



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:18 AM UTC

PDB ID : 1LBE / pdb_00001lbe
Title : APLYSIA ADP RIBOSYL CYCLASE
Authors : Prasad, G.S.; Mcree, D.E.; Stura, E.A.; Levitt, D.G.; Lee, H.C.; Stout, C.D.
Deposited on : 1996-09-18
Resolution : 2.40 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

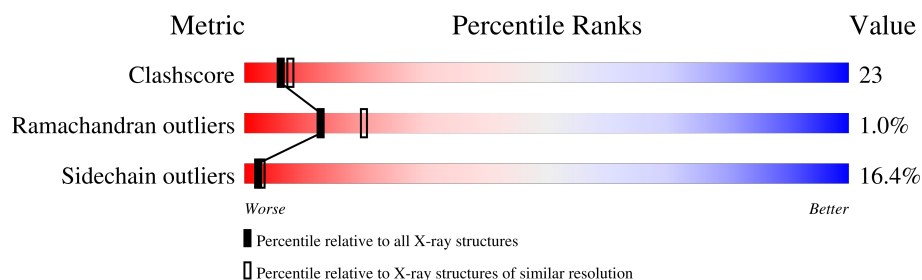
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	258	 48% 39% 8% . .
1	B	258	 45% 36% 13% . .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4064 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 ADP RIBOSYL CYCLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	21	0	0
			2007	1285	341	367	14			
1	B	248	Total	C	N	O	S	13	0	0
			1988	1273	336	365	14			

- Molecule 2 is water.

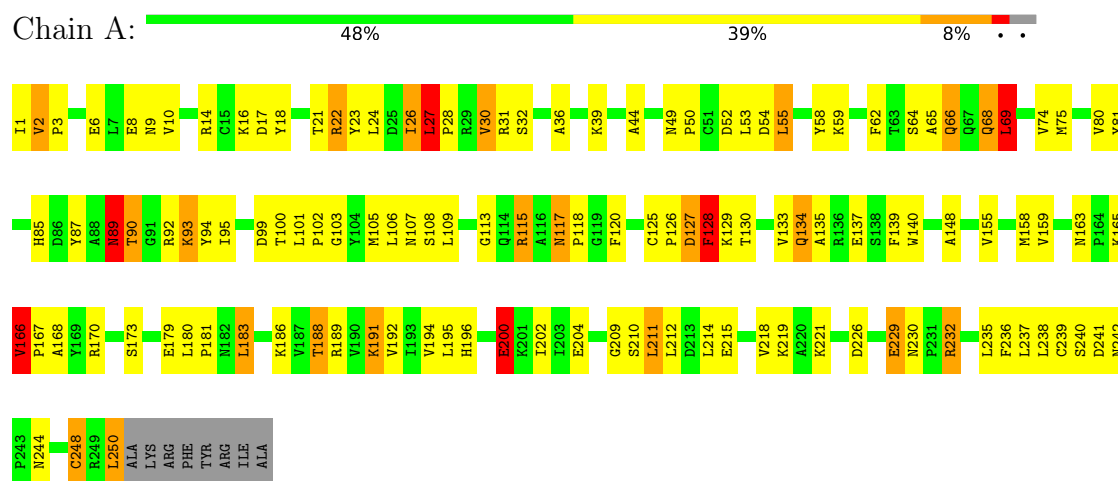
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	25	Total	O	0	0
			25	25		

