Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:42 PM GMT

PDB ID	:	4J91
Title	:	Diamond-shaped octameric structure of KtrA with ADP bound
Authors	:	Vieira-Pires, R.S.; Morais-Cabral, J.H.
Deposited on	:	2013-02-15
Resolution	:	2.93 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 ⓘ symbol.

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

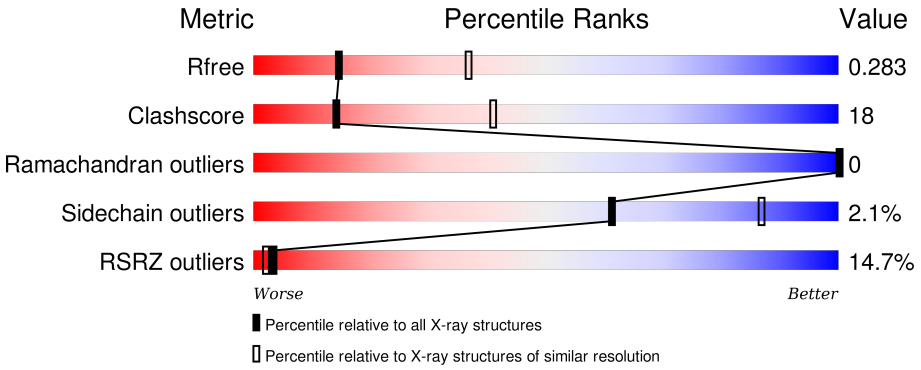
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	2057 (2.98-2.90)
Clashscore	102246	2308 (2.98-2.90)
Ramachandran outliers	100387	2245 (2.98-2.90)
Sidechain outliers	100360	2247 (2.98-2.90)
RSRZ outliers	91569	2065 (2.98-2.90)

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	222	17% 66% 25% • 8%
1	B	222	8% 72% 24% • •
1	C	222	20% 66% 27% • • 5%
1	D	222	12% 67% 27% • 5%

2 Entry composition

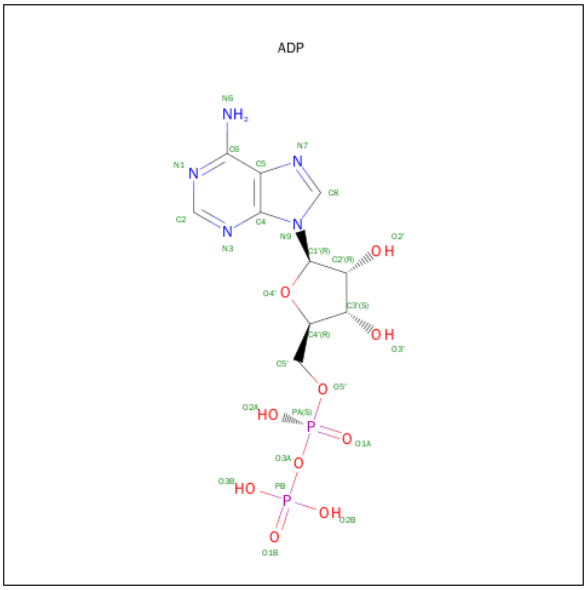
There are 2 unique types of molecules in this entry. The entry contains 6734 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ktr system potassium uptake protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1601	1016	275	302	8			
1	B	215	Total	C	N	O	S	0	0	0
			1689	1071	290	320	8			
1	C	212	Total	C	N	O	S	0	0	0
			1666	1058	284	316	8			
1	D	212	Total	C	N	O	S	0	0	0
			1670	1058	287	317	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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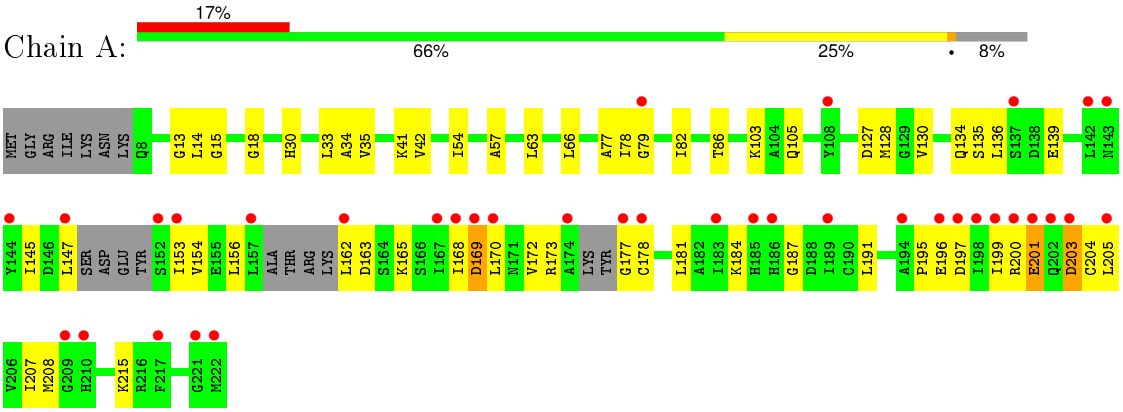
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

