



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:58 pm GMT

PDB ID : 3VPC
Title : ArgX from Sulfolobus tokodaii complexed with ADP
Authors : Tomita, T.; Horie, A.; Kuzuyama, T.; Nishiyama, M.
Deposited on : 2012-02-29
Resolution : 1.87 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

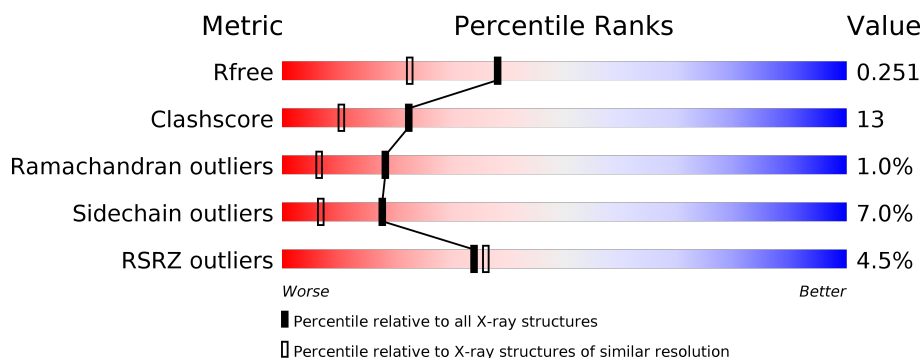
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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}	100719	7505 (1.90-1.86)
Clashscore	112137	8369 (1.90-1.86)
Ramachandran outliers	110173	8279 (1.90-1.86)
Sidechain outliers	110143	8280 (1.90-1.86)
RSRZ outliers	101464	7571 (1.90-1.86)

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 $\leq 5\%$. 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	282	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>.</div> </div> </div>
1	B	282	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
1	C	282	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>.</div> </div> </div>
1	D	282	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

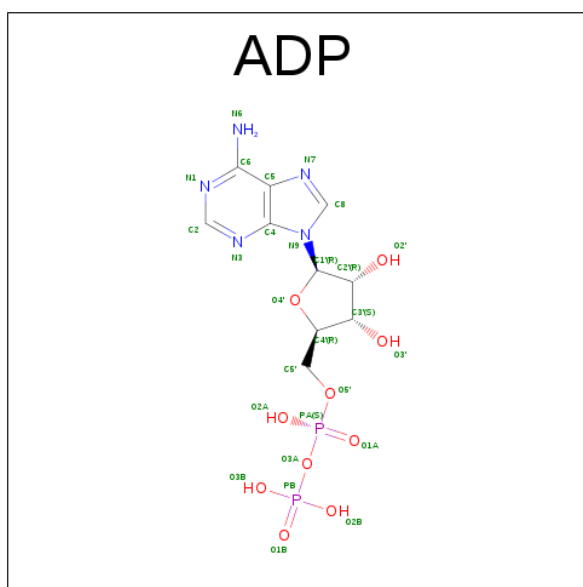
There are 3 unique types of molecules in this entry. The entry contains 10021 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Putative acetylornithine deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	5	0
			2246	1440	382	417	7			
1	B	282	Total	C	N	O	S	0	8	0
			2260	1450	382	421	7			
1	C	275	Total	C	N	O	S	0	7	0
			2213	1420	375	411	7			
1	D	282	Total	C	N	O	S	0	3	0
			2238	1435	379	417	7			

- 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		

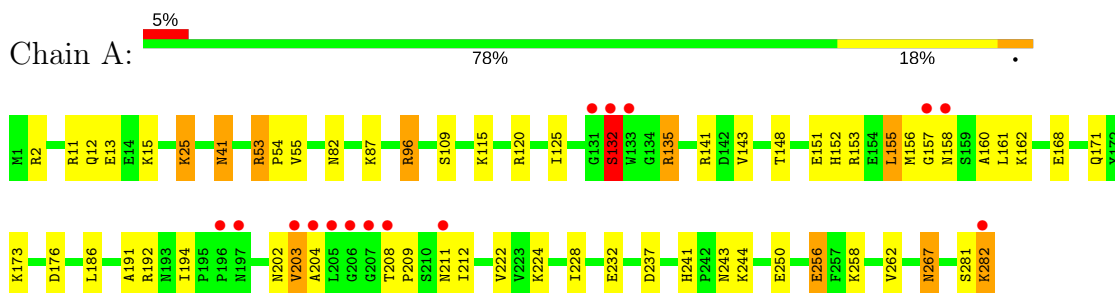
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	247	Total	O	0	0
			247	247		
3	B	270	Total	O	0	0
			270	270		
3	C	221	Total	O	0	0
			221	221		
3	D	218	Total	O	0	0
			218	218		

