



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:00 PM UTC

PDB ID : 4NP6 / pdb_00004np6
Title : Crystal Structure of Adenylate Kinase from *Vibrio cholerae* O1 biovar eltor
Authors : Kim, Y.; Zhou, M.; Grimshaw, S.; Anderson, W.F.; Joachimiak, A.; Center
for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-11-20
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

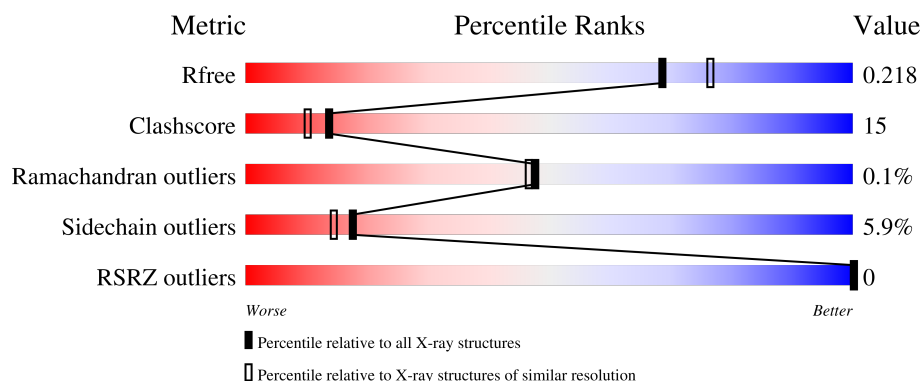
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	217	 66% 29% 5%
1	B	217	 60% 35% . .
1	C	217	 68% 30% .
1	D	217	 70% 24% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6704 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 Adenylate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	Se	0	0	0
			1648	1038	285	319	1	5			
1	B	215	Total	C	N	O	S	Se	0	0	0
			1640	1034	283	317	1	5			
1	C	216	Total	C	N	O	S	Se	0	1	0
			1657	1043	286	322	1	5			
1	D	211	Total	C	N	O	S	Se	0	1	0
			1622	1024	280	311	1	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KTB7
A	-1	ASN	-	expression tag	UNP Q9KTB7
A	0	ALA	-	expression tag	UNP Q9KTB7
B	-2	SER	-	expression tag	UNP Q9KTB7
B	-1	ASN	-	expression tag	UNP Q9KTB7
B	0	ALA	-	expression tag	UNP Q9KTB7
C	-2	SER	-	expression tag	UNP Q9KTB7
C	-1	ASN	-	expression tag	UNP Q9KTB7
C	0	ALA	-	expression tag	UNP Q9KTB7
D	-2	SER	-	expression tag	UNP Q9KTB7
D	-1	ASN	-	expression tag	UNP Q9KTB7
D	0	ALA	-	expression tag	UNP Q9KTB7

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	29	Total	O	0	0
			29	29		
2	B	46	Total	O	0	0
			46	46		

Continued on next page...

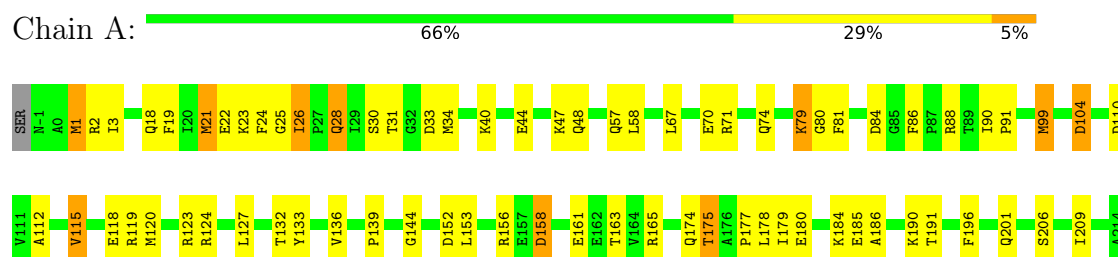
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	39	Total	O	0	0
			39	39		
2	D	23	Total	O	0	0
			23	23		