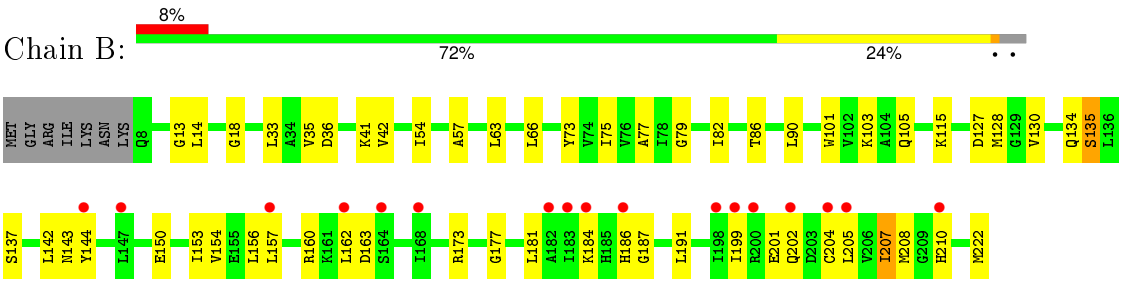
3 Residue-property plots (i)

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.

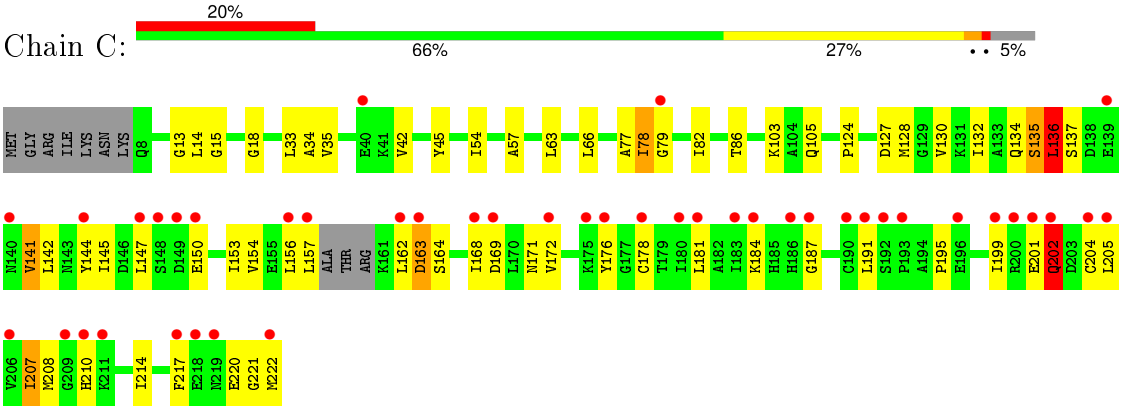
- Molecule 1: Ktr system potassium uptake protein A



- Molecule 1: Ktr system potassium uptake protein A

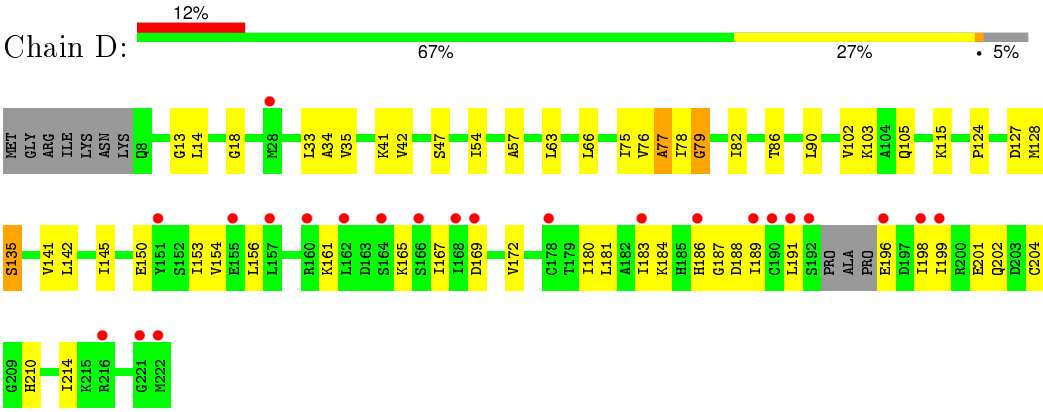


- Molecule 1: Ktr system potassium uptake protein A



- Molecule 1: Ktr system potassium uptake protein A

Chain D:


12%
67%
27%
• 5%
MET GLY ARG ILE LYS ASN LYS Q8 G13 L14 G18 M28 L33 A34 V35 K41 V42 S47 I54 A57 L63 L66 I75 V76 A77 I78 G79 I82 T86 L90 V102 K103 A104 Q105 K115 P124 D127 M128 G129 V130 Q134
S135 V141 L142 I145 E150 Y151 S152 I153 V154 E155 L156 L157 R160 K161 L162 D163 S164 K165 S166 I167 I168 D169 V172 C178 T179 I180 L181 A182 I183 K184 H185 H186 G187 D188 I189 C190 L191 S192 PRO ALA PRO E196 D197 I198 I199 R200 E201 Q202 D203 C204 L205 V206 I207 M208
G209 H210 I214 K215 R216 G221 M222

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	147.93Å 84.63Å 113.67Å 90.00° 128.37° 90.00°	Depositor
Resolution (Å)	89.12 – 2.93 42.31 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.7 (89.12-2.93) 99.6 (42.31-2.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.252 , 0.278 0.253 , 0.283	Depositor DCC
R_{free} test set	1192 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	72.7	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.1	EDS
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 27727 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6734	wwPDB-VP
Average B, all atoms (Å^2)	96.0	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: ADP

