:LEU:HD21	1.83	0.59
4:J:13:DT:H2"	4:J:14:DG:C8	2.37	0.59
1:A:972:LYS:HG3	1:A:1000:GLU:HB3	1.85	0.59
1:B:389:ASN:HB3	1:B:591:ARG:HH21	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:ARG:HD3	3:I:17:DC:H3'	1.84	0.58
1:B:659:CYS:HA	1:B:664:TRP:CD2	2.38	0.58
1:A:784:GLY:HA3	1:A:817:LEU:HD21	1.85	0.58
1:A:759:CYS:O	1:A:761:LYS:N	2.37	0.57
1:A:759:CYS:O	1:A:762:PHE:HD1	1.85	0.57
1:A:679:ARG:CZ	4:G:14:DG:H3'	2.35	0.57
1:B:775:GLN:HE22	1:B:996:LYS:HG3	1.69	0.56
1:A:492:GLN:CD	5:E:12:DT:H3'	2.25	0.56
1:B:972:LYS:HG3	1:B:1000:GLU:HB3	1.86	0.56
1:A:493:LYS:HE3	5:E:11:DC:OP1	2.06	0.56
1:A:738:VAL:HG23	1:A:743:ARG:HB2	1.87	0.56
1:B:426:LEU:HD13	1:B:537:ILE:HG22	1.88	0.55
1:B:840:THR:HG21	1:B:918:SER:H	1.70	0.55
1:A:775:GLN:HE22	1:A:996:LYS:HG3	1.71	0.55
1:B:739:ARG:HG3	1:B:953:HIS:CD2	2.41	0.55
1:B:700:CYS:N	1:B:701:PRO:HD3	2.21	0.55
1:A:400:GLU:HA	1:A:403:ILE:HD12	1.88	0.55
1:A:555:THR:CG2	1:A:861:ASN:HD21	2.16	0.55
1:B:716:HIS:HB2	1:B:725:THR:HG21	1.87	0.55
1:A:682:MET:HB3	1:A:685:GLU:CG	2.23	0.54
1:B:555:THR:HG21	1:B:861:ASN:ND2	2.21	0.54
1:B:468:VAL:HG21	1:B:524:LEU:HD12	1.90	0.54
1:B:713:LEU:HD23	1:B:713:LEU:C	2.28	0.54
1:A:571:LEU:HD12	1:A:571:LEU:H	1.73	0.53
1:A:895:GLU:O	1:A:899:ARG:HG3	2.08	0.53
1:B:980:ASN:HD21	2:L:5:DA:H2'	1.71	0.53
1:A:677:LEU:HD13	1:A:685:GLU:HB2	1.90	0.53
1:A:468:VAL:HG21	1:A:524:LEU:HD12	1.91	0.52
1:B:444:THR:N	1:B:445:PRO:HD2	2.24	0.52
1:B:551:LEU:HD21	1:B:602:LEU:CD1	2.38	0.52
1:B:918:SER:HB2	1:B:921:ARG:HB2	1.91	0.52
4:J:12:DG:H2'	4:J:13:DT:C7	2.39	0.52
1:B:738:VAL:HG23	1:B:743:ARG:HB2	1.92	0.52
1:B:759:CYS:O	1:B:761:LYS:N	2.42	0.52
1:A:700:CYS:N	1:A:701:PRO:HD3	2.25	0.52
1:B:723:GLU:HB3	1:B:724:PRO:HD3	1.92	0.51
1:A:750:ALA:HB1	1:A:765:LEU:HD22	1.93	0.51
1:A:393:MET:HA	1:A:393:MET:HE3	1.93	0.51
4:G:12:DG:H2'	4:G:13:DT:C7	2.41	0.51
1:A:716:HIS:HB2	1:A:725:THR:HG21	1.92	0.51
1:B:393:MET:CE	1:B:393:MET:HA	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:977:LYS:HD2	1:B:981:ASP:O	2.11	0.50
1:A:444:THR:N	1:A:445:PRO:HD2	2.26	0.50
1:B:833:GLY:HA3	1:B:837:THR:OG1	2.12	0.50
1:A:733:LEU:O	1:A:743:ARG:NH2	2.44	0.50
