



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:30 PM UTC

PDB ID : 1T6M / pdb_00001t6m
Title : X-ray Structure of the R70D PI-PLC enzyme: Insight into the role of calcium and surrounding amino acids on active site geometry and catalysis.
Authors : Apiyo, D.; Zhao, L.; Tsai, M.-D.; Selby, T.L.
Deposited on : 2004-05-06
Resolution : 2.11 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)	:	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

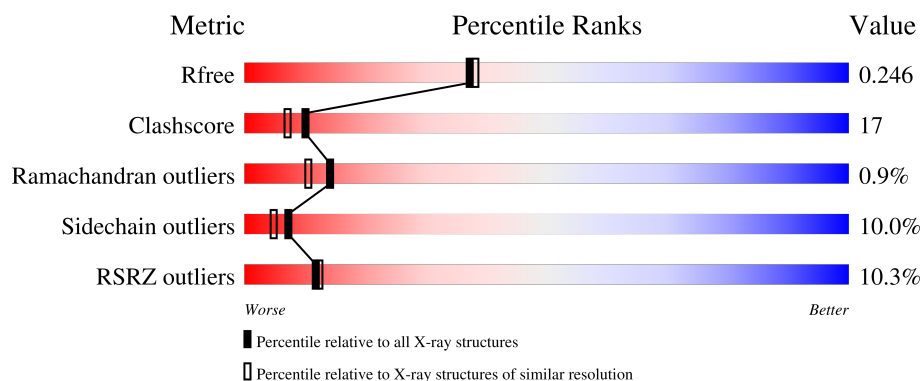
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.11 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	299	11% 68% 22% 7% ..
1	B	299	9% 69% 25% 5% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5066 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 1-phosphatidylinositol phosphodiesterase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2417	1540	399	471	7			
1	B	296	Total	C	N	O	S	0	0	0
			2417	1540	399	471	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP P08954
A	73	ASP	ARG	engineered mutation	UNP P08954
B	4	MET	-	initiating methionine	UNP P08954
B	73	ASP	ARG	engineered mutation	UNP P08954

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		
2	B	2	Total	Ca	0	0
			2	2		

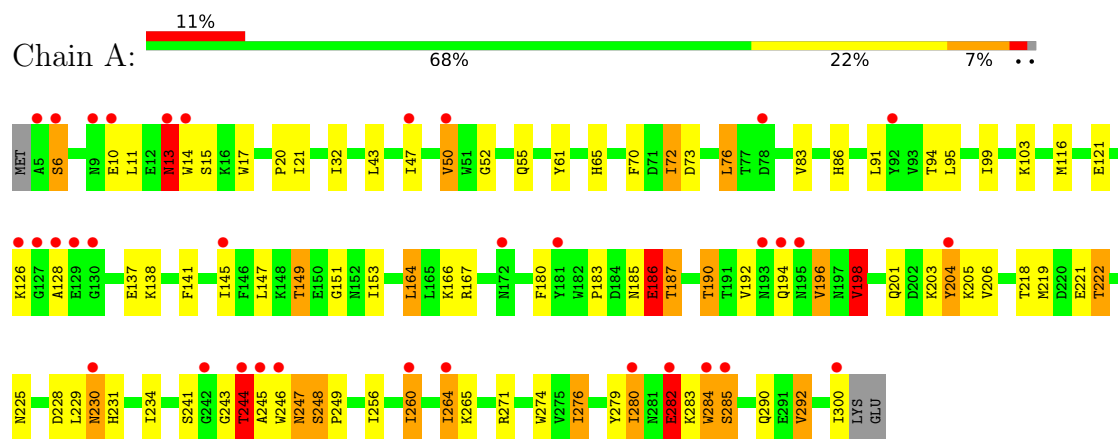
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	113	Total	O	0	0
			113	113		
3	B	115	Total	O	0	0
			115	115		