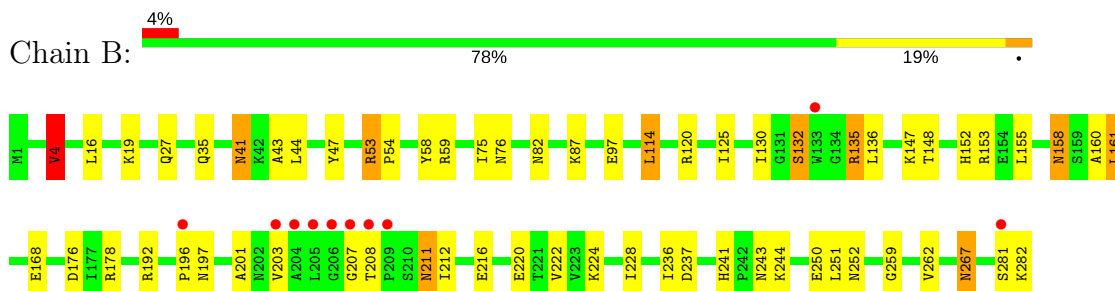
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

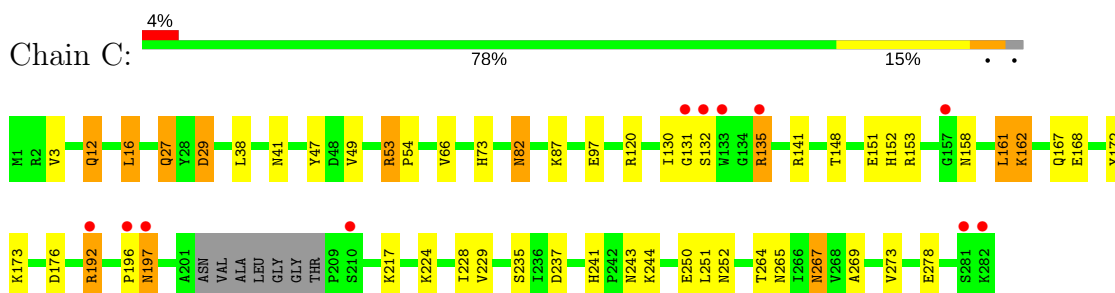
• Molecule 1: Putative acetylornithine deacetylase



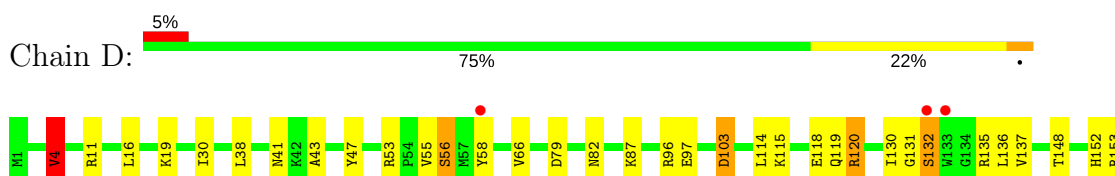
• Molecule 1: Putative acetylornithine deacetylase

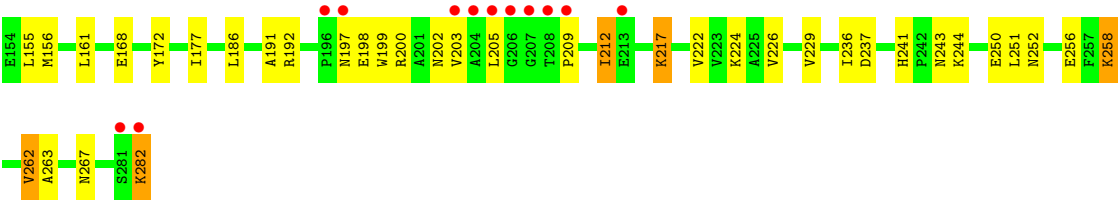


• Molecule 1: Putative acetylornithine deacetylase



• Molecule 1: Putative acetylornithine deacetylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.27Å 67.84Å 80.03Å 87.77° 75.29° 67.03°	Depositor
Resolution (Å)	34.96 – 1.87 34.96 – 1.87	Depositor EDS
% Data completeness (in resolution range)	95.6 (34.96-1.87) 93.8 (34.96-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 1.87Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.198 , 0.253 0.197 , 0.251	Depositor DCC
R_{free} test set	4684 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10021	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.54	0/2301	0.66	0/3117
1	B	0.56	0/2321	0.69	1/3146 (0.0%)
1	C	0.53	0/2273	0.66	0/3076
1	D	0.55	0/2287	0.69	1/3099 (0.0%)
All	All	0.55	0/9182	0.68	2/12438 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	4	VAL	CB-CA-C	-5.86	100.27	111.40
1	D	4	VAL	CB-CA-C	-5.33	101.27	111.40

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	2246	0	2316	70	0
1	B	2260	0	2331	69	0
1	C	2213	0	2282	65	0
1	D	2238	0	2299	61	0
2	A	27	0	12	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	27	0	12	2	0
2	C	27	0	12	2	0
2	D	27	0	12	0	0
3	A	247	0	0	8	0
3	B	270	0	0	7	0
3	C	221	0	0	7	0
3	D	218	0	0	7	0
All	All	10021	0	9276	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 13.

