



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:43 AM UTC

PDB ID : 1ECP / pdb_00001ecp
Title : PURINE NUCLEOSIDE PHOSPHORYLASE
Authors : Mao, C.; Ealick, S.E.
Deposited on : 1995-07-13
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
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

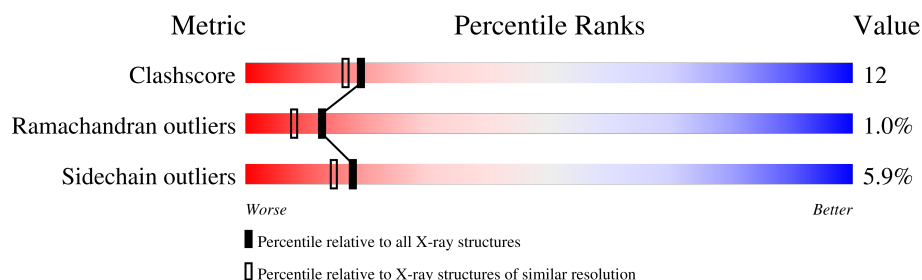
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	73% 24% .
1	B	238	71% 25% .
1	C	238	74% 23% .
1	D	238	74% 24% .
1	E	238	75% 22% ..
1	F	238	66% 31% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11238 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 PURINE NUCLEOSIDE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	B	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	C	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	D	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	E	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			
1	F	237	Total	C	N	O	S	0	0	0
			1793	1132	307	339	15			

- Molecule 2 is water.

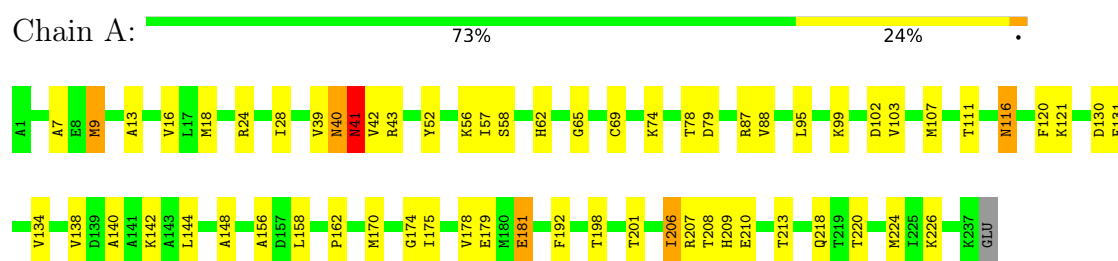
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	80	Total	O	0	0
			80	80		
2	B	76	Total	O	0	0
			76	76		
2	C	82	Total	O	0	0
			82	82		
2	D	85	Total	O	0	0
			85	85		
2	E	79	Total	O	0	0
			79	79		
2	F	78	Total	O	0	0
			78	78		

3 Residue-property plots

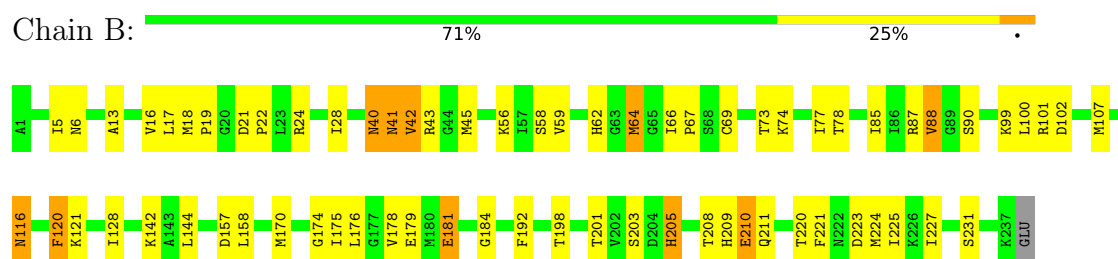
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