3 Residue-property plots

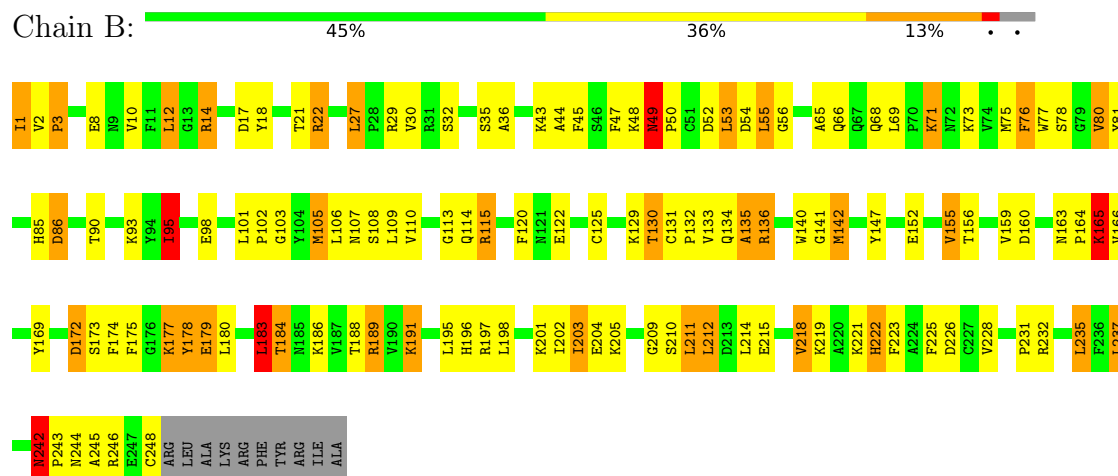
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ADP RIBOSYL CYCLASE



• Molecule 1: ADP RIBOSYL CYCLASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	70.20Å 72.30Å 125.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.40)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.214 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4064	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	1.11	2/2059 (0.1%)	1.50	35/2786 (1.3%)
1	B	1.07	3/2040 (0.1%)	1.38	22/2761 (0.8%)
All	All	1.09	5/4099 (0.1%)	1.44	57/5547 (1.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	THR	CA-CB	6.21	1.62	1.53
1	A	230	ASN	CA-C	-5.65	1.48	1.53
1	B	95	ILE	CA-CB	5.06	1.60	1.54
1	B	3	PRO	CA-C	5.06	1.57	1.52
1	A	148	ALA	CA-CB	-5.00	1.45	1.53

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	ILE	N-CA-C	11.92	121.86	110.30
1	B	135	ALA	N-CA-C	-9.86	98.53	111.24
1	A	135	ALA	N-CA-C	-9.09	99.82	112.45
1	B	105	MET	N-CA-C	8.90	121.06	111.36
1	A	186	LYS	N-CA-C	-8.31	102.92	113.23
1	A	22	ARG	N-CA-C	8.15	128.16	110.80
1	A	117	ASN	N-CA-C	-8.08	98.93	110.08
1	B	68	GLN	N-CA-C	-7.40	98.50	110.20
1	A	74	VAL	N-CA-C	6.90	118.68	109.37
1	B	66	GLN	N-CA-C	6.75	120.16	110.10
1	B	49	ASN	N-CA-C	-6.71	100.44	110.24
1	A	200	GLU	N-CA-C	6.67	125.01	110.80
1	A	21	THR	N-CA-C	6.65	124.39	113.89
1	A	242	ASN	CA-C-N	6.57	126.35	119.05
1	A	242	ASN	C-N-CA	6.57	126.35	119.05
1	A	89	ASN	N-CA-C	6.36	120.33	111.74
1	B	165	LYS	N-CA-C	6.29	120.05	112.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	LEU	CA-CB-CG	6.22	138.06	116.30
1	A	69	LEU	N-CA-C	6.20	117.89	110.07
1	B	242	ASN	CA-C-N	6.14	126.32	119.32
1	B	242	ASN	C-N-CA	6.14	126.32	119.32
1	A	191	LYS	CA-C-N	-6.06	115.28	123.10
1	A	191	LYS	C-N-CA	-6.06	115.28	123.10
1	B	2	VAL	N-CA-C	-5.90	96.14	108.88
1	B	130	THR	N-CA-C	5.90	119.52	110.20
1	A	140	TRP	N-CA-C	5.89	118.66	111.82
1	A	188	THR	N-CA-CB	-5.84	101.95	110.47
1	A	210	SER	N-CA-C	-5.83	105.42	112.54
1	A	99	ASP	N-CA-C	-5.78	106.39	113.50
1	B	218	VAL	CB-CA-C	-5.72	104.58	112.24
1	A	68	GLN	N-CA-C	-5.54	100.96	109.76
1	B	86	ASP	N-CA-C	-5.52	105.16	111.07
1	A	230	ASN	CB-CA-C	-5.51	107.29	111.20
1	A	248	CYS	N-CA-C	5.45	118.94	112.72
1	B	179	GLU	N-CA-C	5.44	119.47	111.04
1	B	141	GLY	N-CA-C	-5.43	105.92	112.49
1	A	27	LEU	CA-C-N	5.41	125.88	120.14
1	A	27	LEU	C-N-CA	5.41	125.88	120.14
1	B	76	PHE	N-CA-C	-5.38	101.39	109.95
1	B	106	LEU	CA-CB-CG	-5.38	97.48	116.30
1	B	178	TYR	N-CA-C	5.35	120.17	113.43
1	B	183	LEU	N-CA-C	-5.27	102.25	110.10
1	A	64	SER	N-CA-C	5.26	117.09	111.36
1	B	177	LYS	N-CA-C	5.25	117.08	111.36
1	A	166	VAL	CA-C-N	5.23	125.17	119.78
1	A	166	VAL	C-N-CA	5.23	125.17	119.78
1	A	36	ALA	N-CA-C	-5.22	105.50	111.14
1	B	21	THR	N-CA-C	5.20	121.93	114.39
1	A	2	VAL	CA-C-N	5.18	125.18	120.21
1	A	2	VAL	C-N-CA	5.18	125.18	120.21
1	A	9	ASN	N-CA-C	5.14	116.96	111.36
1	B	48	LYS	N-CA-C	-5.09	101.67	109.41
1	A	105	MET	N-CA-C	5.08	117.71	111.82
1	A	232	ARG	N-CA-C	5.07	117.20	111.11
1	A	44	ALA	N-CA-C	5.05	117.90	111.69
1	B	36	ALA	N-CA-C	-5.04	105.69	111.14
1	A	173	SER	N-CA-C	-5.00	101.77	109.52