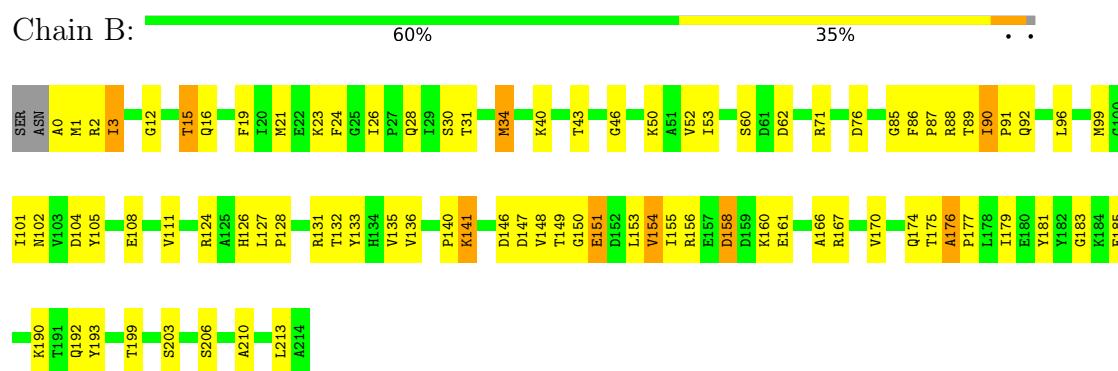
3 Residue-property plots

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.

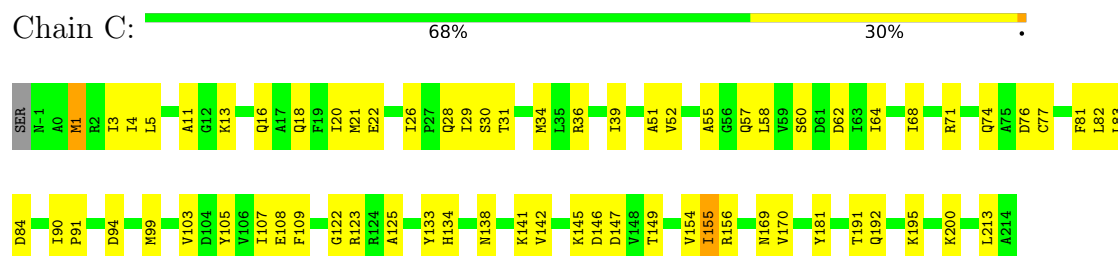
• Molecule 1: Adenylate kinase



• Molecule 1: Adenylate kinase

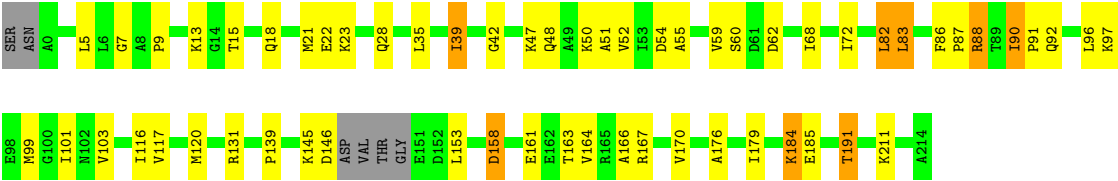


• Molecule 1: Adenylate kinase



• Molecule 1: Adenylate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	101.62Å 101.62Å 89.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.45 – 2.00 45.45 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.45-2.00) 99.6 (45.45-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1161)	Depositor
R, R_{free}	0.186 , 0.222 0.185 , 0.218	Depositor DCC
R_{free} test set	3077 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.469 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	0 of 60974 reflections	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6704	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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](#)

