



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:23 AM UTC

PDB ID : 6F5I / pdb_00006f5i
Title : Crystal structure of H. pylori purine nucleoside phosphorylase
Authors : Stefanic, Z.
Deposited on : 2017-12-01
Resolution : 2.30 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

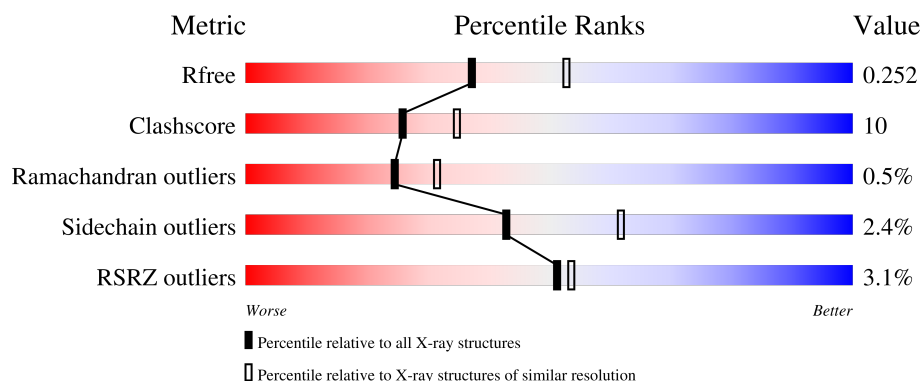
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	233	3% 80% 17% ..
1	B	233	11% 73% 21% ..
1	C	233	4% 85% 15% .
1	D	233	85% 14% .
1	E	233	90% 10%

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Mol	Chain	Length	Quality of chain
1	F	233	 82%18%

2 Entry composition [i](#)

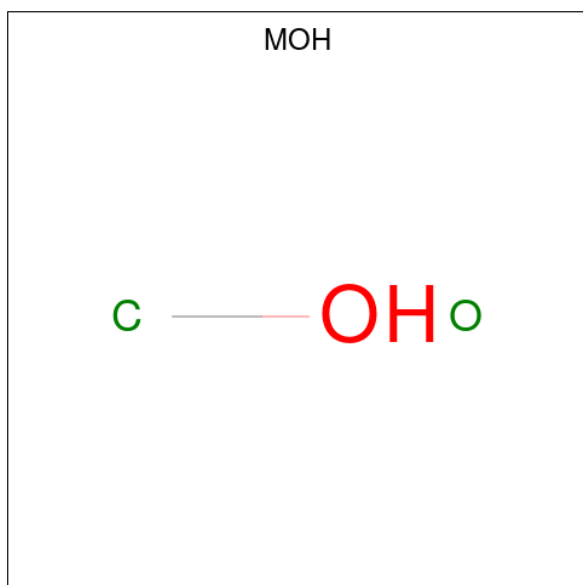
There are 3 unique types of molecules in this entry. The entry contains 11367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DeoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	B	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	C	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	D	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	E	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			
1	F	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			

- Molecule 2 is METHANOL (CCD ID: MOH) (formula: CH₄O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 2 1 1	0	0
2	A	1	Total C O 2 1 1	0	0
2	B	1	Total C O 2 1 1	0	0
2	E	1	Total C O 2 1 1	0	0

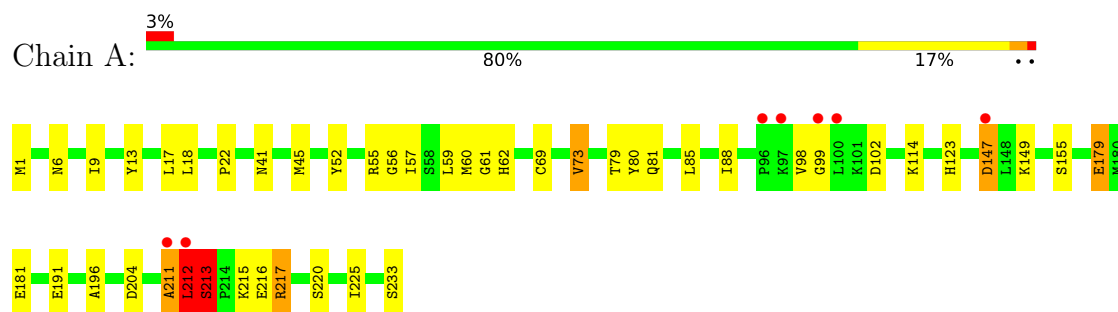
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	74	Total O 74 74	0	0
3	B	96	Total O 96 96	0	0
3	C	93	Total O 93 93	0	0
3	D	88	Total O 88 88	0	0
3	E	105	Total O 105 105	0	0
3	F	91	Total O 91 91	0	0