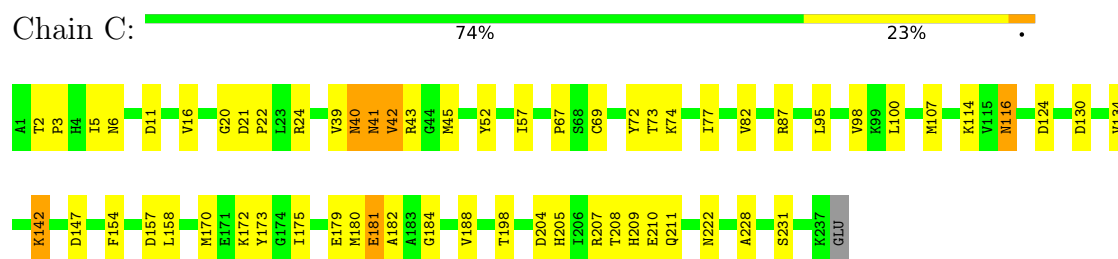
• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



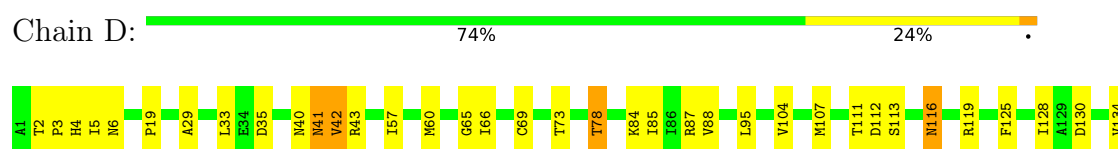
• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE





• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE

Chain E: 75% 22% ..



• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE

Chain F: 66% 31% .



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.50Å 110.60Å 74.60Å 90.00° 111.70° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-2.00)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.200 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11238	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	0.42	0/1822	0.95	7/2457 (0.3%)
1	B	0.38	0/1822	0.90	3/2457 (0.1%)
1	C	0.40	0/1822	0.90	1/2457 (0.0%)
1	D	0.41	0/1822	0.94	8/2457 (0.3%)
1	E	0.39	0/1822	0.93	3/2457 (0.1%)
1	F	0.38	0/1822	0.92	2/2457 (0.1%)
All	All	0.40	0/10932	0.92	24/14742 (0.2%)

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	120	PHE	N-CA-C	7.28	120.80	112.57
1	B	120	PHE	N-CA-C	6.74	120.18	112.57
1	A	174	GLY	N-CA-C	6.43	123.82	114.10
1	E	180	MET	N-CA-C	6.34	120.93	112.30
1	D	180	MET	N-CA-C	6.32	121.85	112.94
1	D	78	THR	N-CA-C	6.14	118.94	111.82
1	C	180	MET	N-CA-C	5.91	123.22	113.89
1	D	181	GLU	N-CA-C	5.85	122.81	114.16
1	A	78	THR	N-CA-C	5.82	117.71	111.36
1	B	174	GLY	N-CA-C	5.74	121.85	113.48
1	D	111	THR	N-CA-C	5.68	117.70	109.07
1	D	159	PHE	N-CA-C	-5.63	105.23	111.36
1	B	78	THR	N-CA-C	5.55	117.41	111.36
1	F	180	MET	N-CA-C	5.54	121.94	113.19
1	A	65	GLY	CA-C-N	5.41	123.65	120.24
1	A	65	GLY	C-N-CA	5.41	123.65	120.24
1	A	111	THR	N-CA-C	5.38	117.01	108.79
1	F	78	THR	N-CA-C	5.36	118.99	112.23
1	E	157	ASP	N-CA-C	-5.35	105.02	112.45
1	E	78	THR	N-CA-C	5.32	116.93	111.03
1	A	206	ILE	N-CA-C	5.23	115.67	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	113	SER	N-CA-C	5.07	116.87	110.33
1	D	65	GLY	CA-C-N	5.02	125.25	120.43
1	D	65	GLY	C-N-CA	5.02	125.25	120.43

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	1793	0	1791	38	2
1	B	1793	0	1791	42	0
1	C	1793	0	1791	46	1
1	D	1793	0	1791	46	3
1	E	1793	0	1791	46	1
1	F	1793	0	1791	54	2
2	A	80	0	0	2	0
2	B	76	0	0	2	0
2	C	82	0	0	1	2
2	D	85	0	0	2	1
2	E	79	0	0	1	0
2	F	78	0	0	2	0
All	All	11238	0	10746	253	6

