Full wwPDB X-ray Structure Validation Report ⓘ

Jun 23, 2024 – 04:38 AM EDT

PDB ID	:	6PK5
Title	:	Adenylate kinase from Methanococcus igneus - apo form
Authors	:	Moon, S.; Kim, J.; Bae, E.; Phillips Jr., G.N.
Deposited on	:	2019-06-28
Resolution	:	2.30 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:

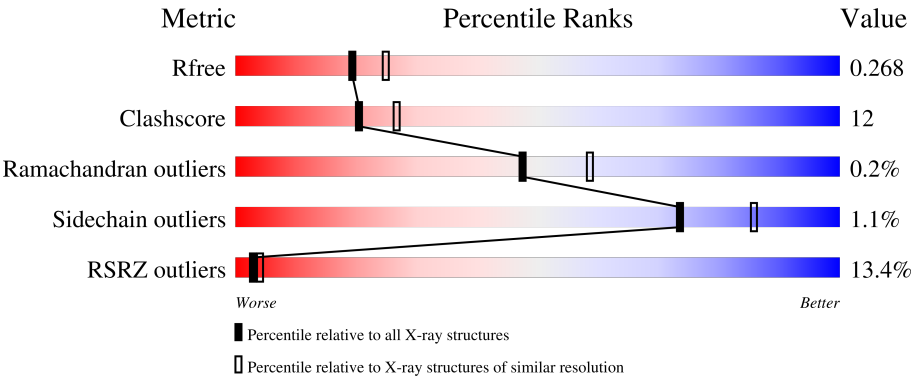
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	200	14% 71% 23% 6%
1	B	200	14% 70% 24% 6%
1	C	200	11% 74% 20% 5%
1	D	200	13% 74% 21%
1	E	200	12% 77% 17% 6%

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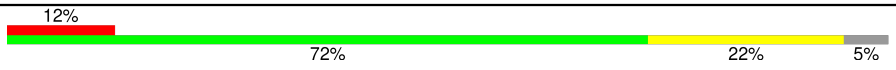
Mol	Chain	Length	Quality of chain
1	F	200	

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
2	CL	F	303	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18234 atoms, of which 9236 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 Adenylate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	188	Total	C	H	N	O	S	0	0	0
			2988	920	1528	249	283	8			
1	B	189	Total	C	H	N	O	S	0	0	0
			3002	924	1534	251	285	8			
1	C	190	Total	C	H	N	O	S	0	0	0
			3019	928	1540	255	288	8			
1	D	191	Total	C	H	N	O	S	0	0	0
			3038	934	1551	256	289	8			
1	E	189	Total	C	H	N	O	S	0	0	0
			3007	924	1536	254	285	8			
1	F	190	Total	C	H	N	O	S	0	0	0
			3026	930	1547	255	286	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	LEU	-	expression tag	UNP P43408
A	194	GLU	-	expression tag	UNP P43408
A	195	HIS	-	expression tag	UNP P43408
A	196	HIS	-	expression tag	UNP P43408
A	197	HIS	-	expression tag	UNP P43408
A	198	HIS	-	expression tag	UNP P43408
A	199	HIS	-	expression tag	UNP P43408
A	200	HIS	-	expression tag	UNP P43408
B	193	LEU	-	expression tag	UNP P43408
B	194	GLU	-	expression tag	UNP P43408
B	195	HIS	-	expression tag	UNP P43408
B	196	HIS	-	expression tag	UNP P43408
B	197	HIS	-	expression tag	UNP P43408
B	198	HIS	-	expression tag	UNP P43408
B	199	HIS	-	expression tag	UNP P43408
B	200	HIS	-	expression tag	UNP P43408
C	193	LEU	-	expression tag	UNP P43408

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Chain	Residue	Modelled	Actual	Comment	Reference
C	194	GLU	-	expression tag	UNP P43408
C	195	HIS	-	expression tag	UNP P43408
C	196	HIS	-	expression tag	UNP P43408
C	197	HIS	-	expression tag	UNP P43408
C	198	HIS	-	expression tag	UNP P43408
C	199	HIS	-	expression tag	UNP P43408
C	200	HIS	-	expression tag	UNP P43408
D	193	LEU	-	expression tag	UNP P43408
D	194	GLU	-	expression tag	UNP P43408
D	195	HIS	-	expression tag	UNP P43408
D	196	HIS	-	expression tag	UNP P43408
D	197	HIS	-	expression tag	UNP P43408
D	198	HIS	-	expression tag	UNP P43408
D	199	HIS	-	expression tag	UNP P43408
D	200	HIS	-	expression tag	UNP P43408
E	193	LEU	-	expression tag	UNP P43408
E	194	GLU	-	expression tag	UNP P43408
E	195	HIS	-	expression tag	UNP P43408
E	196	HIS	-	expression tag	UNP P43408
E	197	HIS	-	expression tag	UNP P43408
E	198	HIS	-	expression tag	UNP P43408
E	199	HIS	-	expression tag	UNP P43408
E	200	HIS	-	expression tag	UNP P43408
F	193	LEU	-	expression tag	UNP P43408
F	194	GLU	-	expression tag	UNP P43408
F	195	HIS	-	expression tag	UNP P43408
F	196	HIS	-	expression tag	UNP P43408
F	197	HIS	-	expression tag	UNP P43408
F	198	HIS	-	expression tag	UNP P43408
F	199	HIS	-	expression tag	UNP P43408
F	200	HIS	-	expression tag	UNP P43408

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Cl 2 2	0	0
2	B	2	Total Cl 2 2	0	0
2	C	3	Total Cl 3 3	0	0
2	D	2	Total Cl 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	3	Total Cl 3 3	0	0
2	F	3	Total Cl 3 3	0	0

- Molecule 3 is water.