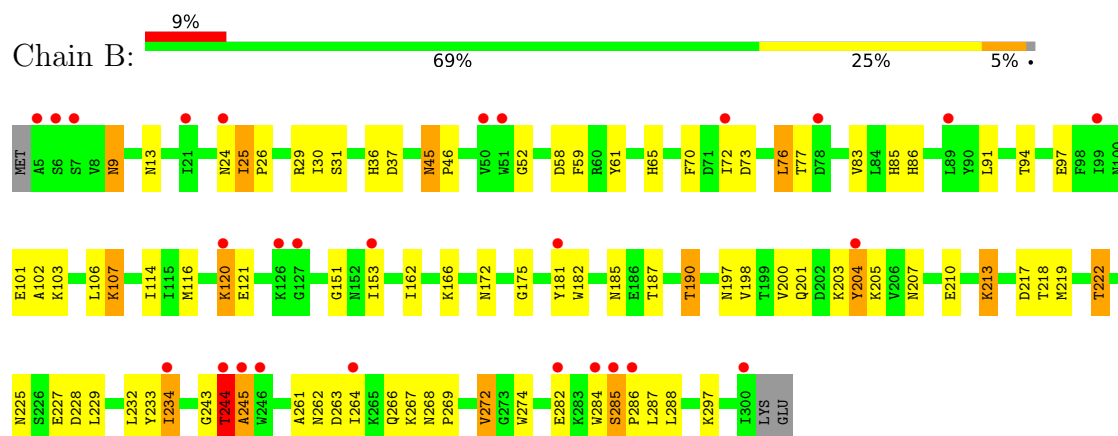
3 Residue-property plots [i](#)

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: 1-phosphatidylinositol phosphodiesterase



- Molecule 1: 1-phosphatidylinositol phosphodiesterase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	91.22Å 147.72Å 96.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.30 – 2.11 43.30 – 2.11	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.30-2.11) 99.9 (43.30-2.11)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.36 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.1.9999, XTALVIEW	Depositor
R, R_{free}	0.223 , 0.240 (Not available) , 0.246	Depositor DCC
R_{free} test set	1912 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5066	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.09	1/2479 (0.0%)	1.17	20/3365 (0.6%)
1	B	0.90	0/2479	1.09	9/3365 (0.3%)
All	All	1.00	1/4958 (0.0%)	1.13	29/6730 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CB-CG	29.49	2.40	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	285	SER	CA-C-N	-11.76	106.34	119.98
1	B	285	SER	C-N-CA	-11.76	106.34	119.98
1	A	13	ASN	N-CA-C	10.84	124.11	111.11
1	A	282	GLU	CB-CG-CD	-8.27	98.54	112.60
1	B	91	LEU	CA-C-N	-8.27	105.75	121.54
1	B	91	LEU	C-N-CA	-8.27	105.75	121.54
1	A	13	ASN	O-C-N	-7.71	114.07	122.09
1	A	91	LEU	CA-C-N	-7.69	106.85	121.54
1	A	91	LEU	C-N-CA	-7.69	106.85	121.54
1	A	198	VAL	CB-CA-C	-7.18	99.85	110.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	LEU	N-CA-C	-7.12	99.33	110.36
1	A	13	ASN	CA-C-N	6.79	133.93	121.70
1	A	13	ASN	C-N-CA	6.79	133.93	121.70
1	B	190	THR	CA-CB-OG1	6.76	119.73	109.60
1	A	183	PRO	CB-CA-C	-6.51	103.06	111.46
1	A	292	VAL	N-CA-C	6.38	116.55	110.42
1	A	6	SER	N-CA-C	6.27	120.83	112.30
1	A	204	TYR	N-CA-C	-6.22	99.56	109.76
1	A	91	LEU	N-CA-C	-6.19	100.82	110.17
1	A	196	VAL	N-CA-C	6.17	116.72	108.27
1	A	13	ASN	CA-C-O	-6.09	114.38	120.90
1	B	182	TRP	N-CA-C	5.94	122.94	109.81
1	B	204	TYR	N-CA-C	-5.69	102.06	110.48
1	A	282	GLU	N-CA-C	-5.64	104.99	112.94
1	A	186	GLU	O-C-N	-5.62	116.37	123.17
1	A	183	PRO	CA-CB-CG	5.39	114.74	104.50
1	A	190	THR	CB-CA-C	-5.38	100.70	113.02
1	B	190	THR	CB-CA-C	-5.34	100.80	113.02
1	A	279	TYR	N-CA-C	5.15	117.46	111.02

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	GLU	Mainchain
1	A	284	TRP	Peptide
1	A	285	SER	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2417	0	2321	92	2
1	B	2417	0	2321	72	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	113	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	115	0	0	6	0
All	All	5066	0	4642	164	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 17.