1:B:389:ASN:HD22	1:B:591:ARG:NH2	2.08	0.50
1:B:849:ILE:HG23	1:B:852:MET:CE	2.41	0.50
4:G:14:DG:O3'	5:E:1:DG:H5'	2.12	0.50
1:B:389:ASN:ND2	1:B:591:ARG:NH2	2.60	0.50
1:B:468:VAL:HG21	1:B:524:LEU:CD1	2.42	0.50
1:A:389:ASN:CB	1:A:591:ARG:NH2	2.67	0.49
1:A:975:GLU:OE2	1:A:977:LYS:NZ	2.35	0.49
1:A:753:LEU:O	1:A:756:SER:HB3	2.13	0.49
1:B:980:ASN:ND2	2:L:5:DA:H2'	2.28	0.49
1:B:392:ASP:HA	1:B:395:LEU:HD12	1.94	0.49
1:B:571:LEU:HD23	1:B:575:LEU:HB3	1.95	0.49
1:B:968:SER:O	1:B:969:ARG:HB2	2.13	0.49
1:B:393:MET:HA	1:B:393:MET:HE3	1.94	0.49
1:B:836:SER:OG	1:B:921:ARG:HD2	2.12	0.49
1:A:526:ARG:HB2	1:A:526:ARG:CZ	2.42	0.49
1:B:496:LEU:O	1:B:500:PHE:HD2	1.96	0.48
1:B:396:PHE:O	1:B:401:LYS:HE3	2.14	0.48
1:B:975:GLU:OE2	1:B:977:LYS:NZ	2.32	0.48
1:B:469:LEU:HA	1:B:472:LEU:HD12	1.96	0.48
1:A:585:PRO:HD3	1:A:913:VAL:O	2.13	0.47
2:F:4:DC:H2"	2:F:5:DA:C8	2.49	0.47
1:A:685:GLU:H	1:A:685:GLU:HG2	1.39	0.47
1:B:466:SER:O	1:B:470:GLU:HB2	2.14	0.47
1:B:605:TYR:HA	1:B:662:VAL:HG13	1.96	0.47
1:A:796:VAL:HG11	1:A:811:LEU:HD13	1.96	0.47
1:A:820:ALA:HA	1:A:823:ARG:NH1	2.30	0.47
1:B:677:LEU:HD13	1:B:685:GLU:HB2	1.97	0.47
1:B:687:VAL:HG13	1:B:711:LEU:HD11	1.96	0.47
1:A:836:SER:HA	1:A:839:SER:HB3	1.96	0.47
1:A:840:THR:HG21	1:A:918:SER:H	1.80	0.47
1:A:496:LEU:O	1:A:500:PHE:HD2	1.98	0.47
1:A:468:VAL:HG21	1:A:524:LEU:CD1	2.44	0.47
1:A:659:CYS:HA	1:A:664:TRP:CG	2.49	0.47
1:B:694:LEU:O	1:B:704:ARG:NH2	2.48	0.47
1:A:880:ARG:HG3	1:A:880:ARG:HH11	1.80	0.47
1:A:373:PRO:HB2	1:A:375:TYR:CE1	2.50	0.47
1:A:377:ARG:HH21	1:A:581:ARG:NH1	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:14:DG:O3'	5:H:1:DG:H5'	2.14	0.46
1:A:687:VAL:HG13	1:A:711:LEU:HD11	1.96	0.46
1:B:556:ASP:HB3	1:B:557:SER:H	1.49	0.46
1:B:840:THR:HG22	1:B:918:SER:H	1.80	0.46
1:A:977:LYS:HD2	1:A:981:ASP:O	2.15	0.46
1:B:750:ALA:HB1	1:B:765:LEU:HD22	1.97	0.46
1:A:739:ARG:HG3	1:A:953:HIS:CD2	2.50	0.46
1:A:855:ILE:O	1:A:858:VAL:HG22	2.16	0.46
1:B:526:ARG:HB2	1:B:526:ARG:CZ	2.44	0.46
1:B:721:ARG:HH21	1:B:723:GLU:HB3	1.80	0.46
1:B:849:ILE:HA	1:B:852:MET:HE2	1.98	0.46
1:A:424:ARG:HD3	3:K:17:DC:H3'	1.97	0.46
1:B:895:GLU:O	1:B:899:ARG:HG3	2.16	0.46