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	0.71	0/1666	1.05	5/2239 (0.2%)
1	B	0.76	0/1658	1.06	9/2228 (0.4%)
1	C	0.75	0/1675	1.02	1/2251 (0.0%)
1	D	0.73	1/1639 (0.1%)	1.04	7/2199 (0.3%)
All	All	0.74	1/6638 (0.0%)	1.04	22/8917 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	90	ILE	CA-CB	-5.93	1.51	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	176	ALA	CA-C-N	-6.72	111.44	119.84
1	D	176	ALA	C-N-CA	-6.72	111.44	119.84
1	B	141	LYS	N-CA-C	-6.35	104.44	111.36
1	B	53	ILE	CB-CA-C	-6.02	104.02	112.14
1	B	150	GLY	N-CA-C	-5.80	106.14	115.08
1	B	90	ILE	CB-CA-C	-5.76	108.24	114.35
1	D	139	PRO	N-CA-C	5.75	117.71	110.70
1	A	115	VAL	CB-CA-C	-5.65	104.51	112.14
1	B	3	ILE	N-CA-C	5.50	116.59	108.45
1	D	90	ILE	CA-C-N	-5.46	114.00	119.56
1	D	90	ILE	C-N-CA	-5.46	114.00	119.56
1	B	161	GLU	N-CA-C	5.31	117.06	111.28
1	A	175	THR	N-CA-C	5.28	117.11	111.36
1	D	55	ALA	N-CA-C	-5.19	106.18	112.88
1	B	176	ALA	CA-C-N	-5.19	114.32	119.56
1	B	176	ALA	C-N-CA	-5.19	114.32	119.56
1	A	178	LEU	N-CA-C	-5.15	105.36	111.69
1	B	52	VAL	CB-CA-C	-5.06	105.50	111.97
1	A	26	ILE	CA-C-N	-5.05	115.52	120.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ILE	C-N-CA	-5.05	115.52	120.52
1	D	88	ARG	N-CA-C	-5.04	107.68	113.88
1	C	107	ILE	N-CA-C	5.02	115.08	107.80

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	1648	0	1671	52	0
1	B	1640	0	1665	68	0
1	C	1657	0	1676	44	0
1	D	1622	0	1649	40	0
2	A	29	0	0	3	0
2	B	46	0	0	5	0
2	C	39	0	0	1	0
2	D	23	0	0	1	0
All	All	6704	0	6661	192	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 15.