All (164) 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:219:MET:SD	1:B:264:ILE:HD11	1.87	1.14
1:B:65:HIS:HE1	1:B:282:GLU:OE1	1.31	1.13
1:B:114:ILE:HB	1:B:162:ILE:HD13	1.32	1.10
1:A:282:GLU:CG	1:A:282:GLU:CB	2.40	0.98
1:B:65:HIS:CE1	1:B:282:GLU:OE1	2.23	0.91
1:A:149:THR:HG23	3:A:513:HOH:O	1.72	0.89
1:A:260:ILE:O	1:A:264:ILE:HD13	1.71	0.89
1:A:256:ILE:O	1:A:260:ILE:HD13	1.74	0.88
1:A:72:ILE:HD13	1:A:116:MET:HG3	1.57	0.86
1:B:25:ILE:HD11	1:B:30:ILE:HG13	1.59	0.84
1:A:192:VAL:CG2	1:A:198:VAL:HG22	2.10	0.80
1:B:114:ILE:HB	1:B:162:ILE:CD1	2.12	0.80
1:A:187:THR:CG2	1:A:203:LYS:HE3	2.13	0.79
1:A:52:GLY:O	1:A:86:HIS:HD2	1.66	0.78
1:B:232:LEU:HG	1:B:234:ILE:HD11	1.66	0.77
1:A:14:TRP:HZ2	1:A:290:GLN:HE21	1.34	0.74
1:B:120:LYS:CG	3:B:536:HOH:O	2.36	0.74
1:A:50:VAL:HG22	1:A:244:THR:OG1	1.87	0.74
1:A:187:THR:HG22	1:A:203:LYS:HE3	1.71	0.73
1:B:73:ASP:HB3	1:B:121:GLU:HB2	1.71	0.72
1:A:14:TRP:CZ2	1:A:290:GLN:HG3	2.25	0.72
1:B:36:HIS:NE2	3:B:509:HOH:O	2.23	0.71
1:A:14:TRP:HZ2	1:A:290:GLN:NE2	1.87	0.71
1:B:153:ILE:H	1:B:153:ILE:HD12	1.55	0.71
1:B:102:ALA:HB1	1:B:162:ILE:HD11	1.73	0.71
1:B:45:ASN:HD22	1:B:46:PRO:HD2	1.56	0.70
1:B:207:ASN:OD1	1:B:210:GLU:HG3	1.90	0.70
1:B:232:LEU:HD11	1:B:274:TRP:CH2	2.27	0.69
1:B:120:LYS:HG3	3:B:536:HOH:O	1.93	0.68
1:B:94:THR:OG1	1:B:97:GLU:HG3	1.94	0.68
1:A:72:ILE:HD13	1:A:116:MET:CG	2.24	0.68
1:B:244:THR:O	1:B:245:ALA:HB2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:O	1:A:14:TRP:CZ3	2.46	0.68
1:A:153:ILE:H	1:A:153:ILE:HD12	1.58	0.68
1:A:14:TRP:CH2	1:A:290:GLN:HG3	2.29	0.67
1:B:25:ILE:HD11	1:B:30:ILE:CG1	2.24	0.67
1:A:234:ILE:HG23	1:A:276:ILE:HD11	1.77	0.67
1:B:213:LYS:NZ	1:B:217:ASP:OD2	2.25	0.67
1:A:218:THR:O	1:A:222:THR:HG23	1.94	0.66
1:A:103:LYS:HE3	1:A:145:ILE:HD13	1.78	0.66