1:A:899:ARG:NH1	1:A:933:SER:OG	2.48	0.46
1:B:682:MET:HB3	1:B:685:GLU:CG	2.28	0.46
1:B:757:PRO:HG2	1:B:758:SER:H	1.80	0.46
1:A:983:LEU:HB3	1:A:988:MET:CE	2.46	0.46
1:A:433:LYS:NZ	5:E:10:DT:OP1	2.49	0.46
1:A:710:ARG:HD2	1:A:710:ARG:HA	1.55	0.46
1:A:735:ASP:OD1	1:A:736:PRO:HD2	2.16	0.46
1:B:735:ASP:OD1	1:B:736:PRO:HD2	2.16	0.46
1:B:899:ARG:NH1	1:B:933:SER:OG	2.49	0.46
1:B:673:PHE:HA	1:B:676:ILE:HD12	1.96	0.45
1:A:393:MET:HA	1:A:393:MET:CE	2.42	0.45
1:B:710:ARG:HD2	1:B:710:ARG:HA	1.56	0.45
1:B:459:GLU:O	1:B:462:LEU:HB3	2.17	0.45
1:A:872:THR:HG22	1:A:873:ASP:N	2.32	0.45
1:A:983:LEU:HB3	1:A:988:MET:HE3	1.99	0.45
1:B:753:LEU:O	1:B:756:SER:HB3	2.16	0.45
1:A:723:GLU:CB	1:A:724:PRO:HD3	2.47	0.44
1:A:466:SER:O	1:A:470:GLU:HB2	2.16	0.44
1:B:716:HIS:HB2	1:B:725:THR:CG2	2.48	0.44
1:B:830:GLY:HA2	1:B:962:VAL:O	2.17	0.44
1:A:469:LEU:HA	1:A:472:LEU:HD12	2.00	0.44
1:B:729:ILE:HA	1:B:746:LEU:HD22	2.00	0.44
2:L:6:DC:H2"	2:L:7:DG:OP2	2.18	0.44
5:E:5:DA:H8	5:E:5:DA:OP2	2.01	0.44
1:A:387:LEU:HD11	1:A:404:VAL:HG11	1.99	0.44
1:A:493:LYS:N	5:E:12:DT:OP2	2.48	0.44
1:A:605:TYR:HA	1:A:662:VAL:HG13	1.99	0.44
1:A:931:LEU:HD11	1:A:962:VAL:HG11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:LEU:C	1:A:713:LEU:HD23	2.38	0.44
1:B:496:LEU:O	1:B:500:PHE:CD2	2.70	0.44
1:A:391:ASP:HB2	1:A:591:ARG:NH2	2.33	0.43
1:A:704:ARG:HD3	1:A:735:ASP:OD2	2.18	0.43
1:B:935:LEU:HA	1:B:971:PHE:CE1	2.54	0.43
2:F:6:DC:H2"	2:F:7:DG:OP2	2.17	0.43
1:B:744:LEU:HB2	1:B:989:ILE:HD11	1.99	0.43
1:A:396:PHE:O	1:A:401:LYS:HE3	2.19	0.43
1:A:918:SER:HB2	1:A:921:ARG:HB2	1.99	0.43
1:B:929:GLN:HA	1:B:932:VAL:HG22	2.00	0.43
2:L:4:DC:H2"	2:L:5:DA:C8	2.53	0.43
4:J:12:DG:H2'	4:J:13:DT:H72	2.01	0.43
1:B:733:LEU:O	1:B:743:ARG:NH2	2.52	0.43
1:A:447:ILE:HG23	1:A:456:LEU:HD23	2.01	0.43
1:B:685:GLU:H	1:B:685:GLU:HG2	1.41	0.43
1:B:373:PRO:HB2	1:B:375:TYR:CE1	2.54	0.42
1:A:520:GLY:HA2	1:A:523:ILE:CD1	2.44	0.42
1:B:670:LEU:O	1:B:673:PHE:HB3	2.19	0.42
1:A:670:LEU:O	1:A:673:PHE:HB3	2.19	0.42
1:A:754:ARG:HG3	1:A:755:GLU:N	2.34	0.42
1:B:537:ILE:HG21	1:B:542:ARG:HH11	1.84	0.42
1:B:659:CYS:HA	1:B:664:TRP:CG	2.55	0.42