All (192) 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:31:THR:HA	1:B:34:MSE:HE3	1.42	0.97
1:B:2:ARG:O	1:B:104:ASP:N	2.21	0.72
1:C:51:ALA:O	1:C:55:ALA:N	2.23	0.71
1:C:13:LYS:NZ	1:C:84:ASP:OD1	2.24	0.70
1:A:88:ARG:NE	2:A:325:HOH:O	2.21	0.69
1:D:97:LYS:NZ	1:D:185:GLU:OE2	2.25	0.69
1:B:3:ILE:HG12	1:B:105:TYR:HB2	1.77	0.67
1:A:70:GLU:O	1:A:74:GLN:NE2	2.28	0.66
1:B:99:MSE:HE2	1:B:101:ILE:HD11	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ILE:O	1:B:160:LYS:NZ	2.29	0.66
1:B:89:THR:HB	1:B:91:PRO:HD2	1.77	0.66
1:A:158:ASP:HA	1:A:163:THR:HG21	1.78	0.65
1:B:158:ASP:N	1:B:158:ASP:OD1	2.30	0.65
1:B:141:LYS:N	1:B:147:ASP:OD2	2.23	0.65
1:C:146:ASP:OD2	1:C:149:THR:N	2.30	0.64
1:A:144:GLY:O	1:A:153:LEU:N	2.30	0.64
1:A:67:LEU:O	1:A:71:ARG:N	2.27	0.63
1:C:71:ARG:HH12	1:C:76:ASP:CG	2.07	0.62
1:C:142:VAL:HB	1:C:145:LYS:HB2	1.79	0.62
1:B:131:ARG:HH11	1:B:146:ASP:CG	2.08	0.62
1:A:44:GLU:O	1:A:48:GLN:HG3	2.01	0.61
1:B:62:ASP:OD1	1:B:62:ASP:N	2.32	0.60
1:A:26:ILE:HB	1:A:81:PHE:HA	1.82	0.60
1:A:33:ASP:OD2	1:B:40:LYS:NZ	2.34	0.60
1:D:131:ARG:HH22	1:D:146:ASP:CG	2.10	0.60
1:A:1:MSE:N	1:A:79:LYS:O	2.34	0.59
1:B:166:ALA:O	1:B:170:VAL:HG23	2.03	0.58
1:A:115:VAL:O	1:A:119:ARG:HG3	2.03	0.58
1:A:2:ARG:N	1:A:104:ASP:OD2	2.27	0.57
1:B:146:ASP:OD1	1:B:149:THR:N	2.37	0.57
1:A:31:THR:HG21	1:A:86:PHE:CD1	2.40	0.56
1:C:90:ILE:HB	1:C:91:PRO:HD3	1.87	0.56
1:D:9:PRO:HG3	1:D:167:ARG:HG2	1.88	0.56
1:A:1:MSE:HE1	1:A:3:ILE:HD11	1.87	0.56
1:C:26:ILE:HB	1:C:81:PHE:HA	1.88	0.56
1:A:127:LEU:O	1:B:167:ARG:NH1	2.40	0.55
1:B:105:TYR:CD1	1:B:192:GLN:HB3	2.42	0.55
1:B:2:ARG:HE	1:B:102:ASN:HB2	1.70	0.55
1:C:28:GLN:NE2	1:C:84:ASP:OD2	2.40	0.55
1:A:175:THR:HG22	1:A:179:ILE:HG13	1.90	0.54
1:B:2:ARG:NE	1:B:102:ASN:HB2	2.22	0.54
1:B:15:THR:HG22	1:B:16:GLN:N	2.22	0.54
1:D:21[A]:MSE:SE	1:D:28:GLN:HE21	2.41	0.54
1:B:181:TYR:O	1:B:185:GLU:HG2	2.07	0.54
1:D:48:GLN:O	1:D:52:VAL:HG23	2.08	0.54
1:A:174:GLN:O	1:A:177:PRO:HD2	2.08	0.54
1:B:0:ALA:HB3	2:B:327:HOH:O	2.08	0.54
1:D:158:ASP:OD1	1:D:158:ASP:N	2.39	0.53
1:B:85:GLY:O	1:B:88:ARG:NH2	2.41	0.53
1:B:111:VAL:HG13	1:B:199:THR:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:GLN:HE22	1:D:50:LYS:HG2	1.74	0.53
1:C:94:ASP:OD1	1:C:181:TYR:OH	2.25	0.53
1:C:141:LYS:N	1:C:147:ASP:OD1	2.35	0.53
1:A:158:ASP:OD1	1:B:156:ARG:NH2	2.24	0.52
1:A:57:GLN:CD	1:C:57:GLN:HE22	2.16	0.52
1:D:164:VAL:HG22	1:D:167:ARG:NH2	2.24	0.52
1:C:123:ARG:O	1:C:155:ILE:HG23	2.10	0.52
1:B:2:ARG:N	1:B:104:ASP:OD2	2.26	0.52
1:C:18:GLN:HE22	1:D:50:LYS:CG	2.23	0.52
1:A:124:ARG:HB2	1:A:133:TYR:HB2	1.91	0.52
1:A:21:MSE:HG2	1:A:26:ILE:O	2.09	0.52
1:A:90:ILE:HB	1:A:91:PRO:HD3	1.92	0.52
1:C:52:VAL:HG13	1:C:57:GLN:HB2	1.92	0.52
1:B:108:GLU:OE1	1:B:193:TYR:OH	2.26	0.51
1:A:18:GLN:OE1	1:B:50:LYS:NZ	2.42	0.51