1:A:103:LYS:HE2	1:A:145:ILE:HG21	1.79	0.65
1:A:219:MET:SD	1:A:264:ILE:HD11	2.36	0.65
1:B:72:ILE:HD13	1:B:116:MET:HG3	1.77	0.65
1:A:72:ILE:CD1	1:A:116:MET:HG3	2.26	0.65
1:A:20:PRO:O	1:A:300:ILE:HD12	1.98	0.63
1:A:55:GLN:HE22	1:A:280:ILE:H	1.45	0.63
1:B:232:LEU:HD11	1:B:274:TRP:CZ2	2.32	0.63
1:A:244:THR:HG21	1:A:248:SER:HA	1.81	0.63
1:A:234:ILE:CG2	1:A:276:ILE:HD11	2.30	0.62
1:A:276:ILE:HD12	1:A:276:ILE:N	2.14	0.61
1:A:228:ASP:OD1	1:A:230:ASN:CG	2.43	0.61
1:A:13:ASN:HD22	1:A:13:ASN:C	2.07	0.61
1:B:285:SER:O	1:B:286:PRO:C	2.40	0.61
1:A:21:ILE:HD13	1:A:300:ILE:CD1	2.30	0.61
1:B:234:ILE:N	1:B:234:ILE:HD12	2.16	0.60
1:A:192:VAL:HG23	1:A:198:VAL:HG22	1.82	0.60
1:A:72:ILE:HD12	1:A:72:ILE:N	2.15	0.60
1:A:276:ILE:HD12	1:A:276:ILE:H	1.66	0.60
1:B:29:ARG:NH1	1:B:227:GLU:OE2	2.35	0.60
1:B:59:PHE:HB2	1:B:101:GLU:HG2	1.85	0.59
1:B:103:LYS:O	1:B:107:LYS:HG2	2.02	0.59
1:A:260:ILE:CD1	1:A:260:ILE:N	2.65	0.58
1:A:20:PRO:HB2	1:A:300:ILE:HD12	1.85	0.58
1:B:120:LYS:HG2	3:B:536:HOH:O	2.00	0.58
1:A:187:THR:HG21	3:A:591:HOH:O	2.04	0.57
1:B:185:ASN:OD1	1:B:204:TYR:O	2.22	0.57
1:A:192:VAL:CG2	1:A:198:VAL:CG2	2.79	0.57
1:A:47:ILE:H	1:A:47:ILE:HD12	1.68	0.57
1:B:31:SER:HB3	1:B:272:VAL:HG12	1.85	0.57
1:A:187:THR:HB	1:A:201:GLN:HA	1.85	0.57
1:B:72:ILE:HD13	1:B:116:MET:CG	2.34	0.57
1:A:167:ARG:HH22	1:A:180:PHE:H	1.53	0.56
1:A:185:ASN:OD1	1:A:204:TYR:O	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:HD21	1:B:297:LYS:HE2	1.71	0.56
1:A:20:PRO:C	1:A:300:ILE:HD12	2.31	0.56
1:A:21:ILE:HD13	1:A:300:ILE:HD11	1.88	0.56
1:B:218:THR:O	1:B:222:THR:HG22	2.06	0.56
1:A:244:THR:H	1:A:247:ASN:HD21	1.51	0.56
1:A:164:LEU:HD13	1:A:166:LYS:HG2	1.89	0.55
1:A:61:TYR:O	1:A:65:HIS:HD2	1.90	0.54
1:A:11:LEU:O	1:A:14:TRP:CE3	2.61	0.54
1:A:32:ILE:HD12	1:A:274:TRP:NE1	2.23	0.54