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	2007	0	1963	82	0
1	B	1988	0	1939	102	0
2	A	44	0	0	6	0
2	B	25	0	0	3	0
All	All	4064	0	3902	178	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 23.

All (178) 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:175:PHE:HA	1:B:179:GLU:HB2	1.46	0.94
1:B:18:TYR:HA	1:B:22:ARG:HB2	1.60	0.84
1:B:184:THR:HG21	2:B:650:HOH:O	1.81	0.81
1:B:132:PRO:HB2	1:B:134:GLN:OE1	1.82	0.80
1:A:89:ASN:HB3	1:A:92:ARG:HB2	1.67	0.77
1:A:189:ARG:NH2	1:A:226:ASP:HB2	2.01	0.76
1:B:103:GLY:O	1:B:107:ASN:HB2	1.87	0.75
1:A:49:ASN:ND2	1:A:115:ARG:HH12	1.85	0.74
1:B:29:ARG:NH1	2:B:669:HOH:O	2.21	0.74
1:A:89:ASN:HB2	1:A:93:LYS:HE2	1.69	0.74
1:B:201:LYS:O	1:B:203:ILE:HD13	1.89	0.73
1:B:115:ARG:HH11	1:B:115:ARG:HG3	1.53	0.73
1:A:163:ASN:HD21	1:A:165:LYS:HG3	1.52	0.73
1:A:69:LEU:HG	1:A:95:ILE:HD11	1.70	0.72
1:B:173:SER:O	1:B:177:LYS:HG3	1.90	0.71
1:A:23:TYR:N	2:A:659:HOH:O	2.25	0.70
1:A:54:ASP:HA	1:A:134:GLN:HG2	1.74	0.69
1:B:80:VAL:HG11	1:B:195:LEU:HD22	1.75	0.68
1:A:26:ILE:H	1:A:26:ILE:HD12	1.57	0.68
1:B:202:ILE:HG21	1:B:205:LYS:HE2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:VAL:HA	1:B:136:ARG:HB3	1.75	0.68
1:B:18:TYR:O	2:B:669:HOH:O	2.11	0.67
1:B:203:ILE:HG22	1:B:204:GLU:HG2	1.77	0.67
1:B:81:TYR:O	1:B:85:HIS:HD2	1.78	0.66
1:B:142:MET:HE2	1:B:142:MET:HA	1.77	0.66
1:A:103:GLY:O	1:A:107:ASN:HB2	1.97	0.65
1:A:107:ASN:O	1:A:108:SER:HB2	1.96	0.65
1:B:69:LEU:HD21	1:B:147:TYR:CD1	2.32	0.65
1:B:1:ILE:HG13	1:B:125:CYS:HB2	1.78	0.64
1:B:221:LYS:O	1:B:222:HIS:HB2	1.97	0.64
1:B:215:GLU:HG2	1:B:219:LYS:HD3	1.79	0.64
1:B:3:PRO:HB3	1:B:125:CYS:SG	2.37	0.64
1:A:101:LEU:HB3	1:A:102:PRO:HD3	1.81	0.63
1:B:115:ARG:HH11	1:B:115:ARG:CG	2.12	0.62
1:A:163:ASN:C	1:A:163:ASN:HD22	2.08	0.62
1:B:1:ILE:HD12	1:B:110:VAL:CG1	2.30	0.61
1:B:201:LYS:HE3	1:B:203:ILE:HD12	1.82	0.61
1:B:65:ALA:HB1	1:B:102:PRO:HD3	1.83	0.60
1:B:198:LEU:HD11	1:B:248:CYS:SG	2.42	0.60
1:A:80:VAL:HG21	1:A:158:MET:HG2	1.83	0.59
1:A:236:PHE:HE2	1:B:243:PRO:HA	1.67	0.59
1:A:39:LYS:N	1:A:39:LYS:HD2	2.18	0.59