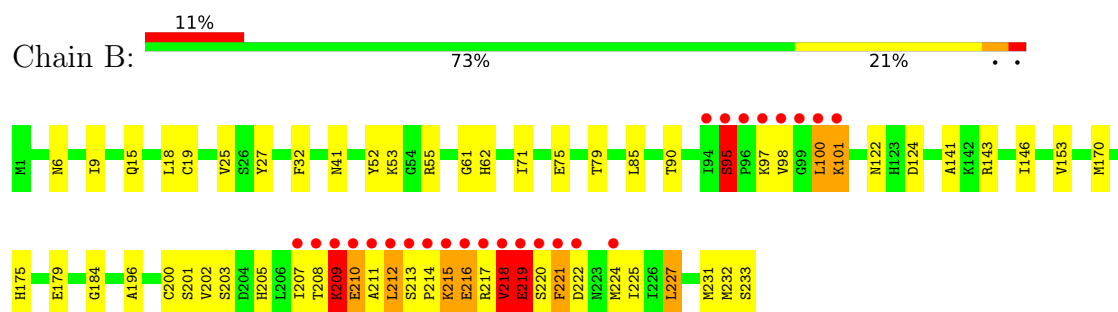
3 Residue-property plots

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.

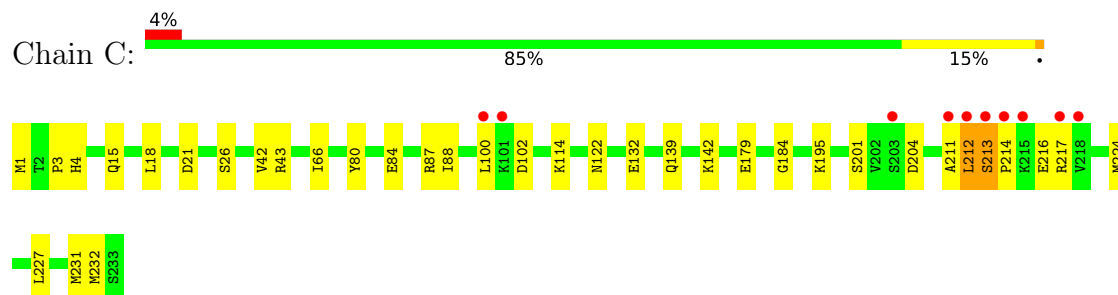
- Molecule 1: Purine nucleoside phosphorylase DeoD-type



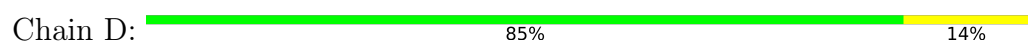
- Molecule 1: Purine nucleoside phosphorylase DeoD-type

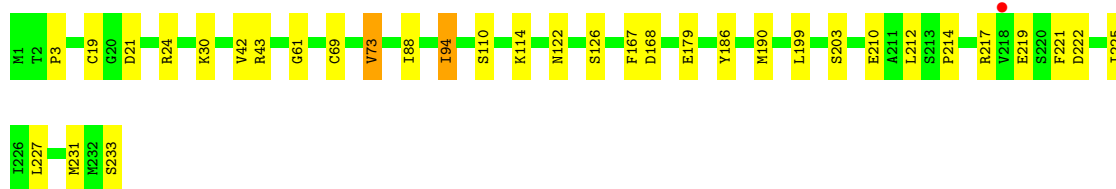


- Molecule 1: Purine nucleoside phosphorylase DeoD-type



- Molecule 1: Purine nucleoside phosphorylase DeoD-type





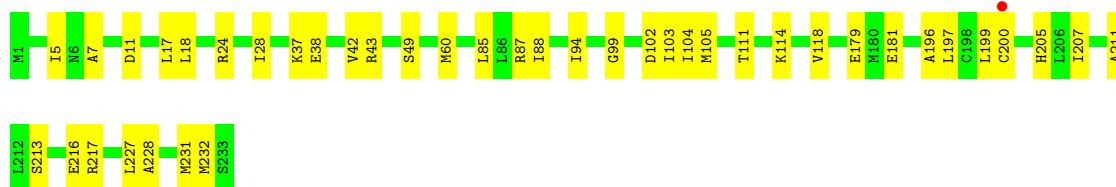
- Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain E: 90% 10%