1:B:201:GLN:NE2	1:B:203:LYS:H	2.06	0.54
1:A:151:GLY:O	1:A:153:ILE:HD12	2.07	0.54
1:B:70:PHE:C	1:B:72:ILE:HD12	2.33	0.54
1:B:151:GLY:O	1:B:153:ILE:HD12	2.08	0.54
1:A:138:LYS:HD2	1:A:138:LYS:N	2.23	0.53
1:A:244:THR:CB	1:A:245:ALA:HA	2.38	0.53
1:A:13:ASN:C	1:A:13:ASN:ND2	2.64	0.53
1:B:13:ASN:HD22	1:B:13:ASN:C	2.17	0.53
1:B:70:PHE:O	1:B:72:ILE:HD12	2.09	0.53
1:A:241:SER:HB2	1:A:249:PRO:HD3	1.91	0.52
1:B:204:TYR:O	1:B:205:LYS:HB3	2.10	0.52
1:A:228:ASP:OD1	1:A:230:ASN:OD1	2.27	0.52
1:B:268:ASN:HD21	1:B:297:LYS:CE	2.23	0.52
1:B:25:ILE:HD12	1:B:26:PRO:O	2.10	0.51
1:B:201:GLN:HE21	1:B:203:LYS:H	1.58	0.51
1:B:37:ASP:OD2	1:B:86:HIS:CE1	2.63	0.51
1:B:243:GLY:O	1:B:245:ALA:N	2.44	0.51
1:A:137:GLU:HA	1:A:141:PHE:HB3	1.93	0.50
1:B:72:ILE:CD1	1:B:116:MET:HG3	2.41	0.50
1:A:70:PHE:C	1:A:72:ILE:HD12	2.36	0.50
1:A:245:ALA:O	1:A:246:TRP:HB2	2.11	0.50
1:B:285:SER:O	1:B:287:LEU:N	2.44	0.50
1:A:192:VAL:HG22	1:A:198:VAL:CG2	2.41	0.50
1:B:244:THR:O	1:B:245:ALA:CB	2.60	0.50
1:A:201:GLN:HE21	1:A:203:LYS:H	1.61	0.49
1:B:72:ILE:HD12	1:B:72:ILE:N	2.28	0.49
1:A:17:TRP:O	1:A:20:PRO:HD2	2.12	0.48
1:A:52:GLY:O	1:A:86:HIS:CD2	2.56	0.48
1:A:13:ASN:HD22	1:A:15:SER:H	1.62	0.48
1:A:83:VAL:HG12	1:A:94:THR:HG22	1.95	0.48
1:B:267:LYS:HB3	1:B:269:PRO:HD3	1.95	0.48
1:A:103:LYS:CE	1:A:145:ILE:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:ASP:HB3	1:A:121:GLU:HB2	1.96	0.48
1:A:99:ILE:HG23	1:A:145:ILE:HD11	1.94	0.47
1:A:76:LEU:HD13	1:A:128:ALA:HB1	1.96	0.47
1:A:70:PHE:O	1:A:72:ILE:HD12	2.15	0.47
1:B:198:VAL:CG2	1:B:234:ILE:HD13	2.45	0.47
1:A:201:GLN:NE2	1:A:203:LYS:H	2.14	0.46
1:B:262:ASN:O	1:B:266:GLN:HG2	2.16	0.46
1:A:50:VAL:HG13	1:A:244:THR:OG1	2.16	0.46
1:A:47:ILE:HD12	1:A:47:ILE:N	2.30	0.46
1:B:198:VAL:HG23	1:B:232:LEU:HB3	1.97	0.46
1:B:233:TYR:C	1:B:234:ILE:HD12	2.41	0.46