1:A:71:ARG:O	1:A:74:GLN:HG2	2.11	0.51
1:D:158:ASP:HA	1:D:163:THR:HG21	1.92	0.51
1:D:146:ASP:HB2	1:D:153:LEU:HD21	1.93	0.51
1:B:2:ARG:HB2	1:B:102:ASN:O	2.11	0.51
1:A:112:ALA:HB3	1:A:115:VAL:HG23	1.91	0.51
1:B:149:THR:OG1	1:B:151:GLU:HB2	2.11	0.51
1:B:133:TYR:HB3	1:B:140:PRO:HD3	1.92	0.50
1:B:90:ILE:HB	1:B:91:PRO:HD3	1.92	0.50
1:B:183:GLY:HA3	2:B:343:HOH:O	2.11	0.50
1:D:39:ILE:HG12	1:D:50:LYS:HB2	1.93	0.50
1:D:88:ARG:N	1:D:92:GLN:OE1	2.35	0.50
1:C:60:SER:OG	1:C:62:ASP:OD1	2.29	0.50
1:C:76:ASP:OD1	1:C:77:CYS:N	2.45	0.50
1:C:3:ILE:HA	1:C:105:TYR:O	2.12	0.50
1:B:174:GLN:O	1:B:177:PRO:HD2	2.12	0.49
1:D:96:LEU:O	1:D:99:MSE:HB2	2.12	0.49
1:D:167:ARG:NH2	2:D:304:HOH:O	2.46	0.49
1:B:21:MSE:HG3	1:B:26:ILE:O	2.13	0.49
1:C:5:LEU:HD21	1:C:13:LYS:HB2	1.93	0.49
1:C:55:ALA:O	1:C:57:GLN:HG3	2.13	0.49
1:D:99:MSE:HB2	1:D:101:ILE:HG12	1.94	0.49
1:A:90:ILE:HG12	2:A:305:HOH:O	2.13	0.49
1:D:99:MSE:HE2	1:D:99:MSE:HB3	1.68	0.49
1:A:104:ASP:N	1:A:104:ASP:OD1	2.44	0.48
1:C:133:TYR:HB3	1:C:138:ASN:O	2.13	0.48
1:D:103:VAL:HG12	1:D:191:THR:OG1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:O	1:C:74:GLN:HG2	2.13	0.48
1:A:1:MSE:O	1:A:80:GLY:HA3	2.14	0.48
1:A:44:GLU:O	1:A:47:LYS:HB2	2.14	0.48
1:B:31:THR:HA	1:B:34:MSE:CE	2.30	0.48
1:C:156:ARG:HD2	2:C:324:HOH:O	2.14	0.48
1:C:16:GLN:O	1:C:20:ILE:HG13	2.14	0.48
1:A:21:MSE:O	1:A:25:GLY:N	2.47	0.48
1:C:191:THR:OG1	1:C:192:GLN:N	2.47	0.47
1:B:146:ASP:N	1:B:151:GLU:O	2.42	0.47
1:B:175:THR:HG22	1:B:179:ILE:HD11	1.96	0.47
1:D:166:ALA:O	1:D:170:VAL:HG23	2.14	0.47
1:B:19:PHE:CE1	1:B:206:SER:HB3	2.50	0.47
1:C:3:ILE:HG12	1:C:105:TYR:HB2	1.97	0.47
1:C:29:ILE:HB	1:C:83:LEU:HD23	1.97	0.47
1:D:7:GLY:HA3	1:D:13:LYS:HD3	1.96	0.47
1:D:86:PHE:CG	1:D:87:PRO:HA	2.49	0.47
1:D:116:ILE:O	1:D:120:MSE:HG2	2.13	0.47
1:B:12:GLY:O	1:B:15:THR:HB	2.15	0.47
1:B:24:PHE:CE2	1:B:213:LEU:HD12	2.50	0.47
1:A:21:MSE:HE2	1:A:21:MSE:HB3	1.75	0.46
1:B:34:MSE:O	2:B:330:HOH:O	2.20	0.46
1:A:124:ARG:N	1:A:133:TYR:O	2.38	0.46
1:B:135:VAL:HG23	1:B:136:VAL:HG23	1.96	0.46
1:B:31:THR:OG1	1:B:88:ARG:NH2	2.49	0.46
1:B:89:THR:N	1:B:92:GLN:OE1	2.49	0.45
1:B:126:HIS:CE1	1:B:128:PRO:HD2	2.51	0.45
1:D:184:LYS:HE2	1:D:184:LYS:HB2	1.46	0.45
1:A:23:LYS:HG3	1:A:24:PHE:CD2	2.51	0.45
1:D:23:LYS:HA	1:D:23:LYS:HD2	1.77	0.45
1:B:1:MSE:SE	1:B:105:TYR:CE2	3.19	0.45
1:B:158:ASP:O	1:B:167:ARG:NH2	2.50	0.45
1:B:16:GLN:NE2	1:B:16:GLN:HA	2.31	0.45
1:A:156:ARG:NH1	1:B:158:ASP:OD2	2.50	0.44
1:D:42:GLY:O	1:D:47:LYS:HE3	2.17	0.44
1:A:44:GLU:HA	1:A:47:LYS:HD2	1.99	0.44
1:A:28:GLN:HB2	1:B:40:LYS:O	2.17	0.44
1:B:60:SER:OG	1:B:62:ASP:OD1	2.29	0.44
1:D:117:VAL:HG11	1:D:161:GLU:HG3	1.99	0.44
1:B:19:PHE:CD1	1:B:206:SER:HB3	2.52	0.44
1:A:99:MSE:HE2	1:A:99:MSE:HB2	1.59	0.44
1:A:30:SER:HB2	1:B:40:LYS:HZ3	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:GLU:O	1:A:184:LYS:HG3	2.17	0.44