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (253) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:HD22	1:A:40:ASN:C	1.53	1.12
1:B:5:ILE:HG23	1:B:40:ASN:OD1	1.59	1.01
1:D:167:PHE:HA	1:D:170:MET:HE2	1.48	0.95
1:A:87:ARG:HB3	1:A:198:THR:HG22	1.51	0.90
1:E:40:ASN:HD22	1:E:41:ASN:H	1.16	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:ASN:OD1	1:E:40:ASN:ND2	2.05	0.89
1:E:40:ASN:HD22	1:E:41:ASN:N	1.73	0.86
1:E:115:VAL:HG23	1:E:116:ASN:ND2	1.89	0.85
1:E:115:VAL:HG23	1:E:116:ASN:HD22	1.40	0.83
1:F:40:ASN:HD21	1:F:42:VAL:HG23	1.43	0.81
1:F:40:ASN:HD22	1:F:41:ASN:H	1.26	0.80
1:E:116:ASN:OD1	2:E:310:HOH:O	1.99	0.80
1:A:40:ASN:C	1:A:40:ASN:ND2	2.28	0.79
1:A:88:VAL:HB	1:A:224:MET:HE3	1.62	0.79
1:B:21:ASP:HB3	1:B:24:ARG:HG3	1.65	0.79
1:D:87:ARG:HB3	1:D:198:THR:HG22	1.64	0.78
1:F:87:ARG:HB3	1:F:198:THR:HG22	1.66	0.76
1:A:162:PRO:HG3	1:D:119:ARG:HG2	1.68	0.76
1:D:40:ASN:HD22	1:D:41:ASN:H	1.29	0.76
1:F:40:ASN:HD22	1:F:41:ASN:N	1.83	0.75
1:B:116:ASN:OD1	2:B:1528:HOH:O	2.04	0.75
1:E:40:ASN:HD21	1:E:42:VAL:HG22	1.52	0.74
1:F:6:ASN:OD1	1:F:40:ASN:ND2	2.20	0.74
1:A:41:ASN:C	1:A:41:ASN:HD22	1.95	0.73
1:B:128:ILE:HD12	1:D:107:MET:HE3	1.70	0.73
1:D:73:THR:HG23	1:D:85:ILE:HD12	1.71	0.73
1:F:73:THR:O	1:F:77:ILE:HG12	1.89	0.72
1:C:87:ARG:HB3	1:C:198:THR:HG22	1.72	0.71
1:A:116:ASN:OD1	2:A:256:HOH:O	2.08	0.71
1:B:22:PRO:HG3	1:B:45:MET:SD	2.30	0.71
1:C:5:ILE:HA	1:C:40:ASN:HD21	1.54	0.70
1:A:69:CYS:SG	1:A:181:GLU:HB2	2.32	0.70
1:E:41:ASN:C	1:E:41:ASN:HD22	1.99	0.69
1:F:40:ASN:ND2	1:F:42:VAL:HG23	2.08	0.69
1:F:115:VAL:HG23	1:F:116:ASN:ND2	2.08	0.69
1:C:20:GLY:H	1:C:24:ARG:HH21	1.38	0.69
1:F:115:VAL:HG23	1:F:116:ASN:HD22	1.58	0.68
1:D:40:ASN:HD22	1:D:41:ASN:N	1.92	0.68
1:B:221:PHE:CE2	1:B:225:ILE:HD11	2.29	0.68
1:C:116:ASN:OD1	2:C:1252:HOH:O	2.11	0.68
1:D:88:VAL:HB	1:D:224:MET:HE3	1.75	0.67
1:C:69:CYS:SG	1:C:181:GLU:HB2	2.35	0.67
1:B:6:ASN:OD1	1:B:40:ASN:ND2	2.27	0.67
1:E:170:MET:HB3	1:E:175:ILE:HG12	1.77	0.67
1:B:87:ARG:HB3	1:B:198:THR:HG22	1.77	0.67
1:C:205:HIS:HB3	1:C:208:THR:O	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ASN:HD22	1:A:41:ASN:N	1.93	0.66
1:D:139:ASP:O	1:D:142:LYS:HG2	1.95	0.66