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	0.46	0/1622	0.66	5/2188 (0.2%)
1	B	0.49	2/1715 (0.1%)	0.61	0/2317
1	C	0.47	1/1691 (0.1%)	0.68	6/2283 (0.3%)
1	D	0.51	2/1693 (0.1%)	0.64	4/2283 (0.2%)
All	All	0.48	5/6721 (0.1%)	0.65	15/9071 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	196	GLU	CD-OE1	-9.05	1.15	1.25
1	C	135	SER	CB-OG	7.08	1.51	1.42
1	B	135	SER	CB-OG	5.60	1.49	1.42
1	D	135	SER	CB-OG	5.46	1.49	1.42
1	B	101	TRP	CD2-CE2	5.12	1.47	1.41

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	78	ILE	N-CA-C	-8.15	89.01	111.00
1	C	136	LEU	CA-CB-CG	6.54	130.35	115.30
1	A	201	GLU	CB-CA-C	-6.38	97.63	110.40
1	C	15	GLY	N-CA-C	-5.85	98.48	113.10
1	D	79	GLY	N-CA-C	-5.80	98.61	113.10
1	C	78	ILE	N-CA-C	-5.70	95.60	111.00
1	C	202	GLN	CB-CA-C	-5.36	99.68	110.40
1	D	188	ASP	CB-CG-OD2	5.26	123.03	118.30
1	C	169	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	163	ASP	CB-CG-OD2	5.20	122.98	118.30
1	C	163	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	169	ASP	CB-CG-OD2	5.17	122.95	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	197	ASP	N-CA-CB	5.16	119.89	110.60
1	D	77	ALA	CB-CA-C	5.15	117.83	110.10
1	A	78	ILE	N-CA-C	-5.01	97.48	111.00

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	1601	0	1624	65	1
1	B	1689	0	1711	60	0
1	C	1666	0	1685	85	2
1	D	1670	0	1691	60	2
2	A	27	0	12	2	0
2	B	27	0	12	1	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
All	All	6734	0	6759	245	4

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 18.