1:B:43:LYS:HG2	1:B:44:ALA:N	2.16	0.59
1:A:49:ASN:HB3	1:A:52:ASP:HB2	1.85	0.58
1:A:163:ASN:ND2	1:A:165:LYS:HG3	2.19	0.58
1:A:89:ASN:O	1:A:92:ARG:HG3	2.02	0.58
1:A:126:PRO:HB2	1:A:130:THR:HG21	1.85	0.58
1:A:90:THR:CG2	1:A:90:THR:O	2.52	0.58
1:B:242:ASN:ND2	1:B:244:ASN:O	2.36	0.57
1:A:49:ASN:OD1	1:A:50:PRO:HD2	2.05	0.57
1:B:77:TRP:CH2	1:B:81:TYR:HD2	2.22	0.57
1:B:1:ILE:HD12	1:B:110:VAL:HG11	1.86	0.56
1:B:78:SER:HB2	1:B:159:VAL:HG23	1.85	0.56
1:B:80:VAL:CG1	1:B:195:LEU:HD22	2.34	0.56
1:A:3:PRO:HB3	1:A:125:CYS:SG	2.45	0.56
1:A:165:LYS:HD2	1:A:166:VAL:HG12	1.88	0.56
1:A:87:TYR:CD2	1:A:158:MET:HE1	2.41	0.56
1:A:106:LEU:HD13	1:A:139:PHE:CZ	2.41	0.55
1:B:164:PRO:HG2	1:B:165:LYS:H	1.71	0.55
1:A:18:TYR:HA	1:A:22:ARG:HG2	1.88	0.54
1:A:179:GLU:O	1:A:183:LEU:HD13	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:HIS:CE1	1:A:202:ILE:HG23	2.41	0.54
1:B:235:LEU:HD22	1:B:235:LEU:O	2.07	0.54
1:A:55:LEU:HD23	1:A:134:GLN:HB2	1.89	0.54
1:A:22:ARG:CA	2:A:659:HOH:O	2.56	0.54
1:A:87:TYR:HD2	1:A:158:MET:HE1	1.73	0.54
1:A:133:VAL:O	1:A:137:GLU:N	2.42	0.53
1:B:214:LEU:O	1:B:218:VAL:HG23	2.08	0.53
1:A:17:ASP:OD1	1:B:14:ARG:HD2	2.08	0.53
1:B:140:TRP:C	1:B:174:PHE:HE2	2.16	0.53
1:B:8:GLU:O	1:B:12:LEU:HB2	2.08	0.53
1:B:76:PHE:CE2	1:B:155:VAL:HG13	2.44	0.53
1:A:163:ASN:ND2	1:A:165:LYS:H	2.06	0.52
1:B:53:LEU:O	1:B:135:ALA:HA	2.09	0.52
1:B:85:HIS:HE1	1:B:98:GLU:OE1	1.93	0.52
1:A:163:ASN:HD21	1:A:165:LYS:CG	2.21	0.52
1:B:169:TYR:CD1	1:B:214:LEU:HD13	2.45	0.52
1:A:248:CYS:O	1:B:232:ARG:NH2	2.42	0.52
1:B:172:ASP:O	1:B:177:LYS:HD2	2.10	0.52
1:A:90:THR:O	1:A:90:THR:HG23	2.10	0.51
1:A:163:ASN:OD1	1:A:166:VAL:HG13	2.10	0.51
1:A:163:ASN:HD22	1:A:165:LYS:H	1.57	0.51
1:A:232:ARG:NH1	1:B:243:PRO:O	2.41	0.51
1:B:218:VAL:CG1	1:B:223:PHE:HB2	2.41	0.51
1:A:39:LYS:HD2	1:A:39:LYS:H	1.76	0.51
1:B:228:VAL:CG1	1:B:231:PRO:HG3	2.41	0.51
1:B:55:LEU:O	1:B:142:MET:HE3	2.12	0.50
1:A:89:ASN:O	1:A:90:THR:HB	2.11	0.49
1:B:174:PHE:CD2	1:B:178:TYR:HD2	2.30	0.49
1:B:189:ARG:HD2	1:B:226:ASP:HB2	1.94	0.49
1:B:196:HIS:CE1	1:B:204:GLU:O	2.65	0.49
1:A:18:TYR:HA	1:A:22:ARG:CG	2.42	0.49
