W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:20 pm GMT

PDB ID	:	1OIB
Title	:	PHOSPHATE-BINDING PROTEIN MUTANT T141D
Authors	:	Yao, N.; Choudhary, A.; Ledvina, P.S.; Quiocho, F.A.
Deposited on	:	1995-11-25
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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	Percentile Ranks	Value
Clashscore		16
Ramachandran outliers		1.4%
Sidechain outliers		9.3%
RSRZ outliers		17.8%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
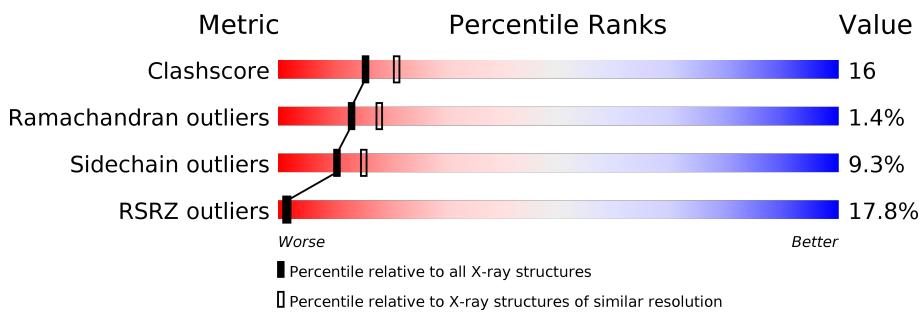
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	321	18% 63% 33% •
1	B	321	17% 64% 31% • •
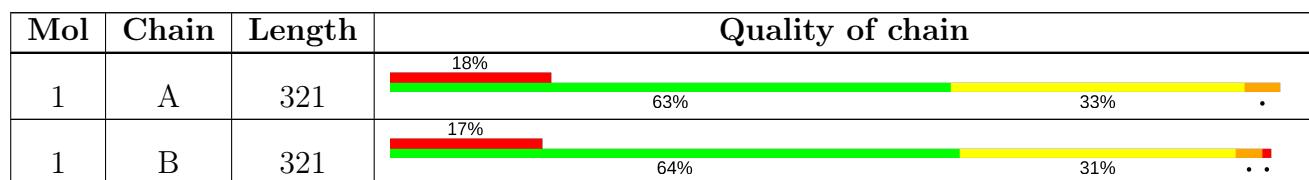
2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4915 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 PHOSPHATE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	0	0	0
			2439	1558	405	476			
1	B	321	Total	C	N	O	0	0	0
			2439	1558	405	476			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ASP	THR	ENGINEERED	UNP P06128
B	141	ASP	THR	ENGINEERED	UNP P06128

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	18	Total	O	0	0
			18	18		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: PHOSPHATE-BINDING PROTEIN
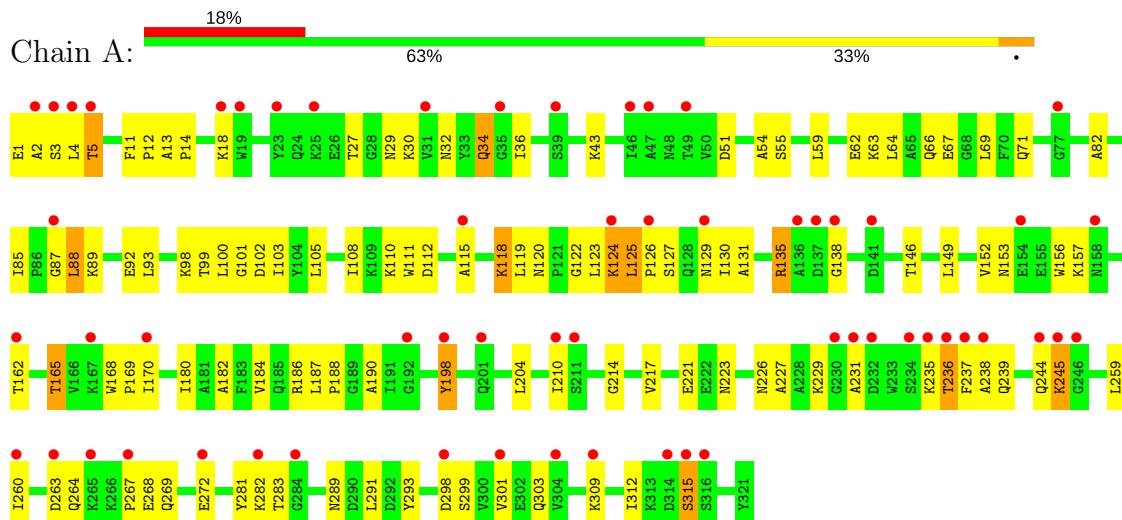
• Molecule 1: PHOSPHATE-BINDING PROTEIN
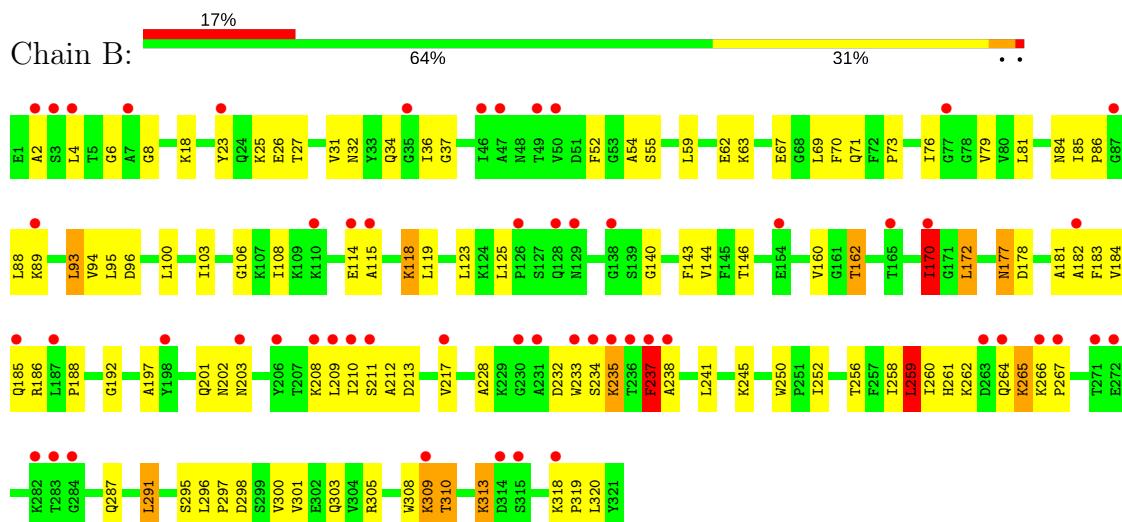
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.22Å　　39.59Å　　113.61Å 90.00°　　92.80°　　90.00°	Depositor
Resolution (Å)	8.00　　–　　2.40 12.01　　–　　1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 67.6 (12.01-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 1.90Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166　　,　　(Not available) 0.299　　,　　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	15.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 100.0	EDS
L-test for twinning[2]	$< |L| > = 0.40, < L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	4915	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.11 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.5446e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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 ⓘ

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	0.62	0/2494	0.84	0/3385
1	B	0.59	0/2494	0.84	6/3385 (0.2%)
All	All	0.60	0/4988	0.84	6/6770 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	259	LEU	CA-CB-CG	7.57	132.70	115.30
1	B	95	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	170	ILE	CB-CA-C	-5.21	101.18	111.60
1	B	232	ASP	N-CA-C	5.21	125.06	111.00
1	B	93	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	237	PHE	N-CA-C	5.17	124.95	111.00

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	2439	0	2414	85	0
1	B	2439	0	2414	75	0
2	A	19	0	0	2	0
2	B	18	0	0	1	0
All	All	4915	0	4828	160	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 16.