- Molecule 1: Purine nucleoside phosphorylase DeoD-type

Chain F: 82% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.33Å 59.61Å 136.44Å 90.00° 102.15° 90.00°	Depositor
Resolution (Å)	44.44 – 2.30 44.44 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (44.44-2.30) 99.5 (44.44-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.252 0.194 , 0.252	Depositor DCC
R_{free} test set	2998 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11367	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: MOH

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	1/1833 (0.1%)	0.72	4/2467 (0.2%)
1	B	0.55	0/1833	0.88	9/2467 (0.4%)
1	C	0.35	0/1833	0.56	0/2467
1	D	0.34	0/1833	0.56	0/2467
1	E	0.37	0/1833	0.58	0/2467
1	F	0.33	0/1833	0.53	0/2467
All	All	0.40	1/10998 (0.0%)	0.65	13/14802 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	SER	C-N	5.67	1.41	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	209	LYS	N-CA-C	9.67	131.40	110.80
1	B	219	GLU	O-C-N	-7.90	113.74	122.12
1	B	219	GLU	CA-C-N	7.52	135.24	121.70
1	B	219	GLU	C-N-CA	7.52	135.24	121.70
1	B	98	VAL	N-CA-C	7.10	118.51	108.36
1	A	212	LEU	N-CA-C	-6.88	91.75	111.00
1	A	213	SER	CA-C-N	-6.80	112.17	119.24
1	A	213	SER	C-N-CA	-6.80	112.17	119.24
1	A	211	ALA	N-CA-C	-6.10	99.25	108.52
1	B	95	SER	N-CA-C	6.05	118.03	108.23
1	B	218	VAL	N-CA-C	5.85	121.51	109.34
1	B	95	SER	O-C-N	5.58	125.76	121.85
1	B	211	ALA	N-CA-C	5.00	117.54	108.69

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	1802	0	1838	61	2
1	B	1802	0	1838	60	0
1	C	1802	0	1838	27	0
1	D	1802	0	1838	21	2
1	E	1802	0	1838	16	0
1	F	1802	0	1836	30	0
2	A	4	0	0	0	0
2	B	2	0	0	0	0
2	E	2	0	0	0	0
3	A	74	0	0	2	0
3	B	96	0	0	7	0
3	C	93	0	0	3	0
3	D	88	0	0	3	0
3	E	105	0	0	3	0
3	F	91	0	0	4	0
All	All	11367	0	11026	208	2

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 10.