1:B:43:THR:OG1	1:B:46:GLY:N	2.38	0.44
1:C:4:ILE:HG13	1:C:103:VAL:HG21	1.98	0.44
1:D:97:LYS:HE3	1:D:97:LYS:HB2	1.82	0.44
1:D:18:GLN:O	1:D:22:GLU:HG3	2.18	0.44
1:C:28:GLN:HE21	1:C:84:ASP:CG	2.26	0.43
1:A:110:ASP:HA	2:A:301:HOH:O	2.18	0.43
1:C:5:LEU:HB2	1:C:82:LEU:HD11	1.99	0.43
1:C:31:THR:O	1:C:34:MSE:HB3	2.19	0.43
1:A:57:GLN:OE1	1:C:57:GLN:NE2	2.45	0.43
1:D:90:ILE:HB	1:D:91:PRO:HD3	2.00	0.43
1:B:96:LEU:O	1:B:99:MSE:N	2.48	0.43
1:C:71:ARG:NH1	1:C:76:ASP:OD2	2.50	0.43
1:A:1:MSE:HE3	1:A:26:ILE:HD13	2.00	0.43
1:B:176:ALA:HB3	1:B:177:PRO:HD3	2.01	0.43
1:C:18:GLN:O	1:C:22:GLU:HG2	2.18	0.43
1:B:141:LYS:H	1:B:147:ASP:CG	2.18	0.43
1:B:1:MSE:HA	1:B:104:ASP:CG	2.44	0.43
1:A:30:SER:HB3	1:A:33:ASP:HB2	2.00	0.43
1:A:19:PHE:CE2	1:A:206:SER:HB3	2.54	0.43
1:D:15:THR:O	1:D:18:GLN:HB2	2.18	0.43
1:A:161:GLU:HG3	1:A:165:ARG:HG3	2.00	0.42
1:A:185:GLU:O	1:A:190:LYS:HB2	2.19	0.42
1:B:23:LYS:HE2	1:B:210:ALA:HB1	2.02	0.42
1:B:85:GLY:O	1:B:86:PHE:HB2	2.19	0.42
1:D:153:LEU:HD23	1:D:153:LEU:HA	1.89	0.42
1:C:1:MSE:SE	1:C:213:LEU:HD13	2.69	0.42
1:A:120:MSE:SE	1:A:123:ARG:CZ	3.17	0.42
1:D:50:LYS:HA	1:D:50:LYS:HD2	1.42	0.42
1:C:5:LEU:HG	1:C:13:LYS:HD2	2.00	0.42
1:D:101:ILE:HG22	1:D:103:VAL:HG23	2.01	0.42
1:D:35:LEU:HD21	1:D:59:VAL:HG21	2.02	0.42
1:D:60:SER:OG	1:D:62:ASP:OD1	2.23	0.42
1:B:203:SER:O	2:B:335:HOH:O	2.21	0.42
1:B:124:ARG:HB3	1:B:153:LEU:HB3	2.02	0.41
1:C:11:ALA:O	1:C:109:PHE:HE2	2.03	0.41
1:C:125:ALA:N	1:C:154:VAL:O	2.36	0.41
1:D:5:LEU:HB2	1:D:82:LEU:HD11	2.01	0.41
1:A:40:LYS:NZ	1:B:28:GLN:OE1	2.51	0.41
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.75	0.41
1:B:71:ARG:HA	1:B:71:ARG:HD2	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:GLN:O	1:D:51:ALA:HB3	2.20	0.41
1:D:83:LEU:HD22	1:D:86:PHE:HB3	2.02	0.41
1:B:76:ASP:O	2:B:331:HOH:O	2.22	0.41
1:C:36:ARG:HA	1:C:39:ILE:HD12	2.01	0.41
1:B:86:PHE:CG	1:B:87:PRO:HA	2.55	0.41
1:C:64:ILE:O	1:C:68:ILE:HG13	2.21	0.41
1:C:83:LEU:HD23	1:C:83:LEU:HA	1.87	0.41
1:C:108:GLU:O	1:C:195:LYS:HA	2.19	0.41
1:C:122:GLY:HA3	1:C:134:HIS:CE1	2.56	0.41
1:A:1:MSE:HE3	1:A:1:MSE:HB3	1.53	0.41
1:A:136:VAL:O	1:A:139:PRO:HD3	2.21	0.41
1:A:153:LEU:HD23	1:A:153:LEU:HA	1.88	0.41
1:A:186:ALA:HA	1:A:191:THR:O	2.21	0.40
1:B:127:LEU:HD21	1:B:154:VAL:HG21	2.03	0.40
1:B:146:ASP:HB3	1:B:151:GLU:H	1.84	0.40
1:D:50:LYS:HE2	1:D:54:ASP:CG	2.46	0.40
1:C:30:SER:HA	1:C:84:ASP:O	2.20	0.40
1:A:196:PHE:CZ	1:A:209:ILE:HA	2.56	0.40
1:D:68:ILE:O	1:D:72:ILE:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	214/217 (99%)	203 (95%)	11 (5%)	0	100	100
1	B	213/217 (98%)	205 (96%)	7 (3%)	1 (0%)	24	21
1	C	215/217 (99%)	202 (94%)	13 (6%)	0	100	100
1	D	208/217 (96%)	197 (95%)	11 (5%)	0	100	100
All	All	850/868 (98%)	807 (95%)	42 (5%)	1 (0%)	48	46