1:F:90:SER:HB3	1:F:203:SER:OG	1.95	0.66
1:C:42:VAL:HG23	1:C:43:ARG:H	1.61	0.65
1:D:42:VAL:HG23	1:D:43:ARG:H	1.60	0.65
1:E:2:THR:HB	1:E:3:PRO:HD2	1.78	0.65
1:B:41:ASN:C	1:B:41:ASN:HD22	2.05	0.65
1:A:170:MET:HB3	1:A:175:ILE:HG12	1.77	0.64
1:B:107:MET:HE3	1:D:128:ILE:HD12	1.78	0.64
1:E:69:CYS:SG	1:E:181:GLU:HB2	2.36	0.64
1:E:40:ASN:ND2	1:E:41:ASN:N	2.44	0.64
1:B:69:CYS:SG	1:B:181:GLU:HB2	2.38	0.64
1:D:69:CYS:SG	1:D:181:GLU:HB2	2.38	0.64
1:A:103:VAL:HG13	1:A:148:ALA:HA	1.79	0.63
1:C:170:MET:HB3	1:C:175:ILE:HG12	1.80	0.63
1:D:6:ASN:OD1	1:D:40:ASN:ND2	2.33	0.62
1:D:41:ASN:N	1:D:41:ASN:HD22	1.98	0.61
1:F:41:ASN:N	1:F:41:ASN:HD22	1.99	0.61
1:D:40:ASN:HD21	1:D:42:VAL:HG22	1.66	0.61
1:E:40:ASN:ND2	1:E:42:VAL:H	1.98	0.61
1:F:201:THR:HG21	1:F:220:THR:HB	1.81	0.61
1:E:13:ALA:HB2	1:E:56:LYS:HG2	1.83	0.61
1:C:5:ILE:HG23	1:C:40:ASN:OD1	2.00	0.61
1:C:52:TYR:HB3	1:C:57:ILE:HD12	1.83	0.60
1:E:135:ARG:HG2	1:E:135:ARG:HH11	1.64	0.60
1:E:212:THR:H	1:E:217:ARG:HH21	1.49	0.60
1:A:16:VAL:HG22	1:A:58:SER:HB2	1.84	0.60
1:E:204:ASP:HB3	1:E:211:GLN:HG2	1.84	0.60
1:A:9:MET:HG2	1:A:79:ASP:O	2.02	0.60
1:A:41:ASN:C	1:A:41:ASN:ND2	2.59	0.59
1:E:11:ASP:HB3	1:E:39:VAL:CG2	2.32	0.59
1:A:121:LYS:HE2	1:E:165:GLU:HG3	1.84	0.59
1:B:17:LEU:HB2	1:B:59:VAL:HG12	1.84	0.59
1:D:170:MET:HB3	1:D:175:ILE:HG12	1.86	0.58
1:C:41:ASN:N	1:C:41:ASN:HD22	2.02	0.58
1:B:13:ALA:HB2	1:B:56:LYS:HG2	1.86	0.57
1:B:66:ILE:HG23	1:B:184:GLY:HA3	1.85	0.57
1:B:73:THR:O	1:B:77:ILE:HG12	2.03	0.57
1:E:116:ASN:HD22	1:E:116:ASN:N	2.02	0.57
1:B:77:ILE:HD11	1:B:85:ILE:HD11	1.85	0.57
1:C:142:LYS:HE3	1:C:142:LYS:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:218:GLN:HA	1:F:218:GLN:NE2	2.20	0.57
1:E:211:GLN:HB3	1:E:217:ARG:HH22	1.70	0.57
1:F:66:ILE:HG23	1:F:184:GLY:HA3	1.85	0.57
1:C:175:ILE:HG13	1:C:175:ILE:O	2.04	0.57
1:F:218:GLN:HA	1:F:218:GLN:HE21	1.68	0.57
1:B:223:ASP:O	1:B:227:ILE:HG13	2.05	0.57
1:A:140:ALA:O	1:A:144:LEU:HD13	2.05	0.56
1:F:5:ILE:HG23	1:F:40:ASN:OD1	2.06	0.56
1:F:94:VAL:O	1:F:207:ARG:HG3	2.06	0.56
1:D:212:THR:HG23	1:D:217:ARG:HG3	1.87	0.56
1:E:41:ASN:C	1:E:41:ASN:ND2	2.62	0.56
1:A:134:VAL:O	1:A:138:VAL:HG23	2.06	0.55