All (208) 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:100:LEU:HD21	1:B:203:SER:O	1.24	1.29
1:B:100:LEU:CD2	1:B:203:SER:O	1.99	1.11
1:B:215:LYS:H	1:B:215:LYS:HD2	1.19	1.05
1:B:218:VAL:N	1:B:220:SER:O	1.92	1.00
1:B:100:LEU:CD2	1:B:203:SER:C	2.35	1.00
1:A:212:LEU:HG	1:A:213:SER:H	1.27	0.99
1:B:212:LEU:HD13	1:B:216:GLU:HG3	1.47	0.93
1:B:216:GLU:C	1:B:217:ARG:HD2	1.94	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:SER:OG	1:B:216:GLU:HG2	1.69	0.92
1:A:212:LEU:HD21	1:A:217:ARG:CZ	2.00	0.91
1:B:100:LEU:HD21	1:B:203:SER:C	1.94	0.91
1:A:45:MET:HE2	1:A:61:GLY:HA3	1.52	0.90
1:A:212:LEU:HD21	1:A:217:ARG:NH1	1.88	0.89
1:A:211:ALA:HB1	1:A:212:LEU:HB3	1.53	0.88
1:B:95:SER:O	1:B:205:HIS:NE2	2.08	0.87
1:B:219:GLU:N	1:B:220:SER:HB3	1.91	0.85
1:C:132:GLU:OE1	1:C:195:LYS:NZ	2.09	0.85
1:B:220:SER:N	1:B:221:PHE:HA	1.92	0.85
1:B:100:LEU:O	1:B:202:VAL:O	1.96	0.83
1:B:215:LYS:HD2	1:B:215:LYS:N	1.94	0.82
1:C:139:GLN:OE1	3:C:301:HOH:O	1.96	0.82
1:A:212:LEU:HD21	1:A:217:ARG:NH2	1.97	0.78
1:B:216:GLU:O	1:B:217:ARG:HD2	1.83	0.77
1:C:211:ALA:O	1:C:217:ARG:NH2	2.17	0.77
1:A:212:LEU:HD11	1:A:217:ARG:CZ	2.15	0.76
1:B:27:TYR:OH	1:B:218:VAL:HG13	1.86	0.75
1:A:80:TYR:O	1:A:81:GLN:HG2	1.86	0.75
1:B:210:GLU:H	1:B:210:GLU:CD	1.96	0.73
1:A:212:LEU:CG	1:A:213:SER:H	2.00	0.73
1:E:83:LYS:NZ	3:E:403:HOH:O	2.21	0.72
1:B:220:SER:H	1:B:221:PHE:HA	1.56	0.71
1:A:147:ASP:O	3:A:402:HOH:O	2.09	0.71
1:A:212:LEU:HD11	1:A:217:ARG:NE	2.06	0.70
1:D:222:ASP:HA	1:D:225:ILE:HD12	1.73	0.70
1:A:98:VAL:HG13	1:A:149:LYS:HZ1	1.56	0.69
1:D:21:ASP:HB3	1:D:24:ARG:HG3	1.74	0.69
1:B:15:GLN:OE1	3:B:401:HOH:O	2.10	0.68
1:B:208:THR:O	1:B:209:LYS:HB2	1.93	0.68
1:B:219:GLU:H	1:B:220:SER:HB3	1.56	0.68
1:E:147:ASP:O	3:E:402:HOH:O	2.12	0.68
1:A:213:SER:OG	1:A:215:LYS:HD3	1.95	0.66
1:A:211:ALA:HA	1:A:212:LEU:HB2	1.77	0.66
1:C:214:PRO:HA	1:C:217:ARG:HD2	1.78	0.66
1:B:222:ASP:HA	1:B:225:ILE:HD12	1.78	0.65
1:A:211:ALA:HB1	1:A:212:LEU:CB	2.25	0.65
1:A:212:LEU:HG	1:A:213:SER:N	2.08	0.65
1:A:213:SER:HB3	1:A:216:GLU:HB2	1.79	0.64
1:C:15:GLN:HB3	1:C:232:MET:HE3	1.80	0.64
1:F:38:GLU:OE1	3:F:303:HOH:O	2.15	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:HB3	1:A:45:MET:HE3	1.81	0.63
1:A:18:LEU:HB3	1:A:62:HIS:HD2	1.64	0.62
1:B:55:ARG:HE	1:B:233:SER:HA	1.64	0.62
1:F:87:ARG:NH2	3:F:308:HOH:O	2.32	0.62
1:C:122:ASN:ND2	3:C:302:HOH:O	2.16	0.62
1:A:204:ASP:OD2	1:A:212:LEU:HD22	2.00	0.61
1:B:217:ARG:HD2	1:B:217:ARG:N	2.12	0.61
1:B:231:MET:HE2	1:B:232:MET:HE3	1.83	0.60
1:E:57:ILE:HD12	1:E:232:MET:HE2	1.84	0.60
1:F:17:LEU:HD11	1:F:228:ALA:HB1	1.84	0.60
1:D:69:CYS:O	1:D:73:VAL:HG13	2.02	0.59
1:F:87:ARG:NH2	1:F:181:GLU:OE1	2.35	0.59
1:C:100:LEU:HD12	1:C:100:LEU:H	1.66	0.59
1:A:212:LEU:HD21	1:A:217:ARG:HH12	1.63	0.58
1:B:200:CYS:SG	3:B:468:HOH:O	2.50	0.57
1:D:42:VAL:HG12	1:D:43:ARG:HG3	1.87	0.57
1:A:1:MET:HE3	1:A:9:ILE:HG23	1.86	0.56
1:D:94:ILE:HD11	1:D:167:PHE:CD2	2.40	0.56
1:A:211:ALA:CA	1:A:212:LEU:CB	2.84	0.56