All (160) 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:211:SER:HB2	1:B:217:VAL:HG21	1.49	0.93
1:A:82:ALA:HB1	1:A:204:LEU:HD12	1.57	0.86
1:A:236:THR:HG23	1:A:237:PHE:H	1.46	0.81
1:A:120:ASN:HB3	1:A:123:LEU:HD22	1.63	0.79
1:B:182:ALA:HB1	1:B:186:ARG:HH11	1.46	0.79
1:A:198:TYR:HB3	2:A:414:HOH:O	1.83	0.76
1:B:118:LYS:HD2	1:B:119:LEU:HG	1.69	0.74
1:A:245:LYS:HD2	1:A:245:LYS:H	1.54	0.72
1:A:64:LEU:HD11	1:A:71:GLN:HE21	1.55	0.71
1:A:263:ASP:OD1	1:A:315:SER:HA	1.91	0.70
1:B:265:LYS:HD3	1:B:266:LYS:HZ3	1.55	0.70
1:A:182:ALA:O	1:A:186:ARG:HD3	1.91	0.70
1:A:2:ALA:HB1	1:A:272:GLU:HG2	1.73	0.70
1:A:227:ALA:O	1:A:244:GLN:HG2	1.92	0.69
1:B:181:ALA:O	1:B:185:GLN:HG3	1.93	0.69
1:B:103:ILE:HG13	1:B:108:ILE:HD12	1.75	0.69
1:B:309:LYS:NZ	1:B:309:LYS:HB2	2.08	0.67
1:A:236:THR:HG23	1:A:237:PHE:N	2.08	0.67
1:B:34:GLN:HB3	1:B:36:ILE:HG23	1.77	0.66
1:B:211:SER:HB2	1:B:217:VAL:CG2	2.25	0.66
1:B:76:ILE:HD13	1:B:228:ALA:HB2	1.78	0.66
1:A:281:TYR:CD2	1:A:301:VAL:HG13	2.31	0.65
1:B:88:LEU:HD21	1:B:123:LEU:HD21	1.77	0.65
1:B:115:ALA:O	1:B:118:LYS:HE3	1.97	0.65
1:B:209:LEU:HD23	1:B:250:TRP:CH2	2.33	0.63
1:B:59:LEU:H	1:B:71:GLN:HE22	1.44	0.63
1:B:18:LYS:HG3	1:B:287:GLN:HE21	1.63	0.63
1:B:298:ASP:O	1:B:301:VAL:HG22	2.00	0.62
1:A:62:GLU:O	1:A:66:GLN:HG3	2.01	0.61
1:B:305:ARG:O	1:B:308:TRP:HB2	2.03	0.58
1:A:226:ASN:O	1:A:229:LYS:HB3	2.04	0.58
1:A:210:ILE:HG23	1:A:214:GLY:O	2.03	0.58
1:A:85:ILE:HD11	1:A:111:TRP:CD2	2.40	0.57
1:A:11:PHE:HB3	1:A:12:PRO:HD3	1.87	0.56
1:B:234:SER:O	1:B:235:LYS:HB2	2.06	0.56
1:B:96:ASP:HB3	1:B:210:ILE:HD12	1.87	0.56
1:A:231:ALA:HB2	1:A:244:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:THR:HB	1:B:162:THR:HA	1.87	0.56
1:A:63:LYS:HG2	1:A:67:GLU:OE1	2.06	0.55
1:B:197:ALA:O	1:B:201:GLN:HG3	2.07	0.55
1:B:23:TYR:O	1:B:27:THR:N	2.40	0.55
1:B:63:LYS:O	1:B:67:GLU:HG2	2.07	0.55
1:B:94:VAL:HG22	1:B:208:LYS:HB2	1.89	0.54
1:A:64:LEU:HD11	1:A:71:GLN:NE2	2.22	0.54
1:A:13:ALA:N	1:A:14:PRO:HD2	2.22	0.54
1:B:233:TRP:HD1	1:B:303:GLN:HE22	1.56	0.54
1:B:313:LYS:HB3	1:B:313:LYS:NZ	2.22	0.54
1:B:318:LYS:HD3	1:B:319:PRO:O	2.08	0.54
1:A:103:ILE:HG23	1:A:130:ILE:HG21	1.89	0.53
1:A:217:VAL:HG12	1:A:223:ASN:HD22	1.74	0.52
1:B:298:ASP:HA	1:B:301:VAL:HG22	1.91	0.52
1:A:102:ASP:HB3	1:A:108:ILE:HG13	1.92	0.52
1:A:236:THR:CG2	1:A:237:PHE:H	2.18	0.52
1:B:265:LYS:HD3	1:B:266:LYS:HG3	1.91	0.52
1:A:312:ILE:HD12	1:A:312:ILE:N	2.24	0.52