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	148	VAL

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	170/166 (102%)	155 (91%)	15 (9%)	9	6
1	B	169/166 (102%)	161 (95%)	8 (5%)	23	22
1	C	171/166 (103%)	163 (95%)	8 (5%)	23	22
1	D	167/166 (101%)	158 (95%)	9 (5%)	20	17
All	All	677/664 (102%)	637 (94%)	40 (6%)	18	14

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	21	MSE
1	A	22	GLU
1	A	28	GLN
1	A	34	MSE
1	A	58	LEU
1	A	79	LYS
1	A	84	ASP
1	A	99	MSE
1	A	104	ASP
1	A	118	GLU
1	A	132	THR
1	A	152	ASP
1	A	158	ASP
1	A	201	GLN
1	B	15	THR
1	B	30	SER
1	B	34	MSE
1	B	132	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	151	GLU
1	B	154	VAL
1	B	158	ASP
1	B	190	LYS
1	C	1	MSE
1	C	21	MSE
1	C	58	LEU
1	C	99	MSE
1	C	155	ILE
1	C	169	ASN
1	C	170	VAL
1	C	200	LYS
1	D	39	ILE
1	D	82	LEU
1	D	83	LEU
1	D	145	LYS
1	D	158	ASP
1	D	179	ILE
1	D	184	LYS
1	D	191	THR
1	D	211	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	16	GLN
1	B	18	GLN
1	B	74	GLN
1	B	174	GLN
1	C	18	GLN
1	C	28	GLN
1	D	16	GLN
1	D	28	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	211/217 (97%)	-1.47	0 100 100	29, 42, 61, 87	1 (0%)
1	B	210/217 (96%)	-1.43	0 100 100	27, 42, 63, 92	3 (1%)
1	C	211/217 (97%)	-1.47	0 100 100	21, 42, 60, 84	2 (0%)
1	D	206/217 (94%)	-1.43	0 100 100	25, 42, 71, 118	3 (1%)
All	All	838/868 (96%)	-1.45	0 100 100	21, 42, 65, 118	9 (1%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.