1:B:218:VAL:HG12	1:B:219:GLU:N	2.21	0.55
1:B:19:CYS:HB2	1:B:25:VAL:HG23	1.87	0.55
1:E:138:TYR:O	1:E:142:LYS:HE2	2.07	0.55
1:C:184:GLY:HA2	3:C:344:HOH:O	2.06	0.55
1:F:37:LYS:HD2	1:F:38:GLU:H	1.72	0.55
1:A:13:TYR:CD1	1:A:56:GLY:HA3	2.42	0.54
1:B:184:GLY:HA2	3:B:455:HOH:O	2.06	0.54
1:B:213:SER:HG	1:B:216:GLU:HG2	1.70	0.54
1:F:17:LEU:HD13	1:F:232:MET:SD	2.48	0.54
1:D:227:LEU:O	1:D:231:MET:HG2	2.08	0.54
1:D:210:GLU:OE1	3:D:301:HOH:O	2.17	0.54
1:A:6:ASN:ND2	1:A:41:ASN:OD1	2.39	0.53
1:B:71:ILE:O	1:B:75:GLU:HG3	2.07	0.53
1:A:45:MET:HE2	1:A:61:GLY:CA	2.31	0.53
1:A:213:SER:O	1:A:217:ARG:HG3	2.09	0.52
1:C:227:LEU:O	1:C:231:MET:HG2	2.10	0.52
1:A:212:LEU:HD21	1:A:217:ARG:HH22	1.73	0.52
1:A:211:ALA:CB	1:A:212:LEU:HB3	2.32	0.51
1:A:55:ARG:HD3	1:A:233:SER:HA	1.92	0.51
1:A:212:LEU:CG	1:A:213:SER:N	2.72	0.51
1:B:52:TYR:CE1	1:B:53:LYS:HE3	2.46	0.51
1:A:62:HIS:CE1	1:A:181:GLU:HG2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:SER:O	1:B:220:SER:OG	2.29	0.51
1:F:42:VAL:HG12	1:F:43:ARG:HG3	1.93	0.51
1:F:88:ILE:HG22	1:F:199:LEU:HB2	1.93	0.50
1:B:122:ASN:OD1	3:B:402:HOH:O	2.20	0.50
1:C:211:ALA:O	1:C:212:LEU:HD23	2.11	0.50
1:A:88:ILE:HD12	1:A:225:ILE:HD12	1.91	0.50
1:C:100:LEU:HD12	1:C:100:LEU:N	2.26	0.50
1:C:114:LYS:HB2	1:F:114:LYS:HB2	1.92	0.50
1:F:114:LYS:O	1:F:118:VAL:HG23	2.11	0.50
1:C:100:LEU:C	1:C:102:ASP:H	2.20	0.50
1:A:217:ARG:HH12	1:D:3:PRO:HB3	1.76	0.50
1:D:203:SER:HA	1:D:212:LEU:HD12	1.93	0.49
1:B:95:SER:C	1:B:205:HIS:CE1	2.89	0.49
1:C:66:ILE:HG23	1:C:184:GLY:HA3	1.93	0.49
1:E:17:LEU:HD12	1:E:86:LEU:O	2.11	0.49
1:A:45:MET:HE3	1:A:45:MET:HA	1.94	0.49
1:A:80:TYR:C	1:A:81:GLN:HG2	2.36	0.49
1:E:132:GLU:OE1	1:E:136:ARG:HG3	2.13	0.49
1:B:124:ASP:O	1:D:110:SER:HB3	2.13	0.49
1:B:100:LEU:HD22	1:B:203:SER:C	2.30	0.49
1:A:18:LEU:HD23	1:A:60:MET:HB3	1.95	0.49
1:A:212:LEU:CD2	1:A:217:ARG:NH2	2.73	0.49
1:B:6:ASN:ND2	1:B:41:ASN:OD1	2.45	0.48
1:A:114:LYS:HB2	1:D:114:LYS:HB2	1.95	0.48
1:D:168:ASP:HB2	3:D:315:HOH:O	2.14	0.48
1:B:219:GLU:CA	1:B:220:SER:HB3	2.43	0.48
1:C:142:LYS:HD3	1:C:142:LYS:C	2.39	0.48
1:B:214:PRO:HB2	1:B:215:LYS:HE2	1.94	0.48
1:A:217:ARG:HH22	1:D:3:PRO:HB3	1.79	0.48
1:A:211:ALA:CB	1:A:212:LEU:CB	2.93	0.47
1:B:227:LEU:O	1:B:231:MET:HG2	2.15	0.47
1:D:19:CYS:O	1:D:61:GLY:HA2	2.15	0.47
1:E:42:VAL:HG12	1:E:43:ARG:HG3	1.96	0.47
1:F:205:HIS:CE1	1:F:207:ILE:HB	2.50	0.47
1:B:9:ILE:HD11	1:B:79:THR:O	2.16	0.46
1:F:17:LEU:HD12	1:F:17:LEU:HA	1.80	0.46
1:A:123:HIS:HB3	1:F:111:THR:O	2.16	0.46
1:A:212:LEU:CD2	1:A:217:ARG:CZ	2.85	0.46
1:A:69:CYS:O	1:A:73:VAL:HG13	2.16	0.46
1:A:212:LEU:HD11	1:A:217:ARG:HG2	1.98	0.46
1:B:32:PHE:HZ	1:B:222:ASP:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:VAL:HG12	1:C:43:ARG:HG3	1.98	0.46
1:B:100:LEU:O	1:B:202:VAL:C	2.59	0.45
1:E:138:TYR:CE2	1:E:142:LYS:HE3	2.51	0.45
1:A:211:ALA:CA	1:A:212:LEU:HB2	2.41	0.45
1:C:100:LEU:HD22	1:C:212:LEU:HB3	1.99	0.45
1:E:33:LEU:HD22	1:E:50:GLY:HA3	1.99	0.45