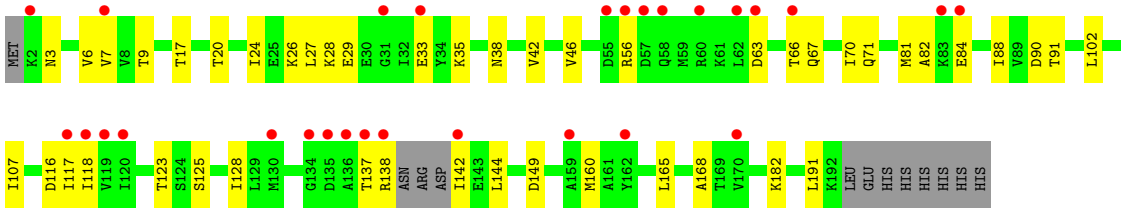
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	18	Total O 18 18	0	0
3	B	11	Total O 11 11	0	0
3	C	17	Total O 17 17	0	0
3	D	33	Total O 33 33	0	0
3	E	37	Total O 37 37	0	0
3	F	23	Total O 23 23	0	0

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.

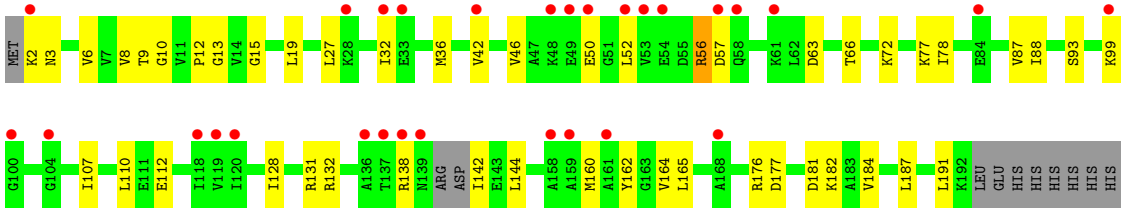
• Molecule 1: Adenylate kinase

Chain A:



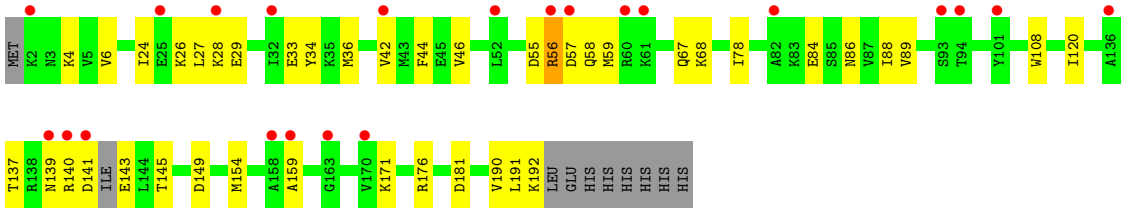
• Molecule 1: Adenylate kinase

Chain B:



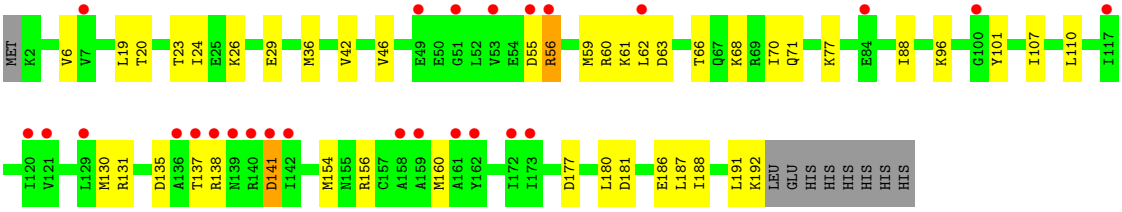
• Molecule 1: Adenylate kinase

Chain C:

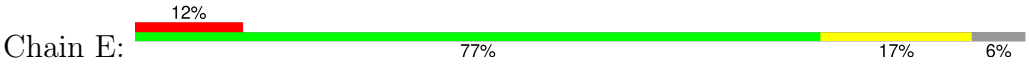


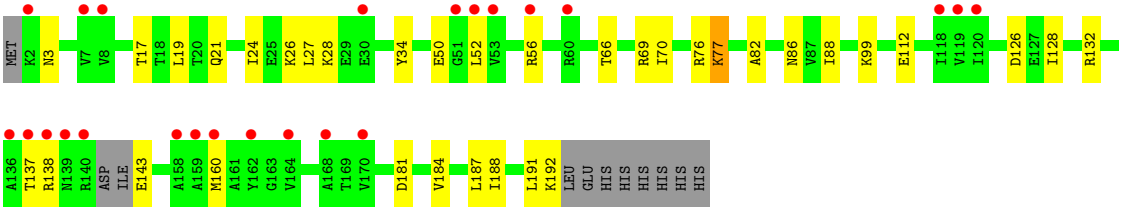
• Molecule 1: Adenylate kinase

Chain D:

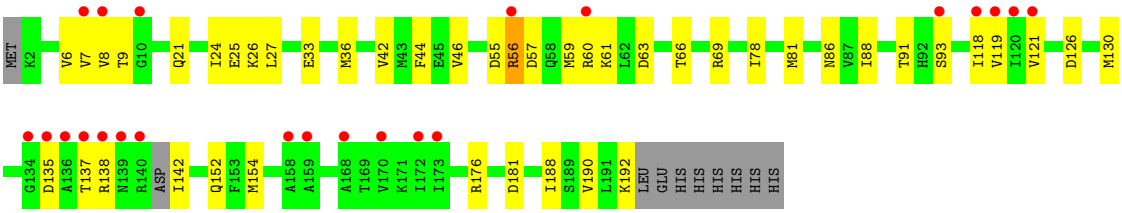


• Molecule 1: Adenylate kinase





• Molecule 1: Adenylate kinase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	68.71Å 68.71Å 257.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	31.33 – 2.30 31.33 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (31.33-2.30) 99.9 (31.33-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.15.2_3472: ???)	Depositor
R, R_{free}	0.229 , 0.267 0.231 , 0.268	Depositor DCC
R_{free} test set	1903 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å^2)	55.5	Xtriage
Anisotropy	0.092	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 54.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.066 for h,-h-k,-l 0.046 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18234	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.33% 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, 0.333 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: CL

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	0.62	0/1473	0.82	0/1982
1	B	0.63	0/1481	0.83	0/1993
1	C	0.67	0/1492	0.86	0/2007
1	D	0.70	2/1501 (0.1%)	0.83	1/2021 (0.0%)
1	E	0.71	1/1484 (0.1%)	0.87	0/1996
1	F	0.74	0/1492	0.90	1/2007 (0.0%)
All	All	0.68	3/8923 (0.0%)	0.85	2/12006 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	186	GLU	CG-CD	6.57	1.61	1.51
1	D	186	GLU	CB-CG	6.49	1.64	1.52
1	E	77	LYS	CB-CG	5.07	1.66	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	156	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	F	181	ASP	CB-CG-OD1	5.24	123.02	118.30

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	1460	1528	1526	38	0
1	B	1468	1534	1532	47	0
1	C	1479	1540	1538	37	0
1	D	1487	1551	1550	41	0
1	E	1471	1536	1534	31	0
1	F	1479	1547	1545	41	0
2	A	2	0	0	0	0
2	B	2	0	0	1	0
2	C	3	0	0	0	0
2	D	2	0	0	1	0
2	E	3	0	0	0	0
2	F	3	0	0	3	0
3	A	18	0	0	7	0
3	B	11	0	0	4	0
3	C	17	0	0	13	0
3	D	33	0	0	6	0
3	E	37	0	0	4	0
3	F	23	0	0	7	0
All	All	8998	9236	9225	224	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 12.