1:A:62:PHE:O	1:A:66:GLN:HB2	2.13	0.49
1:A:236:PHE:CE2	1:B:243:PRO:HA	2.45	0.49
1:B:130:THR:HG22	1:B:131:CYS:O	2.12	0.49
1:A:209:GLY:N	2:A:668:HOH:O	2.44	0.49
1:B:133:VAL:HG12	1:B:136:ARG:HD2	1.94	0.49
1:A:65:ALA:HB1	1:A:102:PRO:HG3	1.94	0.49
1:B:169:TYR:CE1	1:B:214:LEU:HD13	2.48	0.48
1:B:49:ASN:HB3	1:B:115:ARG:NH2	2.28	0.48
1:B:76:PHE:HE2	1:B:155:VAL:CG1	2.26	0.48
1:A:159:VAL:HG21	1:A:168:ALA:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:HIS:HE1	1:B:204:GLU:O	1.95	0.48
1:B:76:PHE:HE2	1:B:155:VAL:HG13	1.79	0.48
1:A:167:PRO:HG2	1:A:170:ARG:HG3	1.96	0.47
1:B:218:VAL:HG21	1:B:225:PHE:CD1	2.49	0.47
1:A:30:VAL:HG13	1:A:32:SER:H	1.80	0.47
1:B:113:GLY:HA2	1:B:120:PHE:HA	1.97	0.47
1:B:10:VAL:CG1	1:B:109:LEU:HD21	2.45	0.46
1:A:221:LYS:NZ	2:A:631:HOH:O	2.46	0.46
1:A:128:PHE:HB2	1:A:129:LYS:H	1.63	0.46
1:B:245:ALA:HB3	1:B:248:CYS:SG	2.56	0.46
1:A:75:MET:HE3	1:A:94:TYR:CD2	2.52	0.45
1:B:10:VAL:HG12	1:B:109:LEU:HD21	1.98	0.45
1:B:211:LEU:HD22	1:B:211:LEU:H	1.81	0.45
1:B:81:TYR:O	1:B:85:HIS:CD2	2.64	0.45
1:B:1:ILE:HD12	1:B:110:VAL:HG13	1.96	0.45
1:A:26:ILE:HD12	1:A:26:ILE:N	2.29	0.45
1:B:47:PHE:HA	1:B:114:GLN:O	2.16	0.45
1:B:177:LYS:HB3	1:B:177:LYS:HE2	1.74	0.45
1:A:194:VAL:HB	1:A:229:GLU:HB3	1.98	0.45
1:A:214:LEU:O	1:A:218:VAL:HG23	2.17	0.45
1:B:75:MET:HA	1:B:156:THR:O	2.17	0.45
1:A:26:ILE:H	1:A:26:ILE:CD1	2.29	0.44
1:B:180:LEU:HA	1:B:183:LEU:HD22	1.98	0.44
1:B:242:ASN:N	1:B:243:PRO:HD3	2.33	0.44
1:B:49:ASN:O	1:B:52:ASP:HB2	2.17	0.44
1:B:133:VAL:HA	1:B:136:ARG:HD2	2.00	0.44
1:B:228:VAL:HG11	1:B:231:PRO:HG3	2.00	0.44
1:A:118:PRO:HB2	1:A:120:PHE:CE1	2.53	0.44
1:B:49:ASN:HB2	1:B:115:ARG:NH1	2.33	0.44
1:A:196:HIS:HE1	1:A:204:GLU:O	2.01	0.43
1:A:211:LEU:HD13	1:A:211:LEU:HA	1.92	0.43
1:B:27:LEU:HD21	1:B:95:ILE:HD13	2.00	0.43
1:A:117:ASN:HD22	1:A:117:ASN:H	1.66	0.43
1:B:45:PHE:HA	1:B:53:LEU:HD11	2.01	0.42
1:B:86:ASP:CB	1:B:237:LEU:HD11	2.50	0.42
1:B:169:TYR:HB3	1:B:210:SER:HB3	2.01	0.42
1:A:58:TYR:HB2	1:A:62:PHE:HE2	1.85	0.42
1:B:54:ASP:O	1:B:56:GLY:N	2.53	0.42
1:A:1:ILE:HG23	1:A:125:CYS:HB2	2.01	0.42