All (245) 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:D:13:GLY:HA3	1:D:77:ALA:O	1.38	1.23
1:B:115:LYS:HG3	1:D:90:LEU:HD11	1.22	1.16
1:C:202:GLN:HG3	1:C:202:GLN:O	1.34	1.13
1:C:13:GLY:HA3	1:C:77:ALA:O	1.46	1.11
1:A:13:GLY:HA3	1:A:77:ALA:O	1.49	1.11
1:A:184:LYS:O	1:A:203:ASP:OD1	1.70	1.08
1:C:154:VAL:HG12	1:C:156:LEU:HD12	1.35	1.05
1:B:90:LEU:HD11	1:D:115:LYS:HG3	1.06	1.05
1:A:170:LEU:HD12	1:A:170:LEU:O	1.57	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:GLY:HA3	1:B:77:ALA:O	1.59	1.02
1:B:154:VAL:HG12	1:B:156:LEU:HD12	1.41	1.02
1:D:154:VAL:HG12	1:D:156:LEU:HD12	1.38	1.01
1:C:128:MET:HG2	1:D:128:MET:HG2	1.43	1.01
1:C:202:GLN:CG	1:C:202:GLN:O	2.07	1.01
1:A:154:VAL:HG12	1:A:156:LEU:HD12	1.39	1.00
1:A:162:LEU:HD22	1:A:170:LEU:CD2	1.95	0.95
1:C:141:VAL:HB	1:C:154:VAL:HG13	1.51	0.93
1:C:162:LEU:HD21	1:C:222:MET:HE3	1.49	0.92
1:B:90:LEU:CD1	1:D:115:LYS:HG3	2.01	0.89
1:C:162:LEU:HD23	1:C:205:LEU:HD11	1.55	0.88
1:C:154:VAL:HG12	1:C:156:LEU:CD1	2.03	0.88
1:C:134:GLN:CB	1:C:144:TYR:OH	2.22	0.88
1:A:128:MET:HG2	1:B:128:MET:HG2	1.55	0.85
1:A:184:LYS:HB3	1:A:204:CYS:HB2	1.56	0.85
1:D:154:VAL:HG12	1:D:156:LEU:CD1	2.06	0.84
1:A:172:VAL:HG12	1:A:178:CYS:O	1.76	0.84
1:B:154:VAL:HG12	1:B:156:LEU:CD1	2.08	0.83
1:A:154:VAL:HG12	1:A:156:LEU:CD1	2.07	0.83
1:A:168:ILE:HG23	1:A:195:PRO:O	1.78	0.82
1:B:13:GLY:O	1:B:18:GLY:HA3	1.80	0.81
1:C:127:ASP:O	1:C:130:VAL:HG22	1.82	0.79
1:A:30:HIS:NE2	1:B:137:SER:HB2	1.99	0.78
1:C:141:VAL:CG2	1:C:141:VAL:O	2.31	0.78
1:D:172:VAL:HG21	1:D:180:ILE:HG13	1.66	0.78
1:B:162:LEU:HD21	1:B:199:ILE:HG21	1.64	0.77
1:A:127:ASP:O	1:A:130:VAL:HG22	1.84	0.77
1:A:79:GLY:HA2	1:A:105:GLN:NE2	1.99	0.76
1:C:13:GLY:O	1:C:18:GLY:HA3	1.85	0.76
1:B:127:ASP:O	1:B:130:VAL:HG22	1.84	0.76
1:A:13:GLY:O	1:A:18:GLY:HA3	1.87	0.74
1:C:141:VAL:HB	1:C:154:VAL:CG1	2.17	0.74
1:D:13:GLY:O	1:D:18:GLY:HA3	1.86	0.74
1:B:162:LEU:CD2	1:B:199:ILE:HG21	2.18	0.74
1:B:79:GLY:HA2	1:B:105:GLN:NE2	2.01	0.74
1:C:162:LEU:CD1	1:C:221:GLY:O	2.35	0.74
1:C:79:GLY:HA2	1:C:105:GLN:NE2	2.02	0.74
1:D:127:ASP:O	1:D:130:VAL:HG22	1.86	0.74
1:A:170:LEU:CD1	1:A:172:VAL:HG23	2.19	0.73
1:C:176:TYR:CE1	1:C:217:PHE:HA	2.23	0.73
1:D:79:GLY:HA2	1:D:105:GLN:NE2	2.04	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HG22	1:C:136:LEU:HD22	1.72	0.72
1:A:165:LYS:HG2	1:A:169:ASP:OD2	1.89	0.72
1:A:162:LEU:HD22	1:A:170:LEU:HD23	1.71	0.72
1:A:30:HIS:CE1	1:B:137:SER:HB2	2.26	0.71
1:B:199:ILE:HD13	1:B:205:LEU:HD21	1.71	0.71
1:C:141:VAL:HG23	1:C:141:VAL:O	1.91	0.71
1:C:154:VAL:CG1	1:C:156:LEU:CD1	2.68	0.70
1:C:134:GLN:HB2	1:C:144:TYR:OH	1.91	0.70
1:C:162:LEU:HD12	1:C:221:GLY:O	1.91	0.69
1:D:199:ILE:HD13	1:D:205:LEU:HD21	1.73	0.69
1:C:199:ILE:HD13	1:C:205:LEU:HD21	1.75	0.69
1:C:134:GLN:HB3	1:C:144:TYR:CZ	2.27	0.69
1:C:181:LEU:O	1:C:191:LEU:O	2.11	0.69
1:A:199:ILE:HD13	1:A:205:LEU:HD21	1.73	0.69
1:C:162:LEU:HD21	1:C:222:MET:CE	2.20	0.69
1:D:154:VAL:CG1	1:D:156:LEU:CD1	2.70	0.68
1:A:154:VAL:CG1	1:A:156:LEU:CD1	2.72	0.68
1:C:162:LEU:HD11	1:C:222:MET:HG3	1.76	0.68
1:A:79:GLY:CA	1:A:105:GLN:NE2	2.56	0.68
1:B:79:GLY:CA	1:B:105:GLN:NE2	2.57	0.68
1:C:162:LEU:HD22	1:C:222:MET:HE2	1.75	0.67
1:A:181:LEU:O	1:A:191:LEU:O	2.11	0.67
1:B:201:GLU:O	1:B:202:GLN:HB3	1.95	0.67
1:C:162:LEU:CD2	1:C:222:MET:CE	2.73	0.67
1:B:154:VAL:CG1	1:B:156:LEU:CD1	2.73	0.66
1:D:79:GLY:CA	1:D:105:GLN:NE2	2.58	0.66
1:A:168:ILE:CG2	1:A:195:PRO:HB3	2.25	0.66
1:C:171:ASN:O	1:C:171:ASN:OD1	2.12	0.66
1:C:79:GLY:CA	1:C:105:GLN:NE2	2.59	0.65
1:C:132:ILE:HG22	1:C:136:LEU:CD2	2.27	0.65