1:B:433:LYS:NZ	5:H:10:DT:OP1	2.52	0.42
4:G:14:DG:O3'	5:E:1:DG:C5'	2.68	0.42
1:A:729:ILE:HA	1:A:746:LEU:HD22	2.00	0.42
1:A:929:GLN:HA	1:A:932:VAL:HG22	2.02	0.42
1:A:555:THR:HB	1:A:864:GLN:HG2	2.01	0.42
1:B:638:TRP:HB2	1:B:666:TYR:CG	2.55	0.42
1:B:395:LEU:HD23	1:B:598:ASP:C	2.39	0.42
1:B:447:ILE:HG23	1:B:456:LEU:HD23	2.01	0.42
1:B:942:GLY:HA3	1:B:997:LEU:CD2	2.50	0.42
1:B:642:LYS:H	1:B:642:LYS:HG2	1.68	0.42
1:B:815:GLU:HG2	1:B:832:HIS:CE1	2.55	0.42
1:B:679:ARG:HD2	1:B:679:ARG:O	2.20	0.41
1:A:496:LEU:O	1:A:500:PHE:CD2	2.72	0.41
1:A:815:GLU:HG2	1:A:832:HIS:NE2	2.35	0.41
1:B:703:SER:HB3	1:B:706:ARG:NH2	2.35	0.41
1:A:465:LEU:HD13	1:A:524:LEU:HB2	2.02	0.41
1:A:650:HIS:HA	1:A:653:LEU:HD12	2.03	0.41
1:B:465:LEU:HD13	1:B:524:LEU:HB2	2.02	0.41
1:B:754:ARG:HG3	1:B:755:GLU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:589:ILE:HD13	1:A:861:ASN:HA	2.02	0.41
1:A:694:LEU:O	1:A:704:ARG:NH2	2.53	0.41
1:A:836:SER:OG	1:A:921:ARG:HD2	2.21	0.41
1:A:721:ARG:HH21	1:A:723:GLU:HB3	1.86	0.41
1:B:704:ARG:HD3	1:B:735:ASP:OD2	2.21	0.41
1:B:762:PHE:HB2	1:B:764:HIS:HD2	1.86	0.41
1:B:820:ALA:HA	1:B:823:ARG:NH1	2.35	0.41
5:H:5:DA:H8	5:H:5:DA:OP2	2.04	0.41
1:B:387:LEU:HD11	1:B:404:VAL:HG11	2.03	0.41
5:H:4:DG:H2"	5:H:5:DA:OP2	2.20	0.41
1:A:392:ASP:HA	1:A:395:LEU:HD12	2.02	0.40
1:A:681:HIS:CE1	4:G:14:DG:OP1	2.74	0.40
1:B:387:LEU:HD22	1:B:393:MET:SD	2.62	0.40
1:B:942:GLY:HA3	1:B:997:LEU:HD21	2.03	0.40
1:A:679:ARG:O	1:A:679:ARG:HD2	2.21	0.40
1:B:697:ARG:HH22	1:B:737:GLU:HG2	1.86	0.40
1:A:407:PHE:CZ	1:A:415:GLN:HG2	2.56	0.40
1:B:589:ILE:HD13	1:B:861:ASN:HA	2.04	0.40
1:B:650:HIS:HA	1:B:653:LEU:HD12	2.03	0.40
1:B:700:CYS:N	1:B:701:PRO:CD	2.85	0.40
1:B:721:ARG:HD2	1:B:721:ARG:HA	1.85	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	607/651 (93%)	549 (90%)	44 (7%)	14 (2%)	6 30
1	B	607/651 (93%)	546 (90%)	52 (9%)	9 (2%)	10 42
All	All	1214/1302 (93%)	1095 (90%)	96 (8%)	23 (2%)	8 36

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	557	SER
1	A	558	MET
1	A	564	ALA
1	B	557	SER
1	A	760	LYS
1	A	761	LYS
1	A	771	GLU
1	B	568	GLN
1	B	760	LYS
1	B	761	LYS
1	B	771	GLU
1	A	895	GLU