All (224) 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:138:ARG:O	3:A:401:HOH:O	1.75	1.03
1:F:142:ILE:O	3:F:401:HOH:O	1.83	0.95
1:C:6:VAL:HB	1:C:88:ILE:HD12	1.51	0.89
1:E:132:ARG:C	1:E:138:ARG:HH21	1.79	0.85
1:E:27:LEU:HD11	1:E:191:LEU:HD12	1.57	0.84
1:C:33:GLU:OE2	3:C:401:HOH:O	1.97	0.82
1:E:132:ARG:HB3	1:E:138:ARG:CZ	2.09	0.81
1:B:12:PRO:HB3	1:B:138:ARG:HH12	1.46	0.81
1:B:142:ILE:N	3:B:402:HOH:O	2.15	0.80
1:B:176:ARG:NH2	3:B:403:HOH:O	2.16	0.79
1:B:15:GLY:HA2	2:B:301:CL:CL	2.22	0.77
1:B:6:VAL:HB	1:B:88:ILE:HD12	1.68	0.75
1:F:63:ASP:OD1	1:F:66:THR:HG23	1.87	0.75
1:D:6:VAL:HB	1:D:88:ILE:HD12	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASP:OD1	3:A:402:HOH:O	2.07	0.73
1:A:24:ILE:HD11	1:A:88:ILE:HG21	1.69	0.72
1:D:137:THR:O	1:D:137:THR:HG22	1.88	0.72
1:B:32:ILE:O	3:B:401:HOH:O	2.09	0.71
1:A:144:LEU:HD11	1:D:130:MET:HB2	1.72	0.71
1:D:42:VAL:O	1:D:46:VAL:HG23	1.90	0.70
1:D:63:ASP:OD1	1:D:66:THR:HG23	1.91	0.70
1:D:192:LYS:O	3:D:401:HOH:O	2.09	0.70
1:B:9:THR:HG21	1:B:93:SER:HB2	1.74	0.69
1:E:192:LYS:O	3:E:401:HOH:O	2.09	0.69
1:F:8:VAL:HG23	1:F:88:ILE:HD11	1.74	0.69
1:A:137:THR:HG22	1:A:137:THR:O	1.92	0.68
1:C:58:GLN:OE1	3:C:402:HOH:O	2.12	0.68
2:F:303:CL:CL	3:F:415:HOH:O	2.47	0.68
1:C:137:THR:HG22	1:C:137:THR:O	1.95	0.67
1:A:142:ILE:HG23	3:A:403:HOH:O	1.94	0.66
2:D:301:CL:CL	3:D:425:HOH:O	2.52	0.65
1:A:6:VAL:HB	1:A:88:ILE:HD12	1.79	0.65
1:E:50:GLU:OE2	3:E:402:HOH:O	2.14	0.65
1:B:36:MET:HA	1:B:88:ILE:HG23	1.78	0.64
1:E:132:ARG:O	1:E:138:ARG:NH2	2.26	0.64
1:F:24:ILE:HD11	1:F:88:ILE:HG21	1.79	0.64
1:F:44:PHE:HA	1:F:59:MET:SD	2.38	0.64
1:C:4:LYS:NZ	3:C:404:HOH:O	2.29	0.63
1:E:137:THR:HG22	1:E:137:THR:O	1.99	0.63
1:A:107:ILE:HD13	1:A:165:LEU:HD13	1.81	0.62
1:B:9:THR:HG22	1:B:10:GLY:N	2.14	0.62
1:C:84:GLU:O	3:C:401:HOH:O	2.15	0.62
1:A:26:LYS:HD3	1:A:29:GLU:OE2	2.00	0.62
1:F:135:ASP:HB3	1:F:138:ARG:HG2	1.80	0.62
1:C:6:VAL:CB	1:C:88:ILE:HD12	2.28	0.62
1:C:24:ILE:HD11	1:C:88:ILE:HG21	1.81	0.62
1:E:3:ASN:HB2	1:E:82:ALA:O	2.00	0.61
1:B:50:GLU:HG3	1:B:50:GLU:O	1.98	0.61
1:F:118:ILE:N	1:F:118:ILE:HD12	2.15	0.61
1:E:143:GLU:N	3:E:405:HOH:O	2.33	0.61
1:B:19:LEU:HD22	1:B:184:VAL:HG22	1.82	0.61
1:D:19:LEU:CD1	1:D:187:LEU:HD22	2.30	0.61
1:F:188:ILE:O	1:F:192:LYS:HG3	2.01	0.60
1:D:20:THR:O	1:D:24:ILE:HG13	2.02	0.59
1:D:55:ASP:OD2	1:D:56:ARG:N	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:LYS:HD3	1:C:29:GLU:OE2	2.03	0.59
1:B:42:VAL:O	1:B:46:VAL:HG23	2.02	0.59