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:B:135:ARG:HD3	1:B:136:LEU:H	1.10	1.16
1:C:135:ARG:HH21	1:C:135:ARG:HG2	1.06	1.13
1:B:135:ARG:CD	1:B:136:LEU:H	1.67	1.06
1:A:96[A]:ARG:HG2	1:A:96[A]:ARG:HH11	0.89	1.06
1:C:192[B]:ARG:HG2	1:C:192[B]:ARG:HH21	0.90	1.03
1:B:135:ARG:HD3	1:B:136:LEU:N	1.73	1.02
1:A:132:SER:HB3	1:A:135:ARG:HB2	1.43	0.98
1:A:153:ARG:HE	1:D:152:HIS:HE1	1.09	0.96
1:B:87:LYS:NZ	1:B:250:GLU:HG2	1.80	0.96
1:B:152:HIS:HE1	1:C:153:ARG:HE	1.07	0.96
1:C:192[B]:ARG:HG2	1:C:192[B]:ARG:NH2	1.66	0.96
1:A:96[A]:ARG:HG2	1:A:96[A]:ARG:NH1	1.67	0.96
1:C:132:SER:O	1:C:135:ARG:HB2	1.66	0.95
1:A:96[A]:ARG:CG	1:A:96[A]:ARG:HH11	1.80	0.94
1:B:87:LYS:NZ	1:B:250:GLU:CG	2.32	0.92
1:C:192[B]:ARG:CG	1:C:192[B]:ARG:HH21	1.81	0.92
1:A:152:HIS:HE1	1:D:153:ARG:HE	1.13	0.89
1:B:153:ARG:HE	1:C:152:HIS:HE1	1.16	0.89
1:B:41:ASN:HD22	1:B:41:ASN:C	1.79	0.86
1:B:87:LYS:HZ3	1:B:250:GLU:CD	1.79	0.85
1:A:153:ARG:HE	1:D:152:HIS:CE1	1.93	0.85
1:A:132:SER:HB3	1:A:135:ARG:CB	2.07	0.85
1:C:176[A]:ASP:OD2	1:C:192[A]:ARG:NH1	2.09	0.84
1:C:224:LYS:O	1:C:228:ILE:HD13	1.76	0.84
1:C:135:ARG:NH2	1:C:135:ARG:HG2	1.86	0.84
1:B:241:HIS:HD2	1:B:243:ASN:H	1.25	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:GLU:HG2	1:D:199:TRP:H	1.43	0.82
1:A:132:SER:O	1:A:135:ARG:HB2	1.79	0.81
1:C:97:GLU:HG2	1:C:228:ILE:HG12	1.62	0.81
1:A:162:LYS:NZ	1:B:59:ARG:HH11	1.78	0.80
1:D:87:LYS:HZ3	1:D:250:GLU:HG2	1.47	0.79
1:A:87:LYS:NZ	1:A:250:GLU:HG2	1.99	0.78
1:A:115:LYS:HE3	1:B:35:GLN:O	1.84	0.78
1:B:241:HIS:CD2	1:B:243:ASN:H	2.01	0.77
1:B:87:LYS:NZ	1:B:250:GLU:CD	2.38	0.76
1:C:135:ARG:CG	1:C:135:ARG:HH21	1.94	0.76
1:B:224:LYS:HD3	3:B:776:HOH:O	1.86	0.76
1:B:152:HIS:CE1	1:C:153:ARG:HE	1.99	0.75
1:B:87:LYS:HZ2	1:B:250:GLU:HG2	1.52	0.75
1:A:87:LYS:HZ3	1:A:250:GLU:HG2	1.51	0.74
1:D:252:ASN:HB2	3:D:608:HOH:O	1.88	0.74
1:A:153:ARG:NE	1:D:152:HIS:HE1	1.85	0.73
1:A:152:HIS:CE1	1:D:153:ARG:HE	2.03	0.73
1:A:12:GLN:HA	1:A:15:LYS:HE2	1.72	0.72
1:D:87:LYS:NZ	1:D:250:GLU:HG2	2.06	0.70
1:D:132:SER:OG	1:D:135:ARG:HB2	1.91	0.70
1:A:168:GLU:OE1	1:A:241:HIS:HE1	1.74	0.70
1:A:241:HIS:CD2	1:A:244:LYS:H	2.11	0.69
1:A:241:HIS:HD2	1:A:244:LYS:H	1.37	0.69
1:D:130:ILE:O	3:D:695:HOH:O	2.10	0.68
1:B:135:ARG:HE	1:C:151:GLU:HG3	1.57	0.68
1:A:162:LYS:HZ2	1:B:59:ARG:NH1	1.91	0.68
1:A:281:SER:O	1:A:282:LYS:HB3	1.93	0.68
1:B:87:LYS:HZ3	1:B:250:GLU:CG	2.00	0.67
1:C:132:SER:HB2	3:C:605:HOH:O	1.95	0.66
1:A:151:GLU:OE2	1:D:135:ARG:HA	1.95	0.66
1:C:73:HIS:HE1	3:C:729:HOH:O	1.77	0.66
1:D:41:ASN:ND2	1:D:43:ALA:HB3	2.11	0.66
1:C:38:LEU:HB3	1:C:66:VAL:HG11	1.78	0.65
1:C:168:GLU:OE1	1:C:241:HIS:HE1	1.80	0.65
1:B:241:HIS:CD2	1:B:244:LYS:H	2.15	0.65