1:F:40:ASN:ND2	1:F:41:ASN:N	2.53	0.55
1:B:90:SER:HB3	1:B:203:SER:OG	2.07	0.55
1:C:42:VAL:HG23	1:C:43:ARG:N	2.22	0.55
1:C:74:LYS:HG2	1:E:160:TYR:CD2	2.41	0.55
1:D:19:PRO:HA	1:D:88:VAL:O	2.07	0.55
1:F:69:CYS:SG	1:F:181:GLU:HB2	2.47	0.55
1:D:5:ILE:HG23	1:D:40:ASN:OD1	2.07	0.54
1:A:74:LYS:HG2	1:D:160:TYR:CD2	2.43	0.54
1:E:211:GLN:HB3	1:E:217:ARG:NH2	2.23	0.54
1:D:221:PHE:O	1:D:225:ILE:HG12	2.07	0.53
1:F:26:LYS:O	1:F:30:GLU:HG2	2.09	0.53
1:A:24:ARG:O	1:A:28:ILE:HG12	2.08	0.53
1:F:154:PHE:HB2	1:F:175:ILE:HD13	1.90	0.53
1:D:167:PHE:HD1	1:D:170:MET:HE2	1.74	0.53
1:F:16:VAL:HG12	1:F:82:VAL:HG11	1.91	0.52
1:A:131:PHE:HA	1:E:107:MET:HE1	1.92	0.52
1:B:221:PHE:O	1:B:225:ILE:HG13	2.09	0.52
1:B:5:ILE:HG23	1:B:40:ASN:CG	2.33	0.52
1:B:41:ASN:C	1:B:41:ASN:ND2	2.65	0.52
1:C:173:TYR:CZ	1:F:119:ARG:HB3	2.45	0.52
1:D:135:ARG:HA	1:D:138:VAL:HG12	1.92	0.52
1:E:21:ASP:H	1:E:24:ARG:HH21	1.56	0.52
1:A:201:THR:HG21	1:A:220:THR:CG2	2.40	0.52
1:D:40:ASN:ND2	1:D:41:ASN:N	2.56	0.52
1:A:95:LEU:HD23	1:A:175:ILE:O	2.10	0.52
1:D:4:HIS:O	1:D:42:VAL:HG21	2.10	0.52
1:C:20:GLY:H	1:C:24:ARG:NH2	2.05	0.52
1:F:105:ILE:HG23	1:F:197:LEU:HD11	1.92	0.52
1:A:42:VAL:HG23	1:A:43:ARG:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:130:ASP:O	1:C:134:VAL:HG23	2.10	0.51
1:F:36:ALA:HA	1:F:49:THR:O	2.11	0.51
1:F:228:ALA:O	1:F:232:VAL:HG23	2.10	0.51
1:C:11:ASP:HB3	1:C:39:VAL:CG1	2.40	0.51
1:D:41:ASN:H	1:D:41:ASN:HD22	1.57	0.51
1:F:2:THR:HB	1:F:3:PRO:HD2	1.92	0.51
1:F:116:ASN:HD22	1:F:116:ASN:N	2.07	0.51
1:F:170:MET:HB3	1:F:175:ILE:HG12	1.93	0.51
1:E:11:ASP:HB3	1:E:39:VAL:HG23	1.91	0.51
1:F:204:ASP:HB3	1:F:211:GLN:HG3	1.91	0.50
1:C:95:LEU:HB2	1:C:98:VAL:HG23	1.93	0.50
1:C:5:ILE:HG23	1:C:40:ASN:CG	2.37	0.50
1:D:41:ASN:N	1:D:41:ASN:ND2	2.60	0.50
1:E:6:ASN:OD1	1:E:42:VAL:HG13	2.12	0.50
1:F:205:HIS:HB3	1:F:208:THR:O	2.12	0.50
1:C:100:LEU:HD22	1:C:100:LEU:H	1.77	0.50
1:A:208:THR:O	1:A:210:GLU:N	2.45	0.50
1:C:124:ASP:O	1:F:110:CYS:HB3	2.12	0.50
1:D:40:ASN:ND2	1:D:42:VAL:H	2.09	0.50
1:B:42:VAL:HG12	1:B:43:ARG:N	2.27	0.49
1:D:73:THR:HG23	1:D:85:ILE:CD1	2.39	0.49
1:B:74:LYS:HD3	1:B:192:PHE:CZ	2.47	0.49