1:B:9:ASN:HD22	1:B:9:ASN:N	2.14	0.46
1:A:260:ILE:N	1:A:260:ILE:HD12	2.30	0.45
1:B:261:ALA:HB2	1:B:288:LEU:HA	1.98	0.45
1:B:222:THR:HB	1:B:233:TYR:CG	2.51	0.45
1:A:32:ILE:HD12	1:A:274:TRP:CE2	2.51	0.45
1:B:61:TYR:O	1:B:65:HIS:HD2	1.99	0.45
1:A:187:THR:HG23	1:A:203:LYS:HE3	1.95	0.45
1:A:244:THR:HB	1:A:245:ALA:HA	1.97	0.45
1:A:244:THR:HG22	1:A:247:ASN:HD22	1.82	0.44
1:B:70:PHE:CB	1:B:72:ILE:HD11	2.48	0.44
1:A:260:ILE:CD1	1:A:260:ILE:H	2.31	0.44
1:B:52:GLY:O	1:B:86:HIS:HD2	1.99	0.44
1:B:243:GLY:O	1:B:244:THR:C	2.61	0.43
1:A:20:PRO:O	1:A:300:ILE:CD1	2.65	0.43
1:B:103:LYS:O	1:B:107:LYS:HE3	2.19	0.43
1:B:166:LYS:HE3	1:B:175:GLY:O	2.18	0.43
1:B:65:HIS:HE1	1:B:282:GLU:CD	2.17	0.43
1:A:103:LYS:HE2	1:A:145:ILE:CG2	2.48	0.42
1:B:58:ASP:OD2	3:B:520:HOH:O	2.22	0.42
1:B:83:VAL:HG12	1:B:94:THR:HG22	2.00	0.42
1:A:70:PHE:CB	1:A:72:ILE:HD11	2.50	0.42
1:A:76:LEU:HD13	1:A:128:ALA:CB	2.50	0.42
1:A:231:HIS:O	1:A:271:ARG:NH2	2.51	0.42
1:A:243:GLY:O	1:A:244:THR:O	2.37	0.42
1:B:45:ASN:HD22	1:B:46:PRO:CD	2.28	0.42
1:A:264:ILE:N	1:A:264:ILE:CD1	2.83	0.42
1:B:198:VAL:HG23	1:B:234:ILE:HD13	2.02	0.41
1:A:247:ASN:HD22	1:A:247:ASN:C	2.28	0.41
1:B:25:ILE:HA	1:B:26:PRO:HD3	1.97	0.41
1:B:76:LEU:HD22	1:B:77:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:ILE:HD12	1:A:153:ILE:N	2.30	0.41
1:B:217:ASP:HB3	3:B:609:HOH:O	2.20	0.41
1:A:6:SER:N	1:A:10:GLU:OE2	2.53	0.41
1:A:20:PRO:C	1:A:300:ILE:CD1	2.93	0.41
1:A:50:VAL:HG22	1:A:244:THR:HG1	1.86	0.41
1:A:50:VAL:CG2	1:A:244:THR:OG1	2.65	0.41
1:B:187:THR:HA	1:B:200:VAL:O	2.22	0.40
1:B:222:THR:HB	1:B:233:TYR:CD2	2.56	0.40
1:A:70:PHE:HB3	1:A:72:ILE:HD11	2.03	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:186:GLU:OE1	1:B:228:ASP:OD2[6_554]	2.11	0.09
1:A:221:GLU:OE2	1:B:213:LYS:NZ[6_554]	2.11	0.09