1:B:252:ASN:HB2	3:B:791:HOH:O	1.97	0.65
2:B:500:ADP:O2B	3:B:620:HOH:O	2.15	0.64
1:B:41:ASN:HD21	1:B:44:LEU:H	1.46	0.64
1:B:135:ARG:HD2	1:B:136:LEU:H	1.61	0.63
1:C:12:GLN:HA	1:C:12:GLN:HE21	1.62	0.63
1:A:176[B]:ASP:OD2	2:A:500:ADP:O3'	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:LYS:NZ	1:A:250:GLU:CG	2.62	0.62
1:D:87:LYS:NZ	1:D:250:GLU:CG	2.63	0.62
1:A:191:ALA:HB2	1:A:212:ILE:HD12	1.82	0.62
1:B:148:THR:O	1:B:152:HIS:HD2	1.81	0.62
1:D:237:ASP:HB2	1:D:250:GLU:HB2	1.81	0.62
1:B:41:ASN:ND2	1:B:41:ASN:C	2.48	0.61
1:D:241:HIS:HD2	1:D:243:ASN:H	1.50	0.60
1:A:96[A]:ARG:CG	1:A:96[A]:ARG:NH1	2.47	0.60
1:D:241:HIS:CD2	1:D:243:ASN:H	2.20	0.60
1:B:135:ARG:NE	1:C:151:GLU:HG3	2.16	0.60
1:D:87:LYS:HE3	3:D:715:HOH:O	2.02	0.59
1:A:115:LYS:CE	1:B:35:GLN:O	2.50	0.59
1:C:241:HIS:HD2	1:C:243[B]:ASN:H	1.50	0.59
1:A:132:SER:O	1:A:135:ARG:HD3	2.03	0.59
1:A:237:ASP:HB2	1:A:250:GLU:HB2	1.84	0.59
1:B:132:SER:OG	1:B:135:ARG:O	2.20	0.58
1:C:241:HIS:HD2	1:C:243[A]:ASN:H	1.50	0.58
1:D:192:ARG:HH21	1:D:203:VAL:HG23	1.66	0.58
1:D:217:LYS:HE2	1:D:217:LYS:H	1.67	0.58
1:B:135:ARG:HG3	1:C:151:GLU:HB3	1.85	0.58
1:A:258:LYS:O	1:A:262:VAL:HG13	2.03	0.58
1:A:162:LYS:NZ	1:B:59:ARG:NH1	2.46	0.58
1:C:87:LYS:HZ3	1:C:250:GLU:HG2	1.68	0.58
1:D:258:LYS:O	1:D:262:VAL:HG13	2.04	0.58
1:C:241:HIS:CD2	1:C:244:LYS:H	2.22	0.57
1:B:153:ARG:HE	1:C:152:HIS:CE1	2.08	0.57
1:A:202:ASN:HB2	1:A:203:VAL:HA	1.87	0.56
1:A:25:LYS:N	1:A:25:LYS:HD3	2.21	0.56
1:C:241:HIS:HD2	1:C:244:LYS:H	1.54	0.56
3:C:650:HOH:O	1:D:79:ASP:HB3	2.06	0.55
1:C:172:TYR:CD1	1:C:173:LYS:HD2	2.42	0.55
1:A:96[A]:ARG:CZ	3:A:711:HOH:O	2.53	0.55
1:D:132:SER:HG	1:D:135:ARG:HB2	1.70	0.55
1:D:209:PRO:HB2	1:D:263:ALA:HB2	1.87	0.55
1:A:250:GLU:OE1	3:A:823:HOH:O	2.18	0.55
1:D:229:VAL:HG21	1:D:251:LEU:HD22	1.89	0.55
1:D:168:GLU:OE1	1:D:241:HIS:HE1	1.90	0.55
1:C:12:GLN:HG3	1:C:16:LEU:HD22	1.89	0.55
1:B:241:HIS:HD2	1:B:244:LYS:H	1.55	0.55
1:D:41:ASN:HD21	1:D:43:ALA:HB3	1.71	0.55
1:A:87:LYS:HZ1	1:A:250:GLU:CG	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:ASN:ND2	1:B:212:ILE:H	2.04	0.55
1:C:158:ASN:HB3	1:C:161:LEU:HD22	1.88	0.55
1:C:176[B]:ASP:OD2	2:C:500:ADP:O3'	2.25	0.55
1:B:241:HIS:HD2	1:B:243:ASN:N	2.02	0.54
1:B:135:ARG:HG3	1:C:151:GLU:OE1	2.07	0.54
1:B:87:LYS:HZ3	1:B:250:GLU:HG2	1.60	0.54
1:B:135:ARG:CD	1:B:136:LEU:N	2.47	0.54
1:C:29[A]:ASP:OD1	1:C:47:TYR:CE1	2.61	0.53
1:C:237:ASP:HB2	1:C:250:GLU:HB2	1.90	0.53
1:D:222:VAL:HG13	1:D:236:ILE:HD13	1.90	0.53
1:A:13:GLU:OE1	1:A:256:GLU:HG3	2.09	0.53
1:B:152:HIS:HE1	1:C:153:ARG:NE	1.91	0.52
1:C:267:ASN:ND2	3:C:682:HOH:O	2.42	0.52
1:A:155:LEU:HD22	1:D:136:LEU:HD11	1.92	0.52