1:D:116:ASN:OD1	2:D:1379:HOH:O	2.20	0.49
1:E:74:LYS:HD3	1:E:74:LYS:C	2.37	0.49
1:B:16:VAL:HG12	1:B:58:SER:HB2	1.95	0.49
1:C:208:THR:O	1:C:210:GLU:N	2.45	0.49
1:E:221:PHE:O	1:E:225:ILE:HG12	2.12	0.49
1:E:11:ASP:HB3	1:E:39:VAL:HG21	1.94	0.49
1:E:4:HIS:O	1:E:42:VAL:HG21	2.12	0.49
1:F:41:ASN:N	1:F:41:ASN:ND2	2.60	0.48
1:C:45:MET:HG2	1:C:72:TYR:CZ	2.48	0.48
1:C:114:LYS:HD3	1:E:114:LYS:HG3	1.95	0.48
1:F:40:ASN:ND2	1:F:42:VAL:H	2.11	0.48
1:E:116:ASN:ND2	1:E:116:ASN:N	2.61	0.48
1:F:20:GLY:HA2	1:F:62:HIS:CE1	2.48	0.48
1:B:19:PRO:HA	1:B:88:VAL:O	2.14	0.48
1:B:74:LYS:HG2	1:F:160:TYR:CD2	2.49	0.48
1:D:60:MET:SD	2:D:1701:HOH:O	2.60	0.48
1:B:18:MET:HE2	1:B:62:HIS:HB3	1.96	0.48
1:B:88:VAL:HB	1:B:224:MET:HE3	1.96	0.47
1:D:66:ILE:HG23	1:D:184:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ASP:HA	1:E:142:LYS:HE3	1.97	0.47
1:A:130:ASP:O	1:A:134:VAL:HG23	2.14	0.47
1:B:28:ILE:HG12	1:B:225:ILE:HD13	1.95	0.47
1:C:2:THR:HB	1:C:3:PRO:HD2	1.96	0.47
1:F:89:GLY:O	1:F:200:CYS:HA	2.14	0.47
1:F:156:ALA:HB1	2:F:492:HOH:O	2.14	0.47
1:A:107:MET:HG3	1:E:107:MET:HE2	1.96	0.47
1:D:167:PHE:HD1	1:D:170:MET:CE	2.27	0.47
1:D:5:ILE:HA	1:D:40:ASN:OD1	2.15	0.47
1:B:157:ASP:O	1:F:67:PRO:HB3	2.15	0.46
1:C:6:ASN:H	1:C:40:ASN:ND2	2.13	0.46
1:B:99:LYS:O	1:B:102:ASP:HB2	2.16	0.46
1:B:144:LEU:HD12	1:B:227:ILE:HG12	1.96	0.46
1:B:201:THR:HG21	1:B:220:THR:HG22	1.97	0.46
1:F:53:LYS:HD2	1:F:233:LEU:CD1	2.45	0.46
1:C:11:ASP:HB3	1:C:39:VAL:HG13	1.98	0.46
1:B:64:MET:HE3	1:F:71:ILE:HD12	1.98	0.46
1:A:74:LYS:HD3	1:A:192:PHE:CZ	2.51	0.45
1:D:40:ASN:ND2	1:D:42:VAL:HG22	2.31	0.45
1:C:107:MET:SD	1:F:107:MET:HE2	2.57	0.45
1:B:74:LYS:HD3	1:B:192:PHE:CE2	2.52	0.45
1:E:66:ILE:HG23	1:E:184:GLY:HA3	1.99	0.45
1:E:101:ARG:HB3	1:E:220:THR:HG21	1.98	0.45
1:C:41:ASN:N	1:C:41:ASN:ND2	2.63	0.44
1:C:184:GLY:O	1:C:188:VAL:HG23	2.16	0.44
1:F:45:MET:HG3	1:F:72:TYR:CZ	2.53	0.44
1:D:130:ASP:O	1:D:134:VAL:HG23	2.18	0.44
1:D:29:ALA:HA	1:D:33:LEU:HD13	2.01	0.43
1:C:21:ASP:HA	1:C:22:PRO:HD3	1.92	0.43
1:E:223:ASP:O	1:E:227:ILE:HG13	2.18	0.43
1:E:105:ILE:HD13	1:E:199:ILE:HG23	2.00	0.43
1:E:95:LEU:HD12	1:E:171:GLU:HG3	2.01	0.43
1:D:228:ALA:O	1:D:232:VAL:HG23	2.19	0.43