1:C:145:THR:OG1	1:E:126:ASP:OD1	2.19	0.59
1:E:26:LYS:HB3	1:E:188:ILE:HD11	1.85	0.58
1:C:55:ASP:HB3	1:C:58:GLN:HG3	1.86	0.58
1:A:125:SER:OG	1:A:149:ASP:OD1	2.22	0.58
1:D:26:LYS:HD3	1:D:29:GLU:OE2	2.03	0.58
1:F:9:THR:CG2	3:F:411:HOH:O	2.51	0.58
1:B:99:LYS:HE3	1:C:190:VAL:O	2.05	0.57
1:C:192:LYS:O	3:C:403:HOH:O	2.17	0.57
1:A:142:ILE:N	3:A:403:HOH:O	2.39	0.56
1:B:9:THR:HG23	1:B:93:SER:H	1.70	0.56
1:B:99:LYS:O	1:C:171:LYS:HB2	2.06	0.56
1:B:8:VAL:HG23	1:B:88:ILE:HD11	1.89	0.55
1:B:9:THR:HG21	1:B:93:SER:CB	2.35	0.55
1:B:50:GLU:HG3	1:B:52:LEU:HG	1.88	0.55
1:B:56:ARG:HD3	1:B:57:ASP:N	2.21	0.55
1:C:42:VAL:O	1:C:46:VAL:HG23	2.06	0.55
1:A:81:MET:HE1	3:A:417:HOH:O	2.05	0.54
1:C:140:ARG:O	1:C:141:ASP:OD1	2.24	0.54
1:E:132:ARG:C	1:E:138:ARG:NH2	2.58	0.54
1:C:27:LEU:HD11	1:C:191:LEU:HD12	1.90	0.54
1:F:60:ARG:HB2	3:F:402:HOH:O	2.08	0.54
1:F:137:THR:HG22	1:F:137:THR:O	2.08	0.53
1:A:3:ASN:HB2	1:A:82:ALA:O	2.09	0.53
1:B:9:THR:CG2	1:B:93:SER:H	2.21	0.53
1:E:24:ILE:HD11	1:E:88:ILE:HD12	1.90	0.53
1:E:66:THR:HG22	1:E:69:ARG:HH12	1.73	0.53
1:A:42:VAL:O	1:A:46:VAL:HG23	2.09	0.53
1:B:99:LYS:NZ	3:C:403:HOH:O	2.41	0.53
1:E:132:ARG:HB3	1:E:138:ARG:NE	2.24	0.53
1:D:181:ASP:N	1:D:181:ASP:OD1	2.41	0.52
1:D:24:ILE:HD11	1:D:88:ILE:HG21	1.92	0.52
1:D:107:ILE:HA	1:D:110:LEU:HD12	1.92	0.52
1:F:66:THR:HG22	1:F:69:ARG:HH22	1.75	0.52
1:B:182:LYS:HD2	1:B:182:LYS:N	2.24	0.52
1:B:8:VAL:CG2	1:B:88:ILE:HD11	2.40	0.52
1:B:144:LEU:HD23	1:F:130:MET:HE3	1.92	0.51
1:F:9:THR:HB	1:F:119:VAL:O	2.11	0.51
1:B:181:ASP:N	1:B:181:ASP:OD1	2.44	0.51
1:E:132:ARG:HB3	1:E:138:ARG:NH2	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:MET:HA	1:B:88:ILE:CG2	2.41	0.51
1:C:143:GLU:N	3:C:406:HOH:O	2.42	0.51
1:A:24:ILE:HG22	1:A:28:LYS:HE3	1.92	0.51
1:B:13:GLY:N	1:B:138:ARG:NH2	2.59	0.51
1:F:7:VAL:HG13	1:F:91:THR:HG22	1.93	0.51
1:D:56:ARG:H	1:D:56:ARG:HD3	1.76	0.51
1:A:38:ASN:O	1:A:42:VAL:HG23	2.12	0.50
1:E:52:LEU:HD12	1:E:70:ILE:HD11	1.94	0.50
1:B:131:ARG:NH2	1:B:177:ASP:OD1	2.40	0.50
1:B:72:LYS:HE2	3:B:409:HOH:O	2.11	0.50
1:D:180:LEU:HB3	3:D:420:HOH:O	2.10	0.50
1:C:24:ILE:HG23	1:C:28:LYS:HE3	1.93	0.49
1:F:56:ARG:HD3	1:F:57:ASP:N	2.27	0.49
1:B:63:ASP:OD1	1:B:66:THR:HG23	2.13	0.49
1:D:60:ARG:HB2	3:D:409:HOH:O	2.11	0.49
1:D:96:LYS:HE2	1:D:101:TYR:CE1	2.48	0.49
1:D:137:THR:O	1:D:137:THR:CG2	2.59	0.49
1:A:123:THR:HG23	1:A:128:ILE:HG13	1.95	0.48
1:C:58:GLN:NE2	3:C:402:HOH:O	2.46	0.48
1:F:21:GLN:O	1:F:25:GLU:HG3	2.13	0.48
1:C:24:ILE:CD1	1:C:36:MET:HB2	2.43	0.48