1:A:170:LEU:HD12	1:A:172:VAL:HG23	1.78	0.64
1:D:13:GLY:CA	1:D:77:ALA:O	2.32	0.63
1:B:181:LEU:O	1:B:191:LEU:O	2.16	0.63
1:A:162:LEU:CD2	1:A:170:LEU:CD2	2.75	0.62
1:A:145:ILE:HG12	1:B:143:ASN:HB3	1.82	0.62
1:A:170:LEU:CD1	1:A:172:VAL:CG2	2.78	0.61
1:A:128:MET:CG	1:B:128:MET:HG2	2.30	0.60
1:C:176:TYR:OH	1:C:220:GLU:HB2	2.01	0.59
1:B:184:LYS:HB3	1:B:204:CYS:HB2	1.83	0.59
1:C:103:LYS:HE3	1:C:105:GLN:HE22	1.68	0.58
1:D:184:LYS:HB3	1:D:204:CYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:MET:HG2	1:B:128:MET:CG	2.30	0.58
1:C:184:LYS:HB3	1:C:204:CYS:HB2	1.84	0.57
1:C:162:LEU:CD2	1:C:222:MET:HE2	2.34	0.57
1:D:181:LEU:HB2	1:D:206:VAL:HG12	1.85	0.57
1:B:153:ILE:HG12	1:B:208:MET:HG3	1.85	0.57
1:B:173:ARG:O	1:B:177:GLY:HA2	2.05	0.57
1:C:154:VAL:CG1	1:C:156:LEU:HD11	2.34	0.56
1:D:154:VAL:CG1	1:D:156:LEU:HD11	2.35	0.56
1:C:128:MET:HG2	1:D:128:MET:CG	2.26	0.56
1:D:103:LYS:HE3	1:D:105:GLN:HE22	1.70	0.56
1:C:128:MET:CG	1:D:128:MET:HG2	2.27	0.56
1:A:170:LEU:CD1	1:A:170:LEU:O	2.43	0.56
1:B:103:LYS:HE3	1:B:105:GLN:HE22	1.70	0.56
1:A:196:GLU:O	1:A:196:GLU:HG2	2.06	0.56
1:C:136:LEU:HD11	1:D:75:ILE:HD11	1.86	0.56
1:B:184:LYS:HE3	1:B:187:GLY:HA2	1.88	0.56
1:D:153:ILE:HG12	1:D:208:MET:HG3	1.88	0.56
1:C:134:GLN:HB3	1:C:144:TYR:OH	2.01	0.55
1:A:153:ILE:HG12	1:A:208:MET:HG3	1.88	0.55
1:A:103:LYS:HE3	1:A:105:GLN:HE22	1.72	0.55
1:A:154:VAL:CG1	1:A:156:LEU:HD11	2.36	0.54
1:C:154:VAL:CG1	1:C:156:LEU:HD12	2.22	0.54
1:A:168:ILE:HG12	1:A:195:PRO:O	2.07	0.54
1:B:154:VAL:CG1	1:B:156:LEU:HD11	2.38	0.54
1:C:153:ILE:HG12	1:C:208:MET:HG3	1.89	0.53
1:B:103:LYS:HE2	2:B:601:ADP:O2B	2.09	0.53
1:D:207:ILE:HG21	1:D:214:ILE:HG12	1.90	0.53
1:A:14:LEU:O	1:A:41:LYS:HD2	2.08	0.53
1:A:147:LEU:O	1:B:184:LYS:HD2	2.08	0.53
1:D:186:HIS:CG	1:D:186:HIS:O	2.60	0.53
1:C:134:GLN:CG	1:C:144:TYR:OH	2.56	0.53
1:B:14:LEU:O	1:B:41:LYS:HD2	2.09	0.53
1:B:162:LEU:CD2	1:B:199:ILE:CG2	2.85	0.53
1:B:162:LEU:HD23	1:B:199:ILE:CG2	2.38	0.52
1:C:134:GLN:HG3	1:C:144:TYR:OH	2.08	0.52
1:A:184:LYS:C	1:A:203:ASP:OD1	2.46	0.52
1:D:14:LEU:O	1:D:41:LYS:HD2	2.09	0.52
1:B:186:HIS:CG	1:B:186:HIS:O	2.63	0.52
1:B:201:GLU:O	1:B:202:GLN:CB	2.57	0.52
1:B:90:LEU:HD11	1:D:115:LYS:CG	2.03	0.52
1:B:82:ILE:O	1:B:86:THR:HG23	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LYS:HE2	2:C:601:ADP:O2B	2.10	0.51
1:C:162:LEU:CD2	1:C:205:LEU:HD11	2.35	0.51
1:A:165:LYS:CG	1:A:169:ASP:OD2	2.56	0.51
1:C:162:LEU:HD11	1:C:221:GLY:O	2.10	0.51
1:D:207:ILE:CG2	1:D:208:MET:N	2.74	0.51
1:D:141:VAL:CG1	1:D:142:LEU:N	2.74	0.51
1:D:202:GLN:O	1:D:202:GLN:HG2	2.11	0.51
1:B:63:LEU:HA	1:B:66:LEU:HD12	1.93	0.51
1:B:115:LYS:HG3	1:D:90:LEU:CD1	2.16	0.50
1:A:103:LYS:HE2	2:A:601:ADP:O2B	2.10	0.50
1:D:141:VAL:HG12	1:D:142:LEU:N	2.26	0.50
1:C:130:VAL:O	1:C:134:GLN:HG2	2.11	0.50
1:C:82:ILE:O	1:C:86:THR:HG23	2.12	0.50
1:B:33:LEU:HD23	1:B:35:VAL:HG23	1.94	0.49
1:C:33:LEU:HD23	1:C:35:VAL:HG23	1.95	0.49
1:A:42:VAL:HG21	1:A:54:ILE:HG13	1.94	0.49
1:B:202:GLN:O	1:B:202:GLN:HG2	2.13	0.49
1:A:63:LEU:HA	1:A:66:LEU:HD12	1.95	0.49
1:D:167:ILE:HD11	1:D:183:ILE:HD11	1.94	0.48
1:C:42:VAL:HG21	1:C:54:ILE:HG13	1.95	0.48
1:D:57:ALA:HA	1:D:63:LEU:HD11	1.95	0.48
1:B:42:VAL:HG21	1:B:54:ILE:HG13	1.94	0.48
1:D:33:LEU:HD23	1:D:35:VAL:HG23	1.96	0.48
1:D:42:VAL:HG21	1:D:54:ILE:HG13	1.96	0.48
1:D:184:LYS:HE3	1:D:187:GLY:HA2	1.96	0.48
1:C:57:ALA:HA	1:C:63:LEU:HD11	1.95	0.48
1:A:57:ALA:HA	1:A:63:LEU:HD11	1.95	0.47
1:C:163:ASP:OD1	1:C:164:SER:N	2.47	0.47
1:C:162:LEU:HD13	1:C:222:MET:HG2	1.95	0.47
1:B:162:LEU:HD11	1:B:205:LEU:HD11	1.96	0.47