1:F:103:ILE:HA	1:F:200:CYS:O	2.17	0.45
1:A:17:LEU:HB2	1:A:59:LEU:HD23	1.98	0.45
1:A:22:PRO:HD3	1:A:45:MET:HE1	1.99	0.45
1:B:32:PHE:CZ	1:B:222:ASP:HB2	2.52	0.45
1:D:186:TYR:O	1:D:190:MET:HG3	2.16	0.45
1:B:90:THR:CG2	1:B:221:PHE:HZ	2.30	0.45
1:C:204:ASP:N	1:C:204:ASP:OD1	2.49	0.45
1:C:213:SER:OG	1:C:216:GLU:OE2	2.35	0.45
1:F:213:SER:O	1:F:217:ARG:HG3	2.16	0.45
1:D:233:SER:O	1:D:233:SER:OG	2.33	0.44
1:B:218:VAL:C	1:B:220:SER:C	2.85	0.44
1:C:212:LEU:CD2	1:C:217:ARG:HE	2.30	0.44
1:B:219:GLU:C	1:B:222:ASP:H	2.26	0.44
1:A:1:MET:HB3	1:A:80:TYR:OH	2.18	0.44
1:B:207:ILE:HD12	1:B:207:ILE:N	2.33	0.44
1:C:84:GLU:HG2	1:C:195:LYS:HE3	1.99	0.44
1:E:43:ARG:HD3	3:E:426:HOH:O	2.18	0.44
1:A:85:LEU:O	1:A:196:ALA:HA	2.17	0.44
1:F:105:MET:HG3	1:F:197:LEU:HD11	2.00	0.44
1:B:170:MET:O	1:B:175:HIS:HB2	2.18	0.44
1:A:216:GLU:O	1:A:220:SER:HB3	2.17	0.44
1:F:18:LEU:HD23	1:F:60:MET:HB3	1.99	0.43
1:F:104:ILE:HB	1:F:200:CYS:HB3	1.99	0.43
1:F:43:ARG:HD3	3:F:320:HOH:O	2.18	0.43
1:B:85:LEU:O	1:B:196:ALA:HA	2.18	0.43
1:D:221:PHE:HD1	1:D:225:ILE:HD11	1.83	0.43
1:C:18:LEU:HB2	1:C:87:ARG:HA	2.01	0.43
1:E:29:ALA:HA	1:E:33:LEU:HB2	1.99	0.43
1:A:62:HIS:HE1	1:A:181:GLU:HG2	1.84	0.43
1:B:18:LEU:HB3	1:B:62:HIS:HD2	1.83	0.42
1:B:214:PRO:HA	1:B:217:ARG:NH2	2.34	0.42
1:B:219:GLU:N	1:B:220:SER:CB	2.71	0.42
1:D:88:ILE:HA	1:D:199:LEU:O	2.19	0.42
1:E:26:SER:O	1:E:30:LYS:HG2	2.19	0.42
1:E:85:LEU:O	1:E:196:ALA:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LYS:N	1:E:142:LYS:HD3	2.34	0.42
1:F:85:LEU:O	1:F:196:ALA:HA	2.20	0.42
1:A:99:GLY:N	1:A:102:ASP:OD2	2.51	0.42
1:A:52:TYR:HB3	1:A:57:ILE:HD12	2.01	0.42
1:A:213:SER:HB3	1:A:216:GLU:CB	2.49	0.42
1:B:95:SER:O	1:B:205:HIS:CE1	2.70	0.42
1:B:101:LYS:O	3:B:403:HOH:O	2.21	0.42
1:F:94:ILE:HA	1:F:207:ILE:HG12	2.02	0.42
1:F:5:ILE:HG22	1:F:7:ALA:H	1.85	0.42
1:C:100:LEU:HD23	1:C:212:LEU:HD22	2.02	0.41
1:D:214:PRO:HA	1:D:217:ARG:HD2	2.01	0.41
1:B:19:CYS:O	1:B:61:GLY:HA2	2.20	0.41
1:C:21:ASP:OD1	1:F:43:ARG:HA	2.20	0.41
1:E:62:HIS:CE1	1:E:181:GLU:HG2	2.55	0.41
1:E:106:ALA:HA	1:E:151:GLY:O	2.20	0.41
1:A:212:LEU:O	1:A:213:SER:CB	2.69	0.41
1:F:211:ALA:HB1	3:F:316:HOH:O	2.20	0.41
1:C:1:MET:HG2	1:C:80:TYR:OH	2.20	0.41
1:C:88:ILE:HB	1:C:224:MET:HE3	2.01	0.41
1:D:122:ASN:ND2	3:D:302:HOH:O	2.18	0.41
1:F:24:ARG:O	1:F:28:ILE:HG13	2.20	0.41
1:A:212:LEU:CD2	1:A:217:ARG:NH1	2.73	0.41
1:B:100:LEU:HD22	1:B:203:SER:O	2.07	0.41
1:F:205:HIS:HE1	1:F:207:ILE:HB	1.85	0.41
1:F:227:LEU:O	1:F:231:MET:HG2	2.21	0.41
1:A:212:LEU:CD1	1:A:217:ARG:HG2	2.52	0.41
3:B:407:HOH:O	1:D:126:SER:HB2	2.20	0.41
1:F:213:SER:OG	1:F:216:GLU:HG3	2.20	0.40
1:A:191:GLU:OE2	3:A:403:HOH:O	2.22	0.40
1:B:141:ALA:HB1	1:B:146:ILE:O	2.21	0.40
1:F:11:ASP:O	1:F:49:SER:OG	2.32	0.40
1:A:13:TYR:CE1	1:A:56:GLY:HA3	2.56	0.40
1:C:3:PRO:HB2	1:C:4:HIS:CE1	2.56	0.40
1:A:155:SER:HA	1:A:179:GLU:O	2.22	0.40
1:B:143:ARG:NH2	3:B:405:HOH:O	2.32	0.40
1:F:99:GLY:O	1:F:102:ASP:HB2	2.21	0.40