1:B:13:GLY:N	1:B:138:ARG:HH22	2.11	0.48
1:D:19:LEU:HD12	1:D:187:LEU:HD22	1.96	0.48
1:A:46:VAL:HG12	1:A:70:ILE:HD12	1.94	0.48
1:D:19:LEU:HD23	3:D:420:HOH:O	2.13	0.48
1:A:28:LYS:HE2	1:A:33:GLU:OE1	2.14	0.48
1:F:60:ARG:O	3:F:402:HOH:O	2.20	0.48
1:C:176:ARG:HH22	1:F:176:ARG:HE	1.62	0.48
1:B:27:LEU:HD11	1:B:191:LEU:HD12	1.96	0.47
1:D:160:MET:HE3	1:F:154:MET:CE	2.44	0.47
1:D:26:LYS:CB	1:D:188:ILE:HD11	2.45	0.47
1:F:135:ASP:HB3	1:F:138:ARG:CG	2.44	0.47
1:E:99:LYS:HE3	1:F:190:VAL:O	2.14	0.47
1:A:160:MET:HE3	1:C:154:MET:CE	2.45	0.47
1:B:9:THR:CG2	1:B:10:GLY:N	2.77	0.47
1:D:63:ASP:OD1	1:D:66:THR:CG2	2.61	0.47
1:F:63:ASP:OD1	1:F:66:THR:CG2	2.61	0.47
1:A:7:VAL:HG13	1:A:91:THR:CG2	2.45	0.47
1:B:99:LYS:HE3	3:C:403:HOH:O	2.15	0.47
1:B:110:LEU:HD11	1:B:162:TYR:CD1	2.50	0.47
1:C:141:ASP:O	1:C:143:GLU:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ILE:HD11	1:C:159:ALA:HB3	1.97	0.47
1:C:137:THR:O	1:C:137:THR:CG2	2.63	0.47
1:E:34:TYR:CD1	1:E:86:ASN:HB3	2.49	0.47
1:D:36:MET:HA	1:D:88:ILE:HG22	1.97	0.46
1:C:44:PHE:HA	1:C:59:MET:SD	2.54	0.46
1:F:9:THR:HG21	1:F:93:SER:HB2	1.97	0.46
1:A:17:THR:OG1	1:A:90:ASP:OD2	2.20	0.46
1:E:34:TYR:CD1	1:E:88:ILE:HG13	2.50	0.46
1:D:188:ILE:O	1:D:192:LYS:HG3	2.16	0.46
1:A:20:THR:O	1:A:24:ILE:HG13	2.16	0.46
1:A:118:ILE:N	1:A:118:ILE:HD12	2.30	0.46
1:A:142:ILE:HD12	1:A:142:ILE:C	2.36	0.46
1:B:12:PRO:HB3	1:B:138:ARG:NH1	2.23	0.46
1:B:19:LEU:CD1	1:B:187:LEU:HD22	2.46	0.46
1:D:26:LYS:HB2	1:D:188:ILE:HD11	1.97	0.46
1:D:42:VAL:HG13	1:D:77:LYS:HD3	1.97	0.46
1:A:9:THR:HA	1:A:91:THR:O	2.16	0.46
1:B:99:LYS:CE	3:C:403:HOH:O	2.63	0.45
1:D:131:ARG:NH2	1:D:177:ASP:OD1	2.31	0.45
1:F:152:GLN:NE2	2:F:303:CL:CL	2.78	0.45
1:E:181:ASP:OD1	1:E:181:ASP:N	2.46	0.45
1:F:142:ILE:O	1:F:142:ILE:HD12	2.16	0.45
1:A:46:VAL:HG12	1:A:70:ILE:CD1	2.47	0.45
1:A:7:VAL:HG13	1:A:91:THR:HG22	1.98	0.45
1:C:34:TYR:CE1	1:C:86:ASN:HB3	2.52	0.45
1:E:19:LEU:HD22	1:E:184:VAL:HG22	1.99	0.45
1:C:68:LYS:HE2	1:C:108:TRP:CG	2.52	0.45
1:D:68:LYS:HA	1:D:71:GLN:OE1	2.17	0.45
1:F:24:ILE:HD11	1:F:88:ILE:CG2	2.47	0.45
1:A:35:LYS:NZ	3:A:406:HOH:O	2.50	0.44
1:C:55:ASP:OD1	1:C:56:ARG:N	2.51	0.44
1:B:2:LYS:O	1:B:3:ASN:C	2.54	0.44
1:B:50:GLU:HG2	1:B:52:LEU:CD1	2.47	0.44
1:D:59:MET:C	1:D:61:LYS:H	2.20	0.44
1:D:36:MET:HA	1:D:88:ILE:CG2	2.48	0.44
1:F:6:VAL:HB	1:F:88:ILE:HD12	1.99	0.44
1:B:78:ILE:HG23	1:B:87:VAL:HG11	1.99	0.44
1:D:138:ARG:HB3	1:D:141:ASP:HB2	1.99	0.44
1:C:181:ASP:OD1	1:C:181:ASP:N	2.50	0.44