1:C:33:LEU:CD2	1:C:35:VAL:CG2	2.93	0.47
1:C:145:ILE:HG13	1:D:145:ILE:CD1	2.44	0.47
1:C:162:LEU:CD1	1:C:222:MET:HG3	2.44	0.47
1:C:103:LYS:HE3	1:C:105:GLN:NE2	2.30	0.47
1:C:176:TYR:CZ	1:C:217:PHE:HA	2.50	0.47
1:C:207:ILE:CG2	1:C:214:ILE:HG12	2.43	0.47
1:A:184:LYS:HE3	1:A:187:GLY:HA2	1.97	0.47
1:B:162:LEU:HD23	1:B:199:ILE:HG22	1.97	0.47
1:A:79:GLY:HA2	1:A:105:GLN:HE21	1.79	0.47
1:B:160:ARG:O	1:B:163:ASP:HB2	2.15	0.47
1:C:147:LEU:HB3	1:D:189:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:LYS:HD2	1:D:169:ASP:HB3	1.97	0.47
1:A:82:ILE:O	1:A:86:THR:HG23	2.15	0.47
1:A:33:LEU:HD23	1:A:35:VAL:HG23	1.97	0.47
1:C:141:VAL:HG22	1:C:141:VAL:O	2.13	0.46
1:B:57:ALA:HA	1:B:63:LEU:HD11	1.96	0.46
1:D:33:LEU:CD2	1:D:35:VAL:CG2	2.94	0.46
1:A:162:LEU:CD2	1:A:170:LEU:HD22	2.45	0.46
1:C:154:VAL:HG11	1:C:156:LEU:HD11	1.96	0.46
1:D:63:LEU:HA	1:D:66:LEU:HD12	1.98	0.46
1:D:82:ILE:O	1:D:86:THR:HG23	2.16	0.46
1:D:207:ILE:HG23	1:D:208:MET:N	2.31	0.46
1:B:33:LEU:CD2	1:B:35:VAL:CG2	2.94	0.46
1:A:33:LEU:CD2	1:A:35:VAL:CG2	2.94	0.46
1:D:181:LEU:O	1:D:191:LEU:O	2.34	0.45
1:A:15:GLY:HA3	2:A:601:ADP:O5'	2.15	0.45
1:D:154:VAL:HG11	1:D:156:LEU:HD11	1.98	0.45
1:C:145:ILE:HG13	1:D:145:ILE:HG13	1.99	0.45
1:C:150:GLU:HB3	1:C:210:HIS:CE1	2.52	0.45
1:B:103:LYS:HE3	1:B:105:GLN:NE2	2.32	0.45
1:A:130:VAL:O	1:A:134:GLN:HG2	2.18	0.44
1:D:183:ILE:O	1:D:189:ILE:HG13	2.16	0.44
1:A:172:VAL:CG1	1:A:178:CYS:O	2.56	0.44
1:C:207:ILE:HD11	1:C:217:PHE:CE2	2.52	0.44
1:A:14:LEU:HD11	1:A:34:ALA:HB1	2.00	0.44
1:A:139:GLU:OE2	1:B:73:TYR:OH	2.34	0.44
1:C:14:LEU:HD13	1:C:45:TYR:CD1	2.52	0.44
1:A:103:LYS:HE3	1:A:105:GLN:NE2	2.32	0.44
1:B:79:GLY:C	1:B:105:GLN:NE2	2.71	0.44
1:A:170:LEU:C	1:A:170:LEU:HD12	2.33	0.44
1:C:184:LYS:HE3	1:C:187:GLY:HA2	1.99	0.44
1:C:142:LEU:HD11	1:C:157:LEU:HB2	1.99	0.44
1:A:154:VAL:HG11	1:A:156:LEU:HD11	2.00	0.44
1:C:63:LEU:HA	1:C:66:LEU:HD12	2.00	0.44
1:C:172:VAL:HG12	1:C:178:CYS:O	2.17	0.43
1:C:128:MET:HG3	1:D:124:PRO:HA	2.01	0.43
1:A:168:ILE:HG23	1:A:195:PRO:HB3	2.00	0.43
1:A:127:ASP:O	1:A:130:VAL:CG2	2.62	0.43
1:A:136:LEU:HD21	1:B:75:ILE:HD11	2.00	0.43
1:B:130:VAL:O	1:B:134:GLN:HG2	2.19	0.43
1:C:124:PRO:HA	1:D:128:MET:HG3	2.01	0.43
1:D:130:VAL:O	1:D:134:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:LYS:HE3	1:D:105:GLN:NE2	2.32	0.43
1:D:79:GLY:C	1:D:105:GLN:NE2	2.72	0.43
1:D:207:ILE:CG2	1:D:214:ILE:HG12	2.48	0.43
1:B:156:LEU:HD23	1:B:222:MET:HE1	2.01	0.43
1:D:201:GLU:O	1:D:202:GLN:HB3	2.18	0.43
1:A:145:ILE:HD11	1:B:144:TYR:CA	2.49	0.42
1:B:150:GLU:HB3	1:B:210:HIS:CE1	2.54	0.42
1:C:201:GLU:O	1:C:202:GLN:CB	2.67	0.42
1:C:14:LEU:HD11	1:C:34:ALA:HB1	2.00	0.42
1:C:162:LEU:CD1	1:C:222:MET:CG	2.98	0.42
1:C:172:VAL:O	1:C:172:VAL:HG12	2.20	0.42
1:D:150:GLU:HB3	1:D:210:HIS:CE1	2.54	0.42
1:A:79:GLY:C	1:A:105:GLN:NE2	2.73	0.41
1:D:79:GLY:O	1:D:105:GLN:CG	2.68	0.41
1:C:79:GLY:O	1:C:105:GLN:CG	2.69	0.41
1:B:142:LEU:HD11	1:B:157:LEU:HB2	2.02	0.41
1:B:33:LEU:CD2	1:B:35:VAL:HG23	2.50	0.41
1:C:141:VAL:CB	1:C:154:VAL:HG13	2.35	0.41
1:A:173:ARG:O	1:A:177:GLY:HA2	2.20	0.41
1:B:207:ILE:HD13	1:B:207:ILE:HG21	1.78	0.41
1:C:79:GLY:C	1:C:105:GLN:NE2	2.75	0.41
1:A:168:ILE:CG2	1:A:195:PRO:O	2.60	0.41
1:B:14:LEU:HD12	1:B:36:ASP:HB2	2.04	0.40
1:C:78:ILE:HA	2:C:601:ADP:H5'2	2.03	0.40
1:C:168:ILE:N	1:C:195:PRO:O	2.51	0.40
1:A:184:LYS:CB	1:A:204:CYS:HB2	2.41	0.40
1:B:160:ARG:HG2	1:B:201:GLU:OE2	2.21	0.40
1:C:145:ILE:HG13	1:D:145:ILE:HD11	2.03	0.40
1:C:127:ASP:O	1:C:130:VAL:CG2	2.62	0.40
1:D:14:LEU:HD11	1:D:34:ALA:HB1	2.03	0.40
1:D:76:VAL:HB	1:D:102:VAL:HG13	2.03	0.40