1	B	895	GLU
1	A	555	THR
1	A	556	ASP
1	A	643	ASN
1	A	758	SER
1	B	398	GLU
1	A	636	ARG
1	A	757	PRO
1	B	770	PRO
1	A	770	PRO
1	B	757	PRO

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	536/563 (95%)	491 (92%)	45 (8%)	11	38
1	B	536/563 (95%)	492 (92%)	44 (8%)	11	39
All	All	1072/1126 (95%)	983 (92%)	89 (8%)	11	39

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	377	ARG
1	A	389	ASN
1	A	424	ARG
1	A	431	MET
1	A	444	THR
1	A	458	THR
1	A	460	SER
1	A	470	GLU
1	A	488	ASN
1	A	522	VAL
1	A	525	LYS
1	A	537	ILE
1	A	547	ARG
1	A	549	LEU
1	A	553	SER
1	A	557	SER
1	A	561	GLU
1	A	571	LEU
1	A	575	LEU
1	A	591	ARG
1	A	592	LYS
1	A	636	ARG
1	A	641	LEU
1	A	642	LYS
1	A	652	ASP
1	A	662	VAL
1	A	674	VAL
1	A	679	ARG
1	A	685	GLU
1	A	710	ARG
1	A	721	ARG
1	A	738	VAL
1	A	754	ARG
1	A	759	CYS
1	A	780	VAL
1	A	787	CYS
1	A	817	LEU
1	A	832	HIS
1	A	834	GLU
1	A	889	LEU
1	A	926	GLN
1	A	967	GLN
1	A	970	HIS

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Mol	Chain	Res	Type
1	A	981	ASP
1	A	995	GLN
1	B	377	ARG
1	B	424	ARG
1	B	431	MET
1	B	444	THR
1	B	458	THR
1	B	460	SER
1	B	470	GLU
1	B	488	ASN
1	B	522	VAL
1	B	525	LYS
1	B	537	ILE
1	B	549	LEU
1	B	556	ASP
1	B	557	SER
1	B	561	GLU
1	B	562	ASP
1	B	565	CYS
1	B	575	LEU
1	B	591	ARG
1	B	592	LYS
1	B	636	ARG
1	B	640	ARG
1	B	641	LEU
1	B	652	ASP
1	B	662	VAL
1	B	674	VAL
1	B	679	ARG
1	B	685	GLU
1	B	710	ARG
1	B	721	ARG
1	B	738	VAL
1	B	754	ARG
1	B	759	CYS
1	B	787	CYS
1	B	817	LEU
1	B	832	HIS
1	B	834	GLU
1	B	840	THR
1	B	889	LEU
1	B	895	GLU

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Mol	Chain	Res	Type
1	B	967	GLN
1	B	970	HIS
1	B	981	ASP
1	B	995	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	423	GLN
1	A	568	GLN
1	A	610	HIS
1	A	681	HIS
1	A	764	HIS
1	A	775	GLN
1	A	926	GLN
1	A	953	HIS
1	A	995	GLN
1	B	423	GLN
1	B	610	HIS
1	B	764	HIS
1	B	775	GLN
1	B	926	GLN
1	B	953	HIS
1	B	995	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 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	613/651 (94%)	0.03	39 (6%) 19 6	31, 54, 145, 173	0
1	B	613/651 (94%)	0.08	42 (6%) 16 5	33, 54, 144, 176	0
2	F	10/10 (100%)	-0.49	0 100 100	55, 67, 79, 86	0