1:D:282:LYS:HA	3:D:751:HOH:O	2.10	0.52
1:A:162:LYS:HD2	1:B:58:TYR:OH	2.10	0.52
1:C:252:ASN:HB2	3:C:629:HOH:O	2.09	0.51
1:D:241:HIS:HD2	1:D:244:LYS:H	1.57	0.51
1:D:250:GLU:OE1	3:D:760:HOH:O	2.19	0.51
1:A:109:SER:HA	1:A:162:LYS:NZ	2.26	0.51
1:C:73:HIS:CE1	3:C:729:HOH:O	2.57	0.51
1:C:241:HIS:CD2	1:C:243[A]:ASN:H	2.28	0.51
1:C:241:HIS:CD2	1:C:243[B]:ASN:H	2.28	0.51
1:B:87:LYS:HE3	3:B:681:HOH:O	2.11	0.51
1:A:176[A]:ASP:HB3	1:A:192:ARG:HD3	1.93	0.51
1:C:97:GLU:HG2	1:C:228:ILE:CG1	2.38	0.50
1:B:216:GLU:OE1	1:B:220:GLU:OE2	2.29	0.50
1:B:97:GLU:HG3	1:B:228:ILE:HG12	1.93	0.50
1:D:103:ASP:HB3	1:D:120:ARG:HH22	1.77	0.50
1:D:258:LYS:HE2	3:D:777:HOH:O	2.10	0.50
1:D:132:SER:HB3	1:D:135:ARG:O	2.12	0.50
1:A:202:ASN:N	1:A:203:VAL:HB	2.27	0.49
1:B:168:GLU:OE1	1:B:241:HIS:HE1	1.94	0.49
1:A:256:GLU:HG3	3:A:772:HOH:O	2.12	0.49
1:C:87:LYS:NZ	1:C:250:GLU:HG2	2.26	0.49
1:B:41:ASN:OD1	1:B:43:ALA:HB3	2.13	0.49
1:C:130:ILE:HG22	1:C:131:GLY:N	2.27	0.49
1:A:53:ARG:N	1:A:54:PRO:CD	2.76	0.49
1:C:148:THR:O	1:C:152:HIS:HD2	1.96	0.48
1:D:56:SER:OG	1:D:58:TYR:CD1	2.62	0.48
1:D:198:GLU:HG2	1:D:200:ARG:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:VAL:HG13	1:D:47:TYR:CZ	2.48	0.48
1:A:232:GLU:OE1	3:A:679:HOH:O	2.20	0.48
1:D:202:ASN:HB2	1:D:205:LEU:HD23	1.95	0.48
1:C:53:ARG:N	1:C:54:PRO:CD	2.76	0.48
1:B:158:ASN:O	1:B:161:LEU:HB2	2.14	0.48
1:B:222:VAL:HG13	1:B:236:ILE:HG21	1.96	0.48
1:A:162:LYS:HZ2	1:B:59:ARG:HH11	1.46	0.48
1:A:87:LYS:HZ3	1:A:250:GLU:CG	2.25	0.47
1:A:241:HIS:CD2	1:A:243:ASN:H	2.32	0.47
1:D:177:ILE:HG12	1:D:212:ILE:HD12	1.95	0.47
1:A:53:ARG:H	1:A:54:PRO:HD3	1.79	0.47
1:C:229:VAL:HG21	1:C:251:LEU:HD22	1.96	0.47
1:A:11:ARG:CZ	1:A:55:VAL:HG22	2.45	0.47
1:B:158:ASN:HD22	1:B:160:ALA:H	1.62	0.47
1:A:41:ASN:HD22	1:A:41:ASN:C	2.17	0.47
1:B:224:LYS:O	1:B:228:ILE:HD12	2.14	0.47
1:A:156:MET:N	1:A:157:GLY:HA2	2.29	0.47
1:A:241:HIS:HD2	1:A:243:ASN:H	1.63	0.47
1:D:241:HIS:CD2	1:D:244:LYS:H	2.32	0.46
1:D:87:LYS:HZ1	1:D:250:GLU:CG	2.27	0.46
1:D:4:VAL:HG22	1:D:47:TYR:CG	2.51	0.46
1:D:156:MET:SD	1:D:161:LEU:HD23	2.55	0.46
1:C:87:LYS:NZ	1:C:250:GLU:CG	2.79	0.46
1:D:130:ILE:HD11	1:D:161:LEU:HD11	1.98	0.46
1:A:53:ARG:N	1:A:54:PRO:HD3	2.31	0.46
1:D:38:LEU:HB3	1:D:66:VAL:HG11	1.97	0.46
1:B:196:PRO:HA	1:B:197:ASN:HA	1.64	0.45
1:B:207:GLY:HA2	1:B:208:THR:HA	1.61	0.45
1:D:186:LEU:HD13	1:D:222:VAL:HG11	1.98	0.45
1:C:167:GLN:NE2	2:C:500:ADP:HN61	2.15	0.45
1:B:237:ASP:HB2	1:B:250:GLU:HB2	1.99	0.45
1:D:11:ARG:CZ	1:D:55:VAL:HG22	2.46	0.45
1:C:131:GLY:HA3	1:C:132:SER:HB2	1.98	0.44
1:D:137:VAL:O	1:D:199:TRP:HH2	2.00	0.44
1:B:259:GLY:HA2	1:B:262:VAL:HG22	2.00	0.44
1:D:226:VAL:CG1	1:D:236:ILE:HD11	2.47	0.44