All (4) 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:C:202:GLN:OE1	1:C:202:GLN:OE1[2_656]	1.03	1.17
1:C:157:LEU:CD2	1:C:201:GLU:OE1[2_656]	1.60	0.60
1:A:173:ARG:NH2	1:D:198:ILE:CD1[1_554]	1.94	0.26
1:D:47:SER:OG	1:D:161:LYS:NZ[4_556]	2.19	0.01

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	197/222 (89%)	193 (98%)	4 (2%)	0	100	100
1	B	213/222 (96%)	209 (98%)	4 (2%)	0	100	100
1	C	208/222 (94%)	203 (98%)	5 (2%)	0	100	100
1	D	208/222 (94%)	204 (98%)	4 (2%)	0	100	100
All	All	826/888 (93%)	809 (98%)	17 (2%)	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	175/190 (92%)	169 (97%)	6 (3%)	44	78
1	B	184/190 (97%)	182 (99%)	2 (1%)	80	94
1	C	182/190 (96%)	176 (97%)	6 (3%)	45	79
1	D	182/190 (96%)	181 (100%)	1 (0%)	92	98
All	All	723/760 (95%)	708 (98%)	15 (2%)	61	87

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	SER
1	A	200	ARG

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Mol	Chain	Res	Type
1	A	201	GLU
1	A	203	ASP
1	A	207	ILE
1	A	215	LYS
1	B	135	SER
1	B	207	ILE
1	C	135	SER
1	C	136	LEU
1	C	137	SER
1	C	141	VAL
1	C	202	GLN
1	C	207	ILE
1	D	135	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	GLN
1	B	105	GLN
1	B	171	ASN
1	B	210	HIS
1	C	105	GLN
1	C	171	ASN
1	C	210	HIS
1	D	105	GLN
1	D	210	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	601	-	22,29,29	1.11	1 (4%)	27,45,45	1.82	4 (14%)
2	ADP	B	601	-	22,29,29	0.98	1 (4%)	27,45,45	1.98	5 (18%)
2	ADP	C	601	-	22,29,29	1.07	1 (4%)	27,45,45	1.85	4 (14%)
2	ADP	D	601	-	22,29,29	1.02	1 (4%)	27,45,45	1.88	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	601	-	-	0/12/32/32	0/3/3/3
2	ADP	B	601	-	-	0/12/32/32	0/3/3/3
2	ADP	C	601	-	-	0/12/32/32	0/3/3/3
2	ADP	D	601	-	-	0/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	ADP	C5-C4	3.10	1.47	1.40
2	D	601	ADP	C5-C4	3.16	1.47	1.40
2	C	601	ADP	C5-C4	3.34	1.48	1.40
2	A	601	ADP	C5-C4	3.46	1.48	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	601	ADP	N3-C2-N1	-7.53	123.12	128.89
2	D	601	ADP	N3-C2-N1	-7.40	123.22	128.89
2	A	601	ADP	N3-C2-N1	-6.98	123.55	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	ADP	N3-C2-N1	-6.31	124.07	128.89
2	C	601	ADP	PA-O3A-PB	-3.68	120.33	132.67
2	C	601	ADP	C4-C5-N7	-3.60	106.17	109.48
2	A	601	ADP	C4-C5-N7	-3.16	106.57	109.48
2	B	601	ADP	PA-O3A-PB	-3.09	122.29	132.67
2	B	601	ADP	C4-C5-N7	-3.00	106.72	109.48
2	D	601	ADP	C4-C5-N7	-2.93	106.79	109.48
2	D	601	ADP	PA-O3A-PB	-2.89	122.99	132.67
2	A	601	ADP	C2'-C1'-N9	-2.28	110.81	114.29
2	C	601	ADP	C2'-C1'-N9	-2.21	110.91	114.29
2	A	601	ADP	PA-O3A-PB	-2.17	125.38	132.67
2	B	601	ADP	C1'-N9-C4	-2.06	123.83	126.94
2	B	601	ADP	C2-N1-C6	2.16	122.63	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ADP	2	0
2	B	601	ADP	1	0
2	C	601	ADP	2	0