1:F:42:VAL:O	1:F:46:VAL:HG23	2.18	0.43
1:F:121:VAL:O	2:F:303:CL:CL	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:LEU:HD21	1:F:188:ILE:HG23	2.01	0.43
1:F:9:THR:HG22	3:F:411:HOH:O	2.18	0.43
1:F:33:GLU:O	1:F:86:ASN:HB2	2.18	0.43
1:F:7:VAL:HG13	1:F:91:THR:CG2	2.47	0.43
1:B:160:MET:O	1:B:164:VAL:HG23	2.19	0.43
1:E:19:LEU:CD1	1:E:187:LEU:HD22	2.49	0.43
1:E:24:ILE:HG23	1:E:28:LYS:HE3	2.00	0.43
1:A:102:LEU:HD12	3:A:413:HOH:O	2.19	0.42
1:A:137:THR:O	1:A:137:THR:CG2	2.62	0.42
1:C:55:ASP:OD1	1:C:56:ARG:HD3	2.19	0.42
1:D:59:MET:O	1:D:62:LEU:HG	2.19	0.42
1:B:50:GLU:CG	1:B:52:LEU:HG	2.49	0.42
1:C:56:ARG:HD3	1:C:57:ASP:N	2.35	0.42
1:D:135:ASP:C	1:D:137:THR:H	2.22	0.42
1:A:84:GLU:O	1:A:84:GLU:HG3	2.18	0.42
1:B:107:ILE:HD13	1:B:165:LEU:HD13	2.00	0.42
1:E:17:THR:O	1:E:21:GLN:HG3	2.19	0.42
1:D:160:MET:CE	1:F:154:MET:CE	2.96	0.42
1:E:137:THR:OG1	3:E:404:HOH:O	2.21	0.42
1:F:26:LYS:NZ	3:F:406:HOH:O	2.52	0.42
1:A:63:ASP:OD1	1:A:66:THR:HG23	2.19	0.42
1:E:128:ILE:O	1:E:132:ARG:HG3	2.19	0.42
1:D:66:THR:O	1:D:70:ILE:HG12	2.19	0.42
1:B:72:LYS:CG	1:B:112:GLU:HG3	2.50	0.41
1:E:66:THR:O	1:E:70:ILE:HG12	2.19	0.41
1:C:78:ILE:HD13	1:C:89:VAL:CG2	2.50	0.41
1:B:128:ILE:O	1:B:132:ARG:HG3	2.20	0.41
1:D:23:THR:HG23	1:D:188:ILE:HG13	2.03	0.41
1:D:154:MET:CE	1:E:160:MET:HE2	2.51	0.41
1:F:55:ASP:OD2	1:F:56:ARG:N	2.53	0.41
1:C:67:GLN:NE2	3:C:410:HOH:O	2.53	0.41
1:C:149:ASP:HA	3:C:405:HOH:O	2.21	0.41
1:A:67:GLN:O	1:A:71:GLN:HG3	2.21	0.41
1:A:118:ILE:CD1	1:A:168:ALA:HB3	2.50	0.41
1:D:154:MET:CE	1:E:160:MET:CE	2.99	0.41
1:F:24:ILE:CD1	1:F:36:MET:HB2	2.49	0.41
1:B:144:LEU:HB3	1:F:126:ASP:OD2	2.21	0.41
1:C:58:GLN:CD	3:C:402:HOH:O	2.56	0.41
1:F:8:VAL:CG2	1:F:88:ILE:HD11	2.47	0.41
1:A:116:ASP:C	1:A:117:ILE:HG13	2.41	0.40
1:A:27:LEU:HD11	1:A:191:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:ASP:OD2	1:D:56:ARG:HD3	2.21	0.40
1:D:60:ARG:C	3:D:409:HOH:O	2.60	0.40
1:A:118:ILE:CD1	1:A:168:ALA:CB	2.99	0.40
1:E:76:ARG:NH2	1:E:112:GLU:OE2	2.52	0.40
1:F:78:ILE:HA	1:F:81:MET:HG2	2.03	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	184/200 (92%)	180 (98%)	4 (2%)	0	100	100
1	B	185/200 (92%)	181 (98%)	4 (2%)	0	100	100
1	C	186/200 (93%)	181 (97%)	5 (3%)	0	100	100
1	D	189/200 (94%)	178 (94%)	9 (5%)	2 (1%)	14	15
1	E	185/200 (92%)	180 (97%)	5 (3%)	0	100	100
1	F	186/200 (93%)	181 (97%)	5 (3%)	0	100	100
All	All	1115/1200 (93%)	1081 (97%)	32 (3%)	2 (0%)	47	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	191	LEU
1	D	141	ASP