1:D:130:ILE:HD12	1:D:131:GLY:H	1.82	0.44
1:D:226:VAL:HG11	1:D:236:ILE:HD11	1.99	0.44
1:C:192[B]:ARG:NH2	1:C:192[B]:ARG:CG	2.51	0.44
1:D:11:ARG:NH1	1:D:256[A]:GLU:OE2	2.51	0.44
1:C:264:THR:O	1:C:265:ASN:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:ALA:O	1:C:273:VAL:HG12	2.18	0.44
1:A:143:VAL:HG23	3:A:635:HOH:O	2.17	0.44
1:A:171:GLN:NE2	3:A:748:HOH:O	2.50	0.44
1:B:178:ARG:HD3	3:B:777:HOH:O	2.18	0.43
1:D:115:LYS:O	1:D:119:GLN:HG3	2.18	0.43
1:C:53:ARG:H	1:C:54:PRO:HD3	1.83	0.43
1:B:259:GLY:O	1:B:262:VAL:HG22	2.18	0.43
1:B:125:ILE:HG13	2:B:500:ADP:C6	2.52	0.43
1:D:96:ARG:NH2	3:D:748:HOH:O	2.51	0.43
1:A:267:ASN:C	1:A:267:ASN:HD22	2.22	0.43
1:B:267:ASN:ND2	3:B:648:HOH:O	2.48	0.43
1:B:53:ARG:N	1:B:54:PRO:CD	2.81	0.43
1:B:176[A]:ASP:OD2	1:B:201:ALA:HB3	2.19	0.43
1:B:4:VAL:HG13	1:B:47:TYR:CZ	2.54	0.43
1:C:3:VAL:HG22	1:C:49:VAL:HG12	2.01	0.43
1:C:87:LYS:HZ1	1:C:250:GLU:CD	2.22	0.43
1:C:130:ILE:CG2	1:C:131:GLY:N	2.81	0.43
1:C:235:SER:OG	1:C:252:ASN:HB3	2.19	0.43
1:D:198:GLU:CG	1:D:199:TRP:H	2.16	0.43
1:A:281:SER:O	1:A:282:LYS:CB	2.65	0.42
1:A:256:GLU:CG	3:A:772:HOH:O	2.66	0.42
1:B:241:HIS:CE1	1:B:244:LYS:HE2	2.54	0.42
1:A:148:THR:O	1:A:152:HIS:HD2	2.02	0.42
1:A:203:VAL:HG13	1:A:203:VAL:O	2.18	0.42
1:B:135:ARG:HD2	1:C:151:GLU:HB3	2.02	0.42
1:C:120:ARG:HD3	3:C:653:HOH:O	2.20	0.42
1:A:162:LYS:HZ3	1:B:59:ARG:HH11	1.65	0.42
1:A:132:SER:HB3	1:A:135:ARG:HB3	1.96	0.42
1:A:224:LYS:O	1:A:228:ILE:HG12	2.20	0.42
1:C:131:GLY:HA3	1:C:132:SER:CB	2.48	0.42
1:A:160:ALA:HB2	3:B:651:HOH:O	2.20	0.42
1:C:135:ARG:CG	1:C:135:ARG:NH2	2.64	0.42
1:B:75:ILE:HA	1:B:76:ASN:HA	1.83	0.41
1:C:27:GLN:HE21	1:C:27:GLN:HB2	1.66	0.41
1:B:114:LEU:HD11	1:B:147:LYS:HE2	2.01	0.41
1:D:217:LYS:HE2	1:D:217:LYS:N	2.33	0.41
1:B:281:SER:O	1:B:282:LYS:HB2	2.21	0.41
1:D:148:THR:O	1:D:152:HIS:HD2	2.02	0.41
1:A:208:THR:HA	1:A:209:PRO:HD3	1.80	0.41
1:B:87:LYS:HZ1	1:B:250:GLU:CG	2.29	0.41
1:D:87:LYS:HZ1	1:D:250:GLU:CD	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:HD11	3:A:756:HOH:O	2.20	0.41
1:D:191:ALA:HB2	1:D:212:ILE:HD11	2.03	0.41
1:B:212:ILE:O	1:B:212:ILE:HG13	2.21	0.41
1:D:114:LEU:O	1:D:118:GLU:HG2	2.19	0.41
1:C:82:ASN:HD22	1:C:82:ASN:HA	1.73	0.41
1:A:186:LEU:HD13	1:A:222:VAL:HG11	2.03	0.40
1:A:87:LYS:HG2	1:A:250:GLU:OE2	2.20	0.40
1:C:196:PRO:HA	1:C:197:ASN:HA	1.61	0.40
1:A:125:ILE:HG13	2:A:500:ADP:C6	2.57	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	285/282 (101%)	272 (95%)	9 (3%)	4 (1%)	13	3
1	B	288/282 (102%)	280 (97%)	5 (2%)	3 (1%)	18	6
1	C	278/282 (99%)	270 (97%)	7 (2%)	1 (0%)	38	25
1	D	283/282 (100%)	274 (97%)	6 (2%)	3 (1%)	17	5
All	All	1134/1128 (100%)	1096 (97%)	27 (2%)	11 (1%)	18	6