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	205/222 (92%)	0.97	37 (18%) 2 1	42, 85, 189, 237	0
1	B	215/222 (96%)	0.42	17 (7%) 15 11	36, 66, 133, 147	0
1	C	212/222 (95%)	0.99	44 (20%) 1 1	54, 86, 189, 220	0
1	D	212/222 (95%)	0.67	26 (12%) 5 3	47, 86, 184, 221	0
All	All	844/888 (95%)	0.76	124 (14%) 3 2	36, 80, 182, 237	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	162	LEU	9.4
1	A	199	ILE	8.9
1	D	196	GLU	8.4
1	C	193	PRO	7.2
1	C	178	CYS	7.2
1	C	156	LEU	6.2
1	C	187	GLY	6.2
1	D	221	GLY	5.7
1	A	222	MET	5.6
1	D	168	ILE	5.5
1	A	221	GLY	5.5
1	C	222	MET	5.2
1	A	152	SER	5.0
1	A	169	ASP	4.8
1	C	184	LYS	4.7
1	D	222	MET	4.7
1	C	186	HIS	4.7
1	C	183	ILE	4.6
1	C	196	GLU	4.6
1	B	205	LEU	4.6
1	C	162	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	139	GLU	4.5
1	A	167	ILE	4.4
1	C	218	GLU	4.4
1	C	206	VAL	4.4
1	D	151	TYR	4.3
1	C	181	LEU	4.3
1	D	189	ILE	4.2
1	C	211	LYS	4.1
1	D	198	ILE	4.1
1	C	199	ILE	4.1
1	C	180	ILE	4.1
1	C	163	ASP	4.0
1	C	210	HIS	4.0
1	A	217	PHE	4.0
1	D	169	ASP	4.0
1	C	202	GLN	3.9
1	C	169	ASP	3.9
1	A	205	LEU	3.9
1	A	144	TYR	3.7
1	C	140	ASN	3.6
1	D	186	HIS	3.6
1	A	194	ALA	3.5
1	D	183	ILE	3.5
1	D	28	MET	3.5
1	A	147	LEU	3.5
1	C	192	SER	3.5
1	C	157	LEU	3.5
1	B	204	CYS	3.4
1	C	204	CYS	3.4
1	A	198	ILE	3.4
1	A	157	LEU	3.3
1	D	199	ILE	3.3
1	B	164	SER	3.3
1	A	79	GLY	3.2
1	C	150	GLU	3.2
1	C	200	ARG	3.2
1	A	178	CYS	3.2
1	D	190	CYS	3.1
1	B	198	ILE	3.1
1	C	176	TYR	3.1
1	C	201	GLU	3.0
1	D	207	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	209	GLY	3.0
1	A	153	ILE	3.0
1	D	208	MET	3.0
1	C	79	GLY	3.0
1	A	174	ALA	2.9
1	D	205	LEU	2.9
1	A	170	LEU	2.9
1	C	219	ASN	2.9
1	A	185	HIS	2.9
1	D	155	GLU	2.8
1	A	168	ILE	2.8
1	C	217	PHE	2.8
1	B	210	HIS	2.8
1	B	183	ILE	2.8
1	A	202	GLN	2.8
1	A	143	ASN	2.7
1	C	144	TYR	2.7
1	D	192	SER	2.7
1	A	197	ASP	2.7
1	C	147	LEU	2.7
1	A	108	TYR	2.7
1	C	168	ILE	2.6
1	A	200	ARG	2.6
1	B	202	GLN	2.6
1	B	182	ALA	2.6
1	C	191	LEU	2.5
1	A	183	ILE	2.5
1	B	199	ILE	2.5
1	A	203	ASP	2.5
1	B	144	TYR	2.4
1	D	160	ARG	2.4
1	A	210	HIS	2.4
1	B	200	ARG	2.4
1	A	186	HIS	2.4
1	D	162	LEU	2.4
1	C	175	LYS	2.4
1	D	157	LEU	2.3
1	B	168	ILE	2.3
1	C	205	LEU	2.3
1	A	189	ILE	2.3
1	A	196	GLU	2.3
1	C	40	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	172	VAL	2.3
1	B	186	HIS	2.2
1	B	184	LYS	2.2
1	B	157	LEU	2.2
1	C	149	ASP	2.2
1	A	142	LEU	2.2
1	D	191	LEU	2.2
1	D	178	CYS	2.1
1	A	201	GLU	2.1
1	B	147	LEU	2.1
1	C	190	CYS	2.1
1	D	216	ARG	2.1
1	C	148	SER	2.1
1	A	209	GLY	2.1
1	D	164	SER	2.1
1	D	166	SER	2.1
1	B	162	LEU	2.0
1	A	137	SER	2.0
1	A	177	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 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
2	ADP	C	601	27/27	0.95	0.17	-0.56	66,73,78,81	0
2	ADP	B	601	27/27	0.97	0.15	-0.74	50,59,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	ADP	D	601	27/27	0.94	0.17	-0.78	66,70,74,75	0
2	ADP	A	601	27/27	0.97	0.16	-0.90	56,64,71,72	0

6.5 Other polymers (i)

There are no such residues in this entry.