All (2) 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:A:81:GLN:OE1	1:D:30:LYS:NZ[2_444]	2.02	0.18
1:A:79:THR:O	1:D:30:LYS:NZ[2_444]	2.12	0.08

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	231/233 (99%)	218 (94%)	10 (4%)	3 (1%)	9	10
1	B	231/233 (99%)	219 (95%)	10 (4%)	2 (1%)	14	17
1	C	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	30	38
1	D	231/233 (99%)	217 (94%)	13 (6%)	1 (0%)	30	38
1	E	231/233 (99%)	223 (96%)	8 (4%)	0	100	100
1	F	231/233 (99%)	223 (96%)	8 (4%)	0	100	100
All	All	1386/1398 (99%)	1317 (95%)	62 (4%)	7 (0%)	24	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	212	LEU
1	A	213	SER
1	C	212	LEU
1	D	219	GLU
1	B	209	LYS
1	A	147	ASP
1	B	218	VAL

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	196/196 (100%)	193 (98%)	3 (2%)	57	75
1	B	196/196 (100%)	180 (92%)	16 (8%)	10	14
1	C	196/196 (100%)	192 (98%)	4 (2%)	48	67
1	D	196/196 (100%)	193 (98%)	3 (2%)	57	75
1	E	196/196 (100%)	195 (100%)	1 (0%)	81	90
1	F	196/196 (100%)	195 (100%)	1 (0%)	81	90
All	All	1176/1176 (100%)	1148 (98%)	28 (2%)	43	62