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	294/299 (98%)	279 (95%)	13 (4%)	2 (1%)	18	15
1	B	294/299 (98%)	279 (95%)	12 (4%)	3 (1%)	12	9
All	All	588/598 (98%)	558 (95%)	25 (4%)	5 (1%)	14	10

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	THR
1	B	244	THR
1	B	245	ALA

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Mol	Chain	Res	Type
1	A	205	LYS
1	B	181	TYR

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	269/272 (99%)	236 (88%)	33 (12%)	4	2
1	B	269/272 (99%)	248 (92%)	21 (8%)	11	9
All	All	538/544 (99%)	484 (90%)	54 (10%)	7	5

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	43	LEU
1	A	50	VAL
1	A	72	ILE
1	A	76	LEU
1	A	95	LEU
1	A	126	LYS
1	A	147	LEU
1	A	149	THR
1	A	164	LEU
1	A	187	THR
1	A	190	THR
1	A	194	GLN
1	A	196	VAL
1	A	198	VAL
1	A	206	VAL
1	A	222	THR
1	A	225	ASN
1	A	229	LEU
1	A	230	ASN
1	A	244	THR

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	248	SER
1	A	260	ILE
1	A	264	ILE
1	A	265	LYS
1	A	276	ILE
1	A	280	ILE
1	A	282	GLU
1	A	283	LYS
1	A	284	TRP
1	A	285	SER
1	A	292	VAL
1	B	9	ASN
1	B	24	ASN
1	B	25	ILE
1	B	45	ASN
1	B	76	LEU
1	B	85	HIS
1	B	106	LEU
1	B	107	LYS
1	B	120	LYS
1	B	172	ASN
1	B	190	THR
1	B	197	ASN
1	B	213	LYS
1	B	222	THR
1	B	225	ASN
1	B	229	LEU
1	B	234	ILE
1	B	244	THR
1	B	263	ASP
1	B	272	VAL
1	B	284	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	49	GLN
1	A	55	GLN
1	A	62	GLN
1	A	80	ASN

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Mol	Chain	Res	Type
1	A	86	HIS
1	A	139	ASN
1	A	194	GLN
1	A	195	ASN
1	A	197	ASN
1	A	201	GLN
1	A	225	ASN
1	A	230	ASN
1	A	231	HIS
1	A	247	ASN
1	B	9	ASN
1	B	13	ASN
1	B	45	ASN
1	B	65	HIS
1	B	86	HIS
1	B	96	HIS
1	B	109	ASN
1	B	152	ASN
1	B	178	ASN
1	B	201	GLN
1	B	225	ASN
1	B	257	ASN
1	B	268	ASN
1	B	277	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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	296/299 (98%)	0.63	34 (11%) 9 10	10, 21, 44, 61	0
1	B	296/299 (98%)	0.54	27 (9%) 15 15	9, 21, 44, 64	0
All	All	592/598 (98%)	0.58	61 (10%) 12 12	9, 21, 44, 64	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	ALA	5.9
1	B	181	TYR	5.6
1	B	244	THR	5.6
1	A	245	ALA	5.1
1	B	245	ALA	5.0
1	A	14	TRP	4.8
1	A	127	GLY	4.7
1	B	246	TRP	4.3
1	A	300	ILE	4.3
1	B	285	SER	4.3
1	A	244	THR	4.2
1	A	285	SER	4.0
1	A	78	ASP	4.0
1	A	282	GLU	3.9
1	A	284	TRP	3.9
1	B	284	TRP	3.7
1	A	246	TRP	3.6
1	A	194	GLN	3.6
1	B	300	ILE	3.6
1	B	6	SER	3.6
1	A	5	ALA	3.5
1	A	129	GLU	3.4
1	A	230	ASN	3.4
1	A	172	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	126	LYS	3.3
1	A	50	VAL	3.1
1	A	145	ILE	3.0
1	B	51	TRP	3.0
1	A	195	ASN	2.9
1	A	204	TYR	2.9
1	B	153	ILE	2.8
1	A	264	ILE	2.8
1	B	24	ASN	2.7
1	B	89	LEU	2.7
1	A	181	TYR	2.7
1	B	286	PRO	2.7
1	A	47	ILE	2.7
1	B	204	TYR	2.6
1	B	99	ILE	2.6
1	B	120	LYS	2.6
1	A	260	ILE	2.6
1	A	13	ASN	2.5
1	B	72	ILE	2.5
1	A	126	LYS	2.4
1	A	92	TYR	2.3
1	B	127	GLY	2.3
1	A	130	GLY	2.3
1	A	9	ASN	2.3
1	A	242	GLY	2.2
1	B	264	ILE	2.2
1	B	78	ASP	2.2
1	A	128	ALA	2.2
1	A	6	SER	2.1
1	A	193	ASN	2.1
1	A	10	GLU	2.1
1	B	21	ILE	2.1
1	B	7	SER	2.1
1	A	280	ILE	2.1
1	B	234	ILE	2.1
1	B	50	VAL	2.0
1	B	282	GLU	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	CA	B	503	1/1	0.83	0.09	25,25,25,25	0
2	CA	A	502	1/1	0.97	0.08	14,14,14,14	0
2	CA	B	504	1/1	0.98	0.08	25,25,25,25	0
2	CA	A	501	1/1	0.99	0.07	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.