1:A:180:ILE:O	1:A:184:VAL:HG23	2.10	0.52
1:A:85:ILE:HD11	1:A:111:TRP:CE3	2.44	0.52
1:A:88:LEU:HD13	1:A:92:GLU:HB3	1.91	0.51
1:A:299:SER:O	1:A:303:GLN:HG3	2.11	0.51
1:B:4:LEU:O	1:B:31:VAL:HA	2.11	0.51
1:B:79:VAL:HB	1:B:252:ILE:CG2	2.40	0.51
1:A:118:LYS:HD2	1:A:119:LEU:HG	1.92	0.51
1:A:59:LEU:HD13	1:A:259:LEU:HD21	1.92	0.51
1:A:264:GLN:O	1:A:267:PRO:HD3	2.11	0.51
1:A:99:THR:O	1:A:103:ILE:HG13	2.11	0.51
1:A:146:THR:HG22	1:A:156:TRP:HZ2	1.75	0.50
1:B:182:ALA:HB1	1:B:186:ARG:NH1	2.22	0.50
1:A:282:LYS:HG3	1:A:283:THR:HG23	1.93	0.50
1:B:94:VAL:HA	1:B:208:LYS:O	2.12	0.50
1:A:82:ALA:CB	1:A:204:LEU:HD12	2.36	0.49
1:A:59:LEU:HD23	1:A:63:LYS:HD3	1.93	0.49
1:A:187:LEU:HD12	1:A:188:PRO:HD2	1.95	0.49
1:A:5:THR:HB	1:A:32:ASN:HB3	1.95	0.49
1:A:122:GLY:O	1:A:123:LEU:HD12	2.12	0.49
1:A:112:ASP:HB3	1:A:126:PRO:O	2.12	0.49
1:A:231:ALA:HB1	1:A:239:GLN:NE2	2.27	0.49
1:A:245:LYS:CD	1:A:245:LYS:H	2.17	0.49
1:B:209:LEU:HD23	1:B:250:TRP:HH2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:N	1:A:269:GLN:HE21	2.11	0.48
1:A:112:ASP:HA	1:A:125:LEU:HB3	1.96	0.48
1:A:217:VAL:CG1	1:A:223:ASN:ND2	2.76	0.48
1:B:182:ALA:O	1:B:186:ARG:HD3	2.13	0.48
1:A:198:TYR:HD1	1:A:198:TYR:H	1.61	0.48
1:A:115:ALA:O	1:A:118:LYS:HE3	2.14	0.48
1:B:234:SER:OG	1:B:303:GLN:HB3	2.14	0.48
1:B:106:GLY:N	1:B:170:ILE:HD11	2.29	0.47
1:B:4:LEU:HB3	1:B:31:VAL:HG22	1.96	0.47
1:A:100:LEU:HG	1:A:149:LEU:HD21	1.96	0.47
1:A:27:THR:OG1	1:A:29:ASN:HB2	2.15	0.47
1:A:131:ALA:HB3	1:A:190:ALA:HA	1.97	0.47
1:A:93:LEU:HD12	1:A:120:ASN:OD1	2.14	0.47
1:B:309:LYS:O	1:B:309:LYS:HG3	2.13	0.47
1:B:309:LYS:HZ2	1:B:309:LYS:HB2	1.79	0.46
1:A:221:GLU:OE2	1:A:289:ASN:O	2.33	0.46
1:A:98:LYS:HD3	1:A:153:ASN:ND2	2.29	0.46
1:B:233:TRP:CG	1:B:300:VAL:HG13	2.49	0.46
1:A:1:GLU:OE2	1:A:3:SER:HB2	2.16	0.46
1:A:14:PRO:HG2	1:A:293:TYR:OH	2.16	0.46
1:B:6:GLY:HA3	1:B:52:PHE:CZ	2.50	0.46
1:B:8:GLY:O	1:B:37:GLY:N	2.48	0.46
1:B:73:PRO:HG2	1:B:296:LEU:HD21	1.97	0.45
1:B:123:LEU:HD23	1:B:125:LEU:HD21	1.97	0.45
1:A:18:LYS:HE3	1:A:291:LEU:HD11	1.98	0.45
1:B:211:SER:O	1:B:213:ASP:N	2.49	0.45
1:A:138:GLY:HA2	1:A:165:THR:HG23	1.98	0.45
1:B:143:PHE:CD1	1:B:143:PHE:C	2.90	0.45
1:B:84:ASN:HB2	1:B:184:VAL:O	2.16	0.45
1:B:291:LEU:HA	1:B:291:LEU:HD12	1.87	0.45
1:A:235:LYS:O	1:A:236:THR:HB	2.17	0.45
1:A:110:LYS:HB3	1:A:112:ASP:OD1	2.17	0.44
1:A:110:LYS:HE3	1:A:112:ASP:OD1	2.17	0.44