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.88	0.42
1:A:168:ALA:HB3	1:A:211:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:TYR:CE2	1:A:85:HIS:CE1	3.08	0.42
1:A:180:LEU:HB3	1:A:181:PRO:HD3	2.01	0.42
1:B:183:LEU:HD12	1:B:183:LEU:HA	1.90	0.42
1:A:27:LEU:HD12	1:A:28:PRO:HD3	2.01	0.42
1:A:244:ASN:HD22	1:B:232:ARG:NH1	2.18	0.42
1:B:50:PRO:HD3	1:B:113:GLY:O	2.19	0.42
1:B:73:LYS:HD3	1:B:93:LYS:O	2.20	0.42
1:B:131:CYS:HB3	1:B:132:PRO:HD2	2.01	0.42
1:A:22:ARG:N	2:A:659:HOH:O	2.52	0.41
1:B:1:ILE:N	1:B:125:CYS:O	2.47	0.41
1:A:50:PRO:HD3	1:A:113:GLY:O	2.20	0.41
1:A:23:TYR:O	1:A:24:LEU:C	2.62	0.41
1:B:131:CYS:O	1:B:132:PRO:C	2.62	0.41
1:A:120:PHE:CD1	1:A:120:PHE:N	2.87	0.41
1:A:215:GLU:O	1:A:219:LYS:HG3	2.21	0.41
1:A:6:GLU:O	1:A:10:VAL:HG23	2.20	0.41
1:A:100:THR:CB	2:A:617:HOH:O	2.68	0.41
1:B:107:ASN:O	1:B:108:SER:HB2	2.20	0.41
1:B:140:TRP:O	1:B:174:PHE:HE2	2.03	0.41
1:B:163:ASN:HA	1:B:164:PRO:HD2	1.91	0.41
1:A:129:LYS:O	1:A:130:THR:C	2.64	0.41
1:A:239:CYS:O	1:A:240:SER:C	2.62	0.41
1:B:55:LEU:HD23	1:B:134:GLN:HB2	2.02	0.41
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.93	0.41
1:B:101:LEU:HG	1:B:105:MET:HE2	2.03	0.41
1:B:215:GLU:HG3	1:B:225:PHE:CD2	2.55	0.41
1:A:127:ASP:HB3	1:A:128:PHE:H	1.73	0.40
1:A:200:GLU:H	1:A:200:GLU:HG2	1.53	0.40
1:A:58:TYR:CB	1:A:62:PHE:CE2	3.04	0.40
1:B:212:LEU:HD22	1:B:212:LEU:O	2.21	0.40
1:B:221:LYS:HB3	1:B:223:PHE:CE2	2.56	0.40
1:B:69:LEU:HD21	1:B:147:TYR:CE1	2.55	0.40
1:B:71:LYS:HG3	1:B:152:GLU:HB2	2.03	0.40
1:B:160:ASP:CG	1:B:197:ARG:HH12	2.28	0.40
1:B:191:LYS:HA	1:B:226:ASP:HB3	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	248/258 (96%)	233 (94%)	13 (5%)	2 (1%)	16	25
1	B	246/258 (95%)	223 (91%)	20 (8%)	3 (1%)	10	16
All	All	494/516 (96%)	456 (92%)	33 (7%)	5 (1%)	12	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	PHE
1	B	55	LEU
1	B	222	HIS
1	B	209	GLY
1	A	127	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	220/226 (97%)	184 (84%)	36 (16%)	2	3
1	B	218/226 (96%)	182 (84%)	36 (16%)	2	3
All	All	438/452 (97%)	366 (84%)	72 (16%)	2	3