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	203	VAL
1	A	204	ALA
1	B	132	SER
1	D	132	SER
1	D	172	TYR

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Mol	Chain	Res	Type
1	B	203	VAL
1	A	53	ARG
1	C	53	ARG
1	B	53	ARG
1	D	53	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/242 (102%)	229 (93%)	18 (7%)	16	6
1	B	250/242 (103%)	231 (92%)	19 (8%)	15	5
1	C	245/242 (101%)	227 (93%)	18 (7%)	16	6
1	D	245/242 (101%)	226 (92%)	19 (8%)	15	5
All	All	987/968 (102%)	913 (92%)	74 (8%)	18	5

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	25	LYS
1	A	41	ASN
1	A	82	ASN
1	A	96[A]	ARG
1	A	96[B]	ARG
1	A	120	ARG
1	A	132	SER
1	A	135	ARG
1	A	141	ARG
1	A	155	LEU
1	A	158	ASN
1	A	161	LEU
1	A	173	LYS
1	A	211	ASN
1	A	256	GLU

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Mol	Chain	Res	Type
1	A	267	ASN
1	A	282	LYS
1	B	4	VAL
1	B	16[A]	LEU
1	B	16[B]	LEU
1	B	19	LYS
1	B	27	GLN
1	B	41	ASN
1	B	82	ASN
1	B	114	LEU
1	B	120[A]	ARG
1	B	120[B]	ARG
1	B	130	ILE
1	B	135	ARG
1	B	155	LEU
1	B	158	ASN
1	B	161	LEU
1	B	192	ARG
1	B	211	ASN
1	B	251	LEU
1	B	267	ASN
1	C	12	GLN
1	C	16	LEU
1	C	27	GLN
1	C	29[A]	ASP
1	C	29[B]	ASP
1	C	41	ASN
1	C	82	ASN
1	C	135	ARG
1	C	141	ARG
1	C	161	LEU
1	C	162[A]	LYS
1	C	162[B]	LYS
1	C	192[A]	ARG
1	C	192[B]	ARG
1	C	197	ASN
1	C	217	LYS
1	C	267	ASN
1	C	278	GLU
1	D	4	VAL
1	D	16	LEU
1	D	19	LYS

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Mol	Chain	Res	Type
1	D	30	ILE
1	D	56	SER
1	D	82	ASN
1	D	97	GLU
1	D	103	ASP
1	D	120	ARG
1	D	155	LEU
1	D	197	ASN
1	D	212	ILE
1	D	217	LYS
1	D	224[A]	LYS
1	D	224[B]	LYS
1	D	258	LYS
1	D	262	VAL
1	D	267	ASN
1	D	282	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	41	ASN
1	A	82	ASN
1	A	119	GLN
1	A	152	HIS
1	A	211	ASN
1	A	241	HIS
1	A	267	ASN
1	A	270	GLN
1	B	12	GLN
1	B	24	ASN
1	B	41	ASN
1	B	82	ASN
1	B	152	HIS
1	B	158	ASN
1	B	193	ASN
1	B	211	ASN
1	B	241	HIS
1	B	267	ASN
1	B	270	GLN
1	B	279	ASN
1	C	12	GLN

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Mol	Chain	Res	Type
1	C	24	ASN
1	C	27	GLN
1	C	35	GLN
1	C	82	ASN
1	C	152	HIS
1	C	167	GLN
1	C	197	ASN
1	C	211	ASN
1	C	241	HIS
1	C	267	ASN
1	C	270	GLN
1	D	24	ASN
1	D	27	GLN
1	D	82	ASN
1	D	119	GLN
1	D	152	HIS
1	D	193	ASN
1	D	197	ASN
1	D	202	ASN
1	D	241	HIS
1	D	267	ASN
1	D	270	GLN