2	L	10/10 (100%)	-0.49	0 100 100	59, 65, 73, 78	0
3	I	9/9 (100%)	-0.54	0 100 100	57, 63, 72, 73	0
3	K	9/9 (100%)	-0.58	0 100 100	53, 62, 70, 70	0
4	G	7/14 (50%)	-0.44	0 100 100	46, 51, 64, 68	0
4	J	7/14 (50%)	-0.59	0 100 100	45, 53, 72, 77	0
5	E	12/12 (100%)	-0.49	0 100 100	62, 79, 83, 84	0
5	H	12/12 (100%)	-0.54	0 100 100	55, 78, 84, 85	0
All	All	1302/1392 (93%)	0.02	81 (6%) 20 7	31, 55, 143, 176	0

All (81) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	568	GLN	9.1
1	A	568	GLN	7.1
1	B	484	PHE	6.4
1	B	796	VAL	6.2
1	B	480	LEU	5.7
1	A	503	LEU	5.6
1	B	501	LEU	5.4
1	A	519	ILE	5.1
1	B	565	CYS	5.1
1	A	506	GLN	5.0
1	B	483	THR	5.0
1	B	509	VAL	4.9
1	B	569	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	562	ASP	4.5
1	B	786	LEU	4.3
1	B	485	HIS	4.3
1	B	1009	VAL	4.2
1	A	787	CYS	4.2
1	B	506	GLN	4.2
1	A	562	ASP	4.1
1	B	521	ALA	4.1
1	A	484	PHE	4.1
1	A	563	ALA	4.1
1	B	567	GLY	4.0
1	A	489	PRO	4.0
1	A	523	ILE	3.9
1	A	499	ALA	3.9
1	A	504	ALA	3.8
1	A	799	MET	3.7
1	A	482	LYS	3.7
1	B	504	ALA	3.7
1	A	485	HIS	3.7
1	B	561	GLU	3.6
1	A	567	GLY	3.5
1	B	486	LEU	3.5
1	B	797	PHE	3.2
1	A	507	ARG	3.2
1	A	493	LYS	3.1
1	A	497	VAL	3.1
1	A	1009	VAL	3.1
1	A	797	PHE	3.1
1	B	508	SER	3.0
1	B	563	ALA	3.0
1	B	505	LYS	3.0
1	A	569	GLY	3.0
1	B	370	THR	3.0
1	B	524	LEU	3.0
1	A	564	ALA	2.9
1	B	495	GLN	2.9
1	B	967	GLN	2.9
1	A	370	THR	2.8
1	A	501	LEU	2.8
1	B	787	CYS	2.7
1	A	502	LYS	2.7
1	B	493	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	476	GLU	2.7
1	B	785	ARG	2.6
1	A	483	THR	2.6
1	B	502	LYS	2.6
1	A	486	LEU	2.5
1	B	766	PHE	2.5
1	B	503	LEU	2.5
1	B	489	PRO	2.5
1	A	811	LEU	2.4
1	B	768	GLN	2.4
1	A	810	VAL	2.4
1	B	497	VAL	2.3
1	B	573	THR	2.3
1	A	796	VAL	2.3
1	A	496	LEU	2.3
1	A	478	LYS	2.3
1	A	786	LEU	2.2
1	A	475	PRO	2.2
1	B	469	LEU	2.1
1	B	522	VAL	2.1
1	B	810	VAL	2.1
1	B	566	GLY	2.1
1	A	766	PHE	2.0
1	A	520	GLY	2.0
1	A	645	PRO	2.0
1	B	520	GLY	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 monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
6	BA	B	1101	1/1	0.99	0.20	61,61,61,61	0
6	BA	A	1101	1/1	1.00	0.19	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.