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL

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Mol	Chain	Res	Type
1	A	8	GLU
1	A	14	ARG
1	A	16	LYS
1	A	27	LEU
1	A	30	VAL
1	A	31	ARG
1	A	53	LEU
1	A	55	LEU
1	A	59	LYS
1	A	66	GLN
1	A	68	GLN
1	A	69	LEU
1	A	89	ASN
1	A	90	THR
1	A	93	LYS
1	A	109	LEU
1	A	115	ARG
1	A	128	PHE
1	A	134	GLN
1	A	155	VAL
1	A	166	VAL
1	A	183	LEU
1	A	188	THR
1	A	191	LYS
1	A	192	VAL
1	A	195	LEU
1	A	200	GLU
1	A	211	LEU
1	A	212	LEU
1	A	229	GLU
1	A	235	LEU
1	A	237	LEU
1	A	238	LEU
1	A	241	ASP
1	A	250	LEU
1	B	1	ILE
1	B	12	LEU
1	B	14	ARG
1	B	17	ASP
1	B	22	ARG
1	B	27	LEU
1	B	30	VAL

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Mol	Chain	Res	Type
1	B	32	SER
1	B	35	SER
1	B	49	ASN
1	B	53	LEU
1	B	71	LYS
1	B	80	VAL
1	B	90	THR
1	B	95	ILE
1	B	115	ARG
1	B	122	GLU
1	B	129	LYS
1	B	136	ARG
1	B	142	MET
1	B	155	VAL
1	B	165	LYS
1	B	166	VAL
1	B	172	ASP
1	B	183	LEU
1	B	186	LYS
1	B	188	THR
1	B	189	ARG
1	B	191	LYS
1	B	203	ILE
1	B	211	LEU
1	B	212	LEU
1	B	235	LEU
1	B	237	LEU
1	B	242	ASN
1	B	246	ARG

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

Mol	Chain	Res	Type
1	A	66	GLN
1	A	117	ASN
1	A	134	GLN
1	A	163	ASN
1	A	196	HIS
1	A	242	ASN
1	A	244	ASN
1	B	85	HIS
1	B	196	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 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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.