1:D:40:ASN:ND2	1:D:41:ASN:H	2.04	0.43
1:D:116:ASN:OD1	1:D:125:PHE:HD2	2.02	0.43
1:F:116:ASN:ND2	1:F:116:ASN:N	2.67	0.43
1:A:206:ILE:H	1:A:206:ILE:HD12	1.84	0.43
1:C:2:THR:OG1	1:C:5:ILE:HB	2.19	0.43
1:B:231:SER:HB2	2:B:1485:HOH:O	2.18	0.42
1:A:156:ALA:HB1	2:A:379:HOH:O	2.19	0.42
1:A:18:MET:HE2	1:A:62:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ASP:HB3	1:E:24:ARG:HE	1.84	0.42
1:A:142:LYS:HE2	1:A:142:LYS:HB3	1.93	0.42
1:B:121:LYS:HD3	1:D:169:VAL:HG21	2.01	0.42
1:B:67:PRO:HD2	1:F:67:PRO:CG	2.50	0.42
1:F:175:ILE:O	1:F:175:ILE:HG13	2.19	0.42
1:A:99:LYS:O	1:A:102:ASP:HB2	2.20	0.42
1:B:208:THR:O	1:B:210:GLU:N	2.52	0.42
1:C:16:VAL:HG12	1:C:82:VAL:HG11	2.01	0.42
1:C:21:ASP:HB3	1:C:24:ARG:HG3	2.01	0.42
1:D:42:VAL:HG23	1:D:43:ARG:N	2.30	0.42
1:B:170:MET:HB3	1:B:175:ILE:HG12	2.02	0.42
1:B:205:HIS:HB3	1:B:208:THR:O	2.19	0.42
1:C:182:ALA:HA	1:C:198:THR:HG21	2.02	0.42
1:C:204:ASP:HA	1:C:210:GLU:O	2.20	0.42
1:D:116:ASN:HD22	1:D:116:ASN:HA	1.64	0.42
1:F:18:MET:HE2	1:F:62:HIS:HB3	2.01	0.42
1:F:70:SER:O	1:F:74:LYS:HB2	2.19	0.42
1:F:100:LEU:O	1:F:101:ARG:HB2	2.21	0.41
1:F:134:VAL:O	1:F:138:VAL:HG23	2.20	0.41
1:C:73:THR:O	1:C:77:ILE:HG13	2.20	0.41
1:E:22:PRO:O	1:E:25:ALA:HB3	2.20	0.41
1:F:60:MET:HE2	1:F:76:LEU:HD11	2.01	0.41
1:B:100:LEU:O	1:B:101:ARG:HB3	2.19	0.41
1:A:7:ALA:HB2	1:A:39:VAL:O	2.20	0.41
1:C:20:GLY:N	1:C:24:ARG:HH21	2.11	0.41
1:C:100:LEU:HD21	1:C:210:GLU:HB2	2.01	0.41
1:C:172:LYS:HG2	2:F:1668:HOH:O	2.21	0.41
1:C:228:ALA:O	1:C:231:SER:HB3	2.20	0.41
1:A:107:MET:HE1	1:E:131:PHE:HA	2.01	0.41
1:C:39:VAL:O	1:C:39:VAL:HG12	2.20	0.41
1:E:88:VAL:HB	1:E:224:MET:HE3	2.02	0.41
1:F:74:LYS:HG2	1:F:192:PHE:CE2	2.56	0.41
1:F:208:THR:O	1:F:210:GLU:N	2.54	0.41
1:A:52:TYR:HB3	1:A:57:ILE:HD12	2.03	0.40
1:D:104:VAL:HG13	1:D:176:LEU:HD13	2.03	0.40
1:A:13:ALA:HB2	1:A:56:LYS:HG2	2.02	0.40
1:A:40:ASN:ND2	1:A:41:ASN:N	2.62	0.40
1:A:170:MET:HB3	1:A:175:ILE:CG1	2.48	0.40
1:F:137:ALA:HA	1:F:231:SER:HB3	2.03	0.40
1:C:67:PRO:HB3	1:E:157:ASP:O	2.22	0.40
1:C:154:PHE:HB2	1:C:175:ILE:HD13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:THR:HB	1:D:3:PRO:HD2	2.02	0.40
1:D:84:LYS:HA	1:D:195:LYS:O	2.22	0.40