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	500	-	25,29,29	1.20	2 (8%)	24,45,45	1.64	3 (12%)
2	ADP	B	500	-	25,29,29	1.08	2 (8%)	24,45,45	1.84	2 (8%)
2	ADP	C	500	-	25,29,29	1.06	1 (4%)	24,45,45	1.81	4 (16%)
2	ADP	D	500	-	25,29,29	1.04	1 (4%)	24,45,45	1.70	2 (8%)

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	500	-	-	0/12/32/32	0/3/3/3
2	ADP	B	500	-	-	0/12/32/32	0/3/3/3
2	ADP	C	500	-	-	0/12/32/32	0/3/3/3
2	ADP	D	500	-	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	ADP	PB-O3A	2.28	1.63	1.60
2	B	500	ADP	C5-C4	2.65	1.46	1.40
2	A	500	ADP	PB-O3A	2.89	1.64	1.60
2	C	500	ADP	C5-C4	3.05	1.47	1.40
2	D	500	ADP	C5-C4	3.05	1.47	1.40
2	A	500	ADP	C5-C4	3.09	1.47	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	N3-C2-N1	-7.28	122.52	128.86
2	C	500	ADP	N3-C2-N1	-6.63	123.08	128.86
2	D	500	ADP	N3-C2-N1	-5.81	123.80	128.86
2	A	500	ADP	N3-C2-N1	-5.50	124.07	128.86
2	C	500	ADP	O2'-C2'-C1'	-2.71	103.15	111.61
2	A	500	ADP	C4-C5-N7	-2.50	107.00	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	ADP	C1'-N9-C4	-2.20	122.84	126.64
2	A	500	ADP	O2'-C2'-C1'	-2.19	104.75	111.61
2	C	500	ADP	O3'-C3'-C4'	-2.03	105.15	111.09
2	C	500	ADP	C4-C5-N7	-2.01	107.47	109.41
2	D	500	ADP	C2-N1-C6	2.10	122.45	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	ADP	2	0
2	B	500	ADP	2	0
2	C	500	ADP	2	0

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, 95th 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	282/282 (100%)	0.01	15 (5%)	27 29	11, 23, 50, 63	0
1	B	282/282 (100%)	0.06	10 (3%)	44 46	12, 23, 43, 60	0
1	C	275/282 (97%)	0.05	11 (4%)	39 41	12, 26, 46, 55	0
1	D	282/282 (100%)	0.08	15 (5%)	27 29	13, 25, 46, 58	0
All	All	1121/1128 (99%)	0.05	51 (4%)	34 36	11, 24, 47, 63	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	207	GLY	11.0
1	A	205	LEU	9.2
1	B	208	THR	8.2
1	C	133	TRP	7.8
1	A	204	ALA	7.6
1	D	203	VAL	6.5
1	D	204	ALA	6.5
1	B	203	VAL	6.1
1	B	205	LEU	5.4
1	C	196	PRO	5.4
1	B	133	TRP	5.2
1	D	133	TRP	5.1
1	A	207	GLY	4.7
1	C	282	LYS	4.6
1	A	157	GLY	4.1
1	C	197	ASN	3.9
1	B	204	ALA	3.9
1	A	282	LYS	3.7
1	A	133	TRP	3.6
1	B	281	SER	3.6
1	A	208	THR	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	196	PRO	3.2
1	A	197	ASN	3.2
1	D	281	SER	3.1
1	A	206	GLY	3.1
1	A	196	PRO	3.0
1	D	196	PRO	3.0
1	D	208	THR	3.0
1	C	131	GLY	2.8
1	C	210	SER	2.8
1	D	282	LYS	2.7
1	D	209	PRO	2.7
1	D	197	ASN	2.6
1	B	206	GLY	2.6
1	A	158	ASN	2.5
1	D	213	GLU	2.5
1	D	207	GLY	2.4
1	C	132	SER	2.4
1	C	157	GLY	2.4
1	C	135	ARG	2.4
1	C	192[A]	ARG	2.4
1	A	211	ASN	2.4
1	A	132	SER	2.3
1	A	203	VAL	2.3
1	D	132	SER	2.3
1	D	206	GLY	2.2
1	A	131	GLY	2.2
1	D	58	TYR	2.2
1	B	209	PRO	2.1
1	D	205	LEU	2.1
1	C	281	SER	2.1

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

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

6.3 Carbohydrates ⓘ

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, 95th 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	500	27/27	0.93	0.11	-0.56	18,25,40,42	0
2	ADP	B	500	27/27	0.95	0.09	-0.83	15,20,33,33	0
2	ADP	A	500	27/27	0.94	0.09	-0.91	17,22,36,38	0
2	ADP	D	500	27/27	0.96	0.09	-0.94	15,22,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.