1:A:129:ASN:N	1:A:129:ASN:HD22	2.16	0.44
1:A:217:VAL:CG1	1:A:223:ASN:HD22	2.31	0.44
1:A:88:LEU:CD1	1:A:92:GLU:HB3	2.48	0.44
1:A:198:TYR:N	1:A:198:TYR:CD1	2.86	0.44
1:A:124:LYS:HB2	1:A:124:LYS:NZ	2.32	0.44
1:A:168:TRP:HA	1:A:169:PRO:HD3	1.81	0.43
1:A:34:GLN:HB3	1:A:36:ILE:HG23	2.00	0.43
1:B:23:TYR:CE1	1:B:27:THR:HG21	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:GLY:O	1:A:89:LYS:HD3	2.18	0.43
1:B:81:LEU:HA	1:B:192:GLY:O	2.19	0.43
1:A:146:THR:HG22	1:A:156:TRP:CZ2	2.53	0.43
1:A:236:THR:CG2	1:A:237:PHE:N	2.77	0.43
1:A:269:GLN:CA	1:A:269:GLN:NE2	2.81	0.43
1:B:182:ALA:C	1:B:186:ARG:HD3	2.38	0.43
1:B:70:PHE:CE1	1:B:237:PHE:CE1	3.07	0.43
1:B:266:LYS:N	1:B:267:PRO:HD3	2.34	0.43
1:A:54:ALA:HB1	2:A:401:HOH:O	2.19	0.43
1:A:239:GLN:HB3	1:A:239:GLN:HE21	1.60	0.43
1:A:260:ILE:CD1	1:A:312:ILE:HG12	2.49	0.43
1:A:135:ARG:HD3	1:A:180:ILE:HD11	2.00	0.43
1:B:264:GLN:HG3	1:B:320:LEU:CD1	2.49	0.42
1:A:269:GLN:HA	1:A:269:GLN:NE2	2.34	0.42
1:A:2:ALA:CB	1:A:272:GLU:HG2	2.47	0.42
1:B:233:TRP:CD1	1:B:300:VAL:HG13	2.55	0.42
1:B:118:LYS:HD2	1:B:119:LEU:CG	2.46	0.42
1:B:217:VAL:O	1:B:250:TRP:HZ3	2.03	0.42
1:B:245:LYS:HB2	1:B:245:LYS:HE3	1.79	0.41
1:A:182:ALA:HB1	1:A:186:ARG:HH11	1.85	0.41
1:B:297:PRO:O	1:B:301:VAL:HG13	2.20	0.41
1:B:69:LEU:O	1:B:262:LYS:HE3	2.20	0.41
1:B:18:LYS:HG3	1:B:287:GLN:NE2	2.31	0.41
1:B:85:ILE:HA	1:B:86:PRO:HD2	1.95	0.41
1:B:309:LYS:HZ3	1:B:309:LYS:HB2	1.84	0.41
1:A:291:LEU:HD23	1:A:291:LEU:HA	1.94	0.41
1:A:43:LYS:HE2	1:A:43:LYS:HB2	1.86	0.41
1:A:149:LEU:HA	1:A:152:VAL:HG22	2.01	0.41
1:B:265:LYS:O	1:B:265:LYS:HG2	2.20	0.41
1:A:236:THR:C	1:A:238:ALA:H	2.24	0.40
1:A:101:GLY:O	1:A:105:LEU:HG	2.21	0.40
1:B:228:ALA:HA	1:B:241:LEU:CD2	2.52	0.40
1:B:177:ASN:HD22	1:B:177:ASN:HA	1.59	0.40
1:B:32:ASN:OD1	1:B:34:GLN:NE2	2.54	0.40
1:B:54:ALA:HB1	2:B:422:HOH:O	2.20	0.40
1:B:140:GLY:O	1:B:144:VAL:HG23	2.21	0.40
1:B:172:LEU:HD23	1:B:183:PHE:CD1	2.57	0.40
1:B:73:PRO:HA	1:B:256:THR:O	2.21	0.40
1:B:59:LEU:HD22	1:B:259:LEU:HD11	2.03	0.40
1:B:69:LEU:HD21	1:B:261:HIS:CE1	2.56	0.40
1:B:71:GLN:HA	1:B:258:ILE:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	319/321 (99%)	294 (92%)	24 (8%)	1 (0%)	44	60
1	B	319/321 (99%)	293 (92%)	18 (6%)	8 (2%)	6	6
All	All	638/642 (99%)	587 (92%)	42 (7%)	9 (1%)	13	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	LYS
1	B	310	THR
1	A	236	THR
1	B	203	ASN
1	B	2	ALA
1	B	212	ALA
1	B	238	ALA