All (6) 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:D:78:THR:CB	2:C:389:HOH:O[1_556]	1.51	0.69
1:A:226:LYS:NZ	1:F:223:ASP:OD1[1_656]	1.59	0.61
1:A:213:THR:OG1	1:F:34:GLU:OE1[1_656]	1.93	0.27
1:C:211:GLN:NE2	1:D:35:ASP:OD1[2_646]	1.95	0.25
1:E:209:HIS:CD2	2:D:1326:HOH:O[1_554]	2.07	0.13
1:D:78:THR:CG2	2:C:389:HOH:O[1_556]	2.19	0.01

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	235/238 (99%)	224 (95%)	8 (3%)	3 (1%)	9	5
1	B	235/238 (99%)	222 (94%)	11 (5%)	2 (1%)	14	9
1	C	235/238 (99%)	222 (94%)	10 (4%)	3 (1%)	9	5
1	D	235/238 (99%)	225 (96%)	8 (3%)	2 (1%)	14	9
1	E	235/238 (99%)	219 (93%)	14 (6%)	2 (1%)	14	9
1	F	235/238 (99%)	222 (94%)	11 (5%)	2 (1%)	14	9
All	All	1410/1428 (99%)	1334 (95%)	62 (4%)	14 (1%)	12	8

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	HIS

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Mol	Chain	Res	Type
1	B	42	VAL
1	C	209	HIS
1	F	209	HIS
1	A	207	ARG
1	B	209	HIS
1	D	42	VAL
1	D	207	ARG
1	E	214	ALA
1	C	207	ARG
1	F	207	ARG
1	A	41	ASN
1	C	42	VAL
1	E	41	ASN

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	187/189 (99%)	178 (95%)	9 (5%)	23	21
1	B	187/189 (99%)	172 (92%)	15 (8%)	11	8
1	C	187/189 (99%)	177 (95%)	10 (5%)	20	18
1	D	187/189 (99%)	180 (96%)	7 (4%)	30	30
1	E	187/189 (99%)	175 (94%)	12 (6%)	16	12
1	F	187/189 (99%)	174 (93%)	13 (7%)	14	10
All	All	1122/1134 (99%)	1056 (94%)	66 (6%)	18	14

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	MET
1	A	40	ASN
1	A	41	ASN
1	A	116	ASN
1	A	158	LEU

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Mol	Chain	Res	Type
1	A	178	VAL
1	A	179	GLU
1	A	181	GLU
1	A	218	GLN
1	B	40	ASN
1	B	41	ASN
1	B	64	MET
1	B	88	VAL
1	B	116	ASN
1	B	120	PHE
1	B	142	LYS
1	B	158	LEU
1	B	176	LEU
1	B	178	VAL
1	B	179	GLU
1	B	181	GLU
1	B	205	HIS
1	B	210	GLU
1	B	211	GLN
1	C	40	ASN
1	C	41	ASN
1	C	116	ASN
1	C	142	LYS
1	C	147	ASP
1	C	157	ASP
1	C	158	LEU
1	C	179	GLU
1	C	181	GLU
1	C	222	ASN
1	D	41	ASN
1	D	57	ILE
1	D	95	LEU
1	D	112	ASP
1	D	116	ASN
1	D	158	LEU
1	D	181	GLU
1	E	41	ASN
1	E	95	LEU
1	E	112	ASP
1	E	116	ASN
1	E	122	ASP
1	E	157	ASP

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Mol	Chain	Res	Type
1	E	158	LEU
1	E	165	GLU
1	E	178	VAL
1	E	179	GLU
1	E	212	THR
1	E	218	GLN
1	F	34	GLU
1	F	41	ASN
1	F	74	LYS
1	F	83	LYS
1	F	116	ASN
1	F	120	PHE
1	F	147	ASP
1	F	157	ASP
1	F	172	LYS
1	F	175	ILE
1	F	179	GLU
1	F	181	GLU
1	F	207	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN
1	A	41	ASN
1	A	116	ASN
1	A	211	GLN
1	B	4	HIS
1	B	41	ASN
1	B	116	ASN
1	B	218	GLN
1	B	222	ASN
1	C	40	ASN
1	C	41	ASN
1	C	116	ASN
1	C	218	GLN
1	C	222	ASN
1	D	40	ASN
1	D	41	ASN
1	D	116	ASN
1	D	211	GLN
1	D	218	GLN

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Mol	Chain	Res	Type
1	E	40	ASN
1	E	41	ASN
1	E	116	ASN
1	E	218	GLN
1	F	40	ASN
1	F	41	ASN
1	F	116	ASN
1	F	218	GLN
1	F	222	ASN

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.