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	163/175 (93%)	161 (99%)	2 (1%)	71	84
1	B	164/175 (94%)	162 (99%)	2 (1%)	71	84
1	C	165/175 (94%)	163 (99%)	2 (1%)	71	84
1	D	166/175 (95%)	165 (99%)	1 (1%)	86	94
1	E	164/175 (94%)	162 (99%)	2 (1%)	71	84
1	F	165/175 (94%)	163 (99%)	2 (1%)	71	84
All	All	987/1050 (94%)	976 (99%)	11 (1%)	73	86

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	182	LYS
1	B	56	ARG
1	B	77	LYS
1	C	56	ARG
1	C	139	ASN
1	D	56	ARG
1	E	56	ARG
1	E	77	LYS
1	F	56	ARG
1	F	61	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 15 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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	188/200 (94%)	0.99	28 (14%)	2 3	56, 73, 96, 113	0
1	B	189/200 (94%)	1.00	29 (15%)	2 3	55, 74, 102, 117	0
1	C	190/200 (95%)	0.78	22 (11%)	4 6	54, 68, 92, 109	0
1	D	191/200 (95%)	0.97	26 (13%)	3 4	51, 70, 87, 98	0
1	E	189/200 (94%)	0.86	24 (12%)	3 5	49, 64, 86, 91	0
1	F	190/200 (95%)	0.77	23 (12%)	4 6	47, 60, 80, 89	0
All	All	1137/1200 (94%)	0.90	152 (13%)	3 4	47, 68, 92, 117	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	ARG	6.6
1	F	140	ARG	6.4
1	D	140	ARG	6.0
1	B	136	ALA	5.7
1	C	140	ARG	5.7
1	F	136	ALA	5.6
1	A	142	ILE	5.5
1	E	140	ARG	5.1
1	E	138	ARG	5.1
1	D	142	ILE	4.8
1	C	139	ASN	4.8
1	A	136	ALA	4.7
1	B	52	LEU	4.6
1	A	137	THR	4.5
1	D	136	ALA	4.5
1	E	139	ASN	4.5
1	A	57	ASP	4.3
1	A	138	ARG	4.2
1	B	139	ASN	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	60	ARG	4.0
1	C	61	LYS	4.0
1	D	7	VAL	4.0
1	B	50	GLU	3.9
1	D	56	ARG	3.9
1	A	33	GLU	3.9
1	B	54	GLU	3.8
1	E	60	ARG	3.7
1	A	58	GLN	3.7
1	B	137	THR	3.7
1	D	49	GLU	3.6
1	F	137	THR	3.6
1	D	138	ARG	3.6
1	F	119	VAL	3.5
1	F	7	VAL	3.5
1	E	2	LYS	3.5
1	C	141	ASP	3.4
1	F	138	ARG	3.3
1	B	53	VAL	3.3
1	F	170	VAL	3.2
1	C	159	ALA	3.2
1	E	137	THR	3.2
1	F	139	ASN	3.2
1	C	57	ASP	3.2
1	D	137	THR	3.2
1	B	99	LYS	3.2
1	C	56	ARG	3.2
1	E	7	VAL	3.1
1	A	84	GLU	3.1
1	B	84	GLU	3.1
1	A	162	TYR	3.1
1	B	2	LYS	3.1
1	C	25	GLU	3.0
1	A	55	ASP	3.0
1	D	120	ILE	3.0
1	F	120	ILE	3.0
1	E	136	ALA	3.0
1	A	56	ARG	2.9
1	A	62	LEU	2.9
1	F	134	GLY	2.9
1	A	60	ARG	2.9
1	F	159	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	168	ALA	2.9
1	A	118	ILE	2.9
1	B	48	LYS	2.9
1	A	7	VAL	2.9
1	A	2	LYS	2.9
1	C	52	LEU	2.8
1	B	28	LYS	2.8
1	A	66	THR	2.8
1	E	8	VAL	2.7
1	A	159	ALA	2.7
1	E	119	VAL	2.7
1	F	121	VAL	2.7
1	D	84	GLU	2.7
1	B	33	GLU	2.7
1	D	139	ASN	2.6
1	E	159	ALA	2.6
1	A	135	ASP	2.6
1	F	135	ASP	2.6
1	D	173	ILE	2.6
1	D	51	GLY	2.6
1	D	121	VAL	2.6
1	A	63	ASP	2.6
1	F	93	SER	2.6
1	C	158	ALA	2.5
1	F	8	VAL	2.5
1	B	32	ILE	2.5
1	B	58	GLN	2.5
1	B	159	ALA	2.5
1	B	168	ALA	2.5
1	C	136	ALA	2.5
1	B	61	LYS	2.5
1	D	55	ASP	2.5
1	B	104	GLY	2.5
1	E	160	MET	2.4
1	C	82	ALA	2.4
1	A	120	ILE	2.4
1	E	118	ILE	2.4
1	F	56	ARG	2.4
1	E	52	LEU	2.4
1	B	158	ALA	2.4
1	A	170	VAL	2.4
1	A	134	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLY	2.4
1	D	100	GLY	2.4
1	E	120	ILE	2.3
1	D	161	ALA	2.3
1	D	172	ILE	2.3
1	B	42	VAL	2.3
1	E	164	VAL	2.3
1	C	170	VAL	2.3
1	E	53	VAL	2.3
1	C	101	TYR	2.3
1	E	56	ARG	2.3
1	D	159	ALA	2.3
1	E	30	GLU	2.2
1	D	129	LEU	2.2
1	E	170	VAL	2.2
1	A	117	ILE	2.2
1	C	42	VAL	2.2
1	E	51	GLY	2.2
1	F	172	ILE	2.2
1	F	173	ILE	2.2
1	B	57	ASP	2.2
1	D	53	VAL	2.2
1	B	49	GLU	2.2
1	C	93	SER	2.2
1	C	2	LYS	2.1
1	D	158	ALA	2.1
1	C	32	ILE	2.1
1	D	141	ASP	2.1
1	F	60	ARG	2.1
1	A	119	VAL	2.1
1	E	158	ALA	2.1
1	E	162	TYR	2.1
1	B	118	ILE	2.1
1	C	163	GLY	2.1
1	D	117	ILE	2.1
1	B	120	ILE	2.1
1	B	161	ALA	2.1
1	F	168	ALA	2.1
1	B	100	GLY	2.1
1	F	10	GLY	2.1
1	C	28	LYS	2.1
1	F	158	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	118	ILE	2.0
1	C	94	THR	2.0
1	A	83	LYS	2.0
1	D	62	LEU	2.0
1	B	119	VAL	2.0
1	D	162	TYR	2.0
1	A	130	MET	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
2	CL	B	301	1/1	0.90	0.08	62,62,62,62	0
2	CL	B	302	1/1	0.91	0.22	62,62,62,62	0
2	CL	D	301	1/1	0.91	0.12	59,59,59,59	0
2	CL	E	303	1/1	0.92	0.06	57,57,57,57	0
2	CL	E	302	1/1	0.93	0.15	57,57,57,57	0
2	CL	E	301	1/1	0.95	0.17	59,59,59,59	0
2	CL	C	302	1/1	0.95	0.19	60,60,60,60	0
2	CL	D	302	1/1	0.95	0.09	57,57,57,57	0
2	CL	F	303	1/1	0.95	0.13	57,57,57,57	0
2	CL	F	302	1/1	0.96	0.12	57,57,57,57	0
2	CL	A	301	1/1	0.97	0.06	60,60,60,60	0
2	CL	F	301	1/1	0.97	0.21	57,57,57,57	0
2	CL	C	303	1/1	0.98	0.07	60,60,60,60	0
2	CL	C	301	1/1	0.98	0.28	57,57,57,57	0
2	CL	A	302	1/1	0.98	0.11	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.