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	VAL
1	A	179	GLU
1	A	217	ARG
1	B	95	SER
1	B	97	LYS
1	B	100	LEU
1	B	101	LYS
1	B	153	VAL
1	B	179	GLU
1	B	201	SER
1	B	209	LYS
1	B	210	GLU
1	B	212	LEU
1	B	215	LYS
1	B	216	GLU
1	B	219	GLU
1	B	221	PHE
1	B	224	MET
1	B	227	LEU
1	C	26	SER
1	C	179	GLU
1	C	201	SER
1	C	213	SER
1	D	73	VAL
1	D	94	ILE
1	D	179	GLU
1	E	73	VAL

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Mol	Chain	Res	Type
1	F	179	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	HIS
1	B	122	ASN
1	C	165	HIS
1	C	223	ASN
1	E	81	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 oligosaccharides 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	MOH	B	301	-	1,1,1	0.15	0	-		
2	MOH	E	301	-	1,1,1	0.11	0	-		
2	MOH	A	301	-	1,1,1	0.02	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MOH	A	302	-	1,1,1	0.02	0	-		

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	233/233 (100%)	-0.01	7 (3%) 52 54	14, 24, 41, 58	0
1	B	233/233 (100%)	0.15	25 (10%) 11 12	11, 19, 59, 103	0
1	C	233/233 (100%)	-0.04	10 (4%) 40 41	12, 21, 46, 79	0
1	D	233/233 (100%)	-0.06	1 (0%) 88 89	11, 24, 41, 53	0
1	E	233/233 (100%)	-0.38	0 100 100	9, 16, 29, 37	0
1	F	233/233 (100%)	-0.07	1 (0%) 88 89	12, 25, 41, 53	0
All	All	1398/1398 (100%)	-0.07	44 (3%) 51 53	9, 21, 43, 103	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	218	VAL	6.0
1	B	217	ARG	5.4
1	B	224	MET	4.9
1	C	212	LEU	4.8
1	B	212	LEU	4.7
1	B	211	ALA	4.6
1	B	208	THR	4.4
1	B	214	PRO	4.1
1	B	220	SER	4.1
1	B	96	PRO	4.0
1	B	215	LYS	3.9
1	A	211	ALA	3.7
1	B	95	SER	3.6
1	B	213	SER	3.6
1	B	98	VAL	3.6
1	F	200	CYS	3.5
1	A	96	PRO	3.5
1	B	101	LYS	3.5
1	B	94	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	211	ALA	3.3
1	C	214	PRO	3.3
1	B	100	LEU	3.2
1	C	100	LEU	3.1
1	C	215	LYS	3.1
1	A	99	GLY	3.1
1	B	219	GLU	3.1
1	B	221	PHE	3.0
1	C	217	ARG	2.9
1	B	210	GLU	2.9
1	B	222	ASP	2.8
1	C	213	SER	2.8
1	C	101	LYS	2.8
1	D	218	VAL	2.7
1	B	209	LYS	2.7
1	B	99	GLY	2.6
1	B	207	ILE	2.3
1	C	218	VAL	2.3
1	A	100	LEU	2.3
1	A	147	ASP	2.2
1	C	203	SER	2.2
1	B	216	GLU	2.1
1	B	97	LYS	2.1
1	A	212	LEU	2.0
1	A	97	LYS	2.0

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MOH	E	301	2/2	0.58	0.26	23,23,23,27	0
2	MOH	A	302	2/2	0.76	0.27	28,28,28,34	0
2	MOH	A	301	2/2	0.85	0.24	23,23,23,26	0
2	MOH	B	301	2/2	0.86	0.21	20,20,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.