1	B	114	GLU
1	B	237	PHE

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	252/252 (100%)	229 (91%)	23 (9%)	11	16
1	B	252/252 (100%)	228 (90%)	24 (10%)	10	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	504/504 (100%)	457 (91%)	47 (9%)	10	15

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	5	THR
1	A	30	LYS
1	A	34	GLN
1	A	51	ASP
1	A	55	SER
1	A	69	LEU
1	A	88	LEU
1	A	118	LYS
1	A	124	LYS
1	A	125	LEU
1	A	127	SER
1	A	135	ARG
1	A	157	LYS
1	A	162	THR
1	A	165	THR
1	A	170	ILE
1	A	198	TYR
1	A	245	LYS
1	A	268	GLU
1	A	298	ASP
1	A	309	LYS
1	A	315	SER
1	B	25	LYS
1	B	26	GLU
1	B	55	SER
1	B	62	GLU
1	B	89	LYS
1	B	93	LEU
1	B	100	LEU
1	B	118	LYS
1	B	160	VAL
1	B	162	THR
1	B	170	ILE
1	B	172	LEU
1	B	177	ASN
1	B	178	ASP

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Mol	Chain	Res	Type
1	B	188	PRO
1	B	202	ASN
1	B	259	LEU
1	B	260	ILE
1	B	265	LYS
1	B	291	LEU
1	B	295	SER
1	B	309	LYS
1	B	310	THR
1	B	313	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	GLN
1	A	129	ASN
1	A	202	ASN
1	A	223	ASN
1	A	269	GLN
1	A	303	GLN
1	B	34	GLN
1	B	44	GLN
1	B	71	GLN
1	B	128	GLN
1	B	158	ASN
1	B	177	ASN
1	B	239	GLN
1	B	264	GLN
1	B	287	GLN
1	B	289	ASN
1	B	303	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	321/321 (100%)	1.25	59 (18%)	1	1	3, 16, 36, 58	0
1	B	321/321 (100%)	1.19	55 (17%)	2	1	3, 16, 37, 57	0
All	All	642/642 (100%)	1.22	114 (17%)	2	1	3, 16, 37, 58	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	SER	13.5
1	B	236	THR	9.3
1	A	235	LYS	6.0
1	A	232	ASP	5.3
1	B	238	ALA	5.3
1	B	237	PHE	4.8
1	B	315	SER	4.7
1	A	237	PHE	4.5
1	B	233	TRP	4.4
1	B	272	GLU	4.4
1	A	201	GLN	4.3
1	B	235	LYS	4.2
1	A	230	GLY	4.1
1	B	230	GLY	4.1
1	A	315	SER	4.1
1	A	126	PRO	4.0
1	B	309	LYS	3.8
1	B	182	ALA	3.8
1	A	267	PRO	3.7
1	A	129	ASN	3.6
1	A	246	GLY	3.5
1	A	316	SER	3.5
1	B	284	GLY	3.5
1	A	31	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	3	SER	3.4
1	B	35	GLY	3.3
1	B	87	GLY	3.3
1	B	282	LYS	3.2
1	B	49	THR	3.2
1	A	236	THR	3.1
1	A	211	SER	3.1
1	A	282	LYS	3.1
1	A	49	THR	3.1
1	A	301	VAL	3.0
1	A	77	GLY	3.0
1	B	314	ASP	3.0
1	A	314	ASP	3.0
1	A	284	GLY	3.0
1	A	39	SER	3.0
1	B	271	THR	3.0
1	B	89	LYS	2.9
1	B	4	LEU	2.9
1	A	170	ILE	2.9
1	B	266	LYS	2.8
1	B	115	ALA	2.8
1	A	25	LYS	2.8
1	A	158	ASN	2.8
1	A	5	THR	2.8
1	B	206	TYR	2.8
1	A	87	GLY	2.7
1	B	47	ALA	2.7
1	B	129	ASN	2.7
1	A	198	TYR	2.7
1	A	47	ALA	2.6
1	A	115	ALA	2.6
1	A	263	ASP	2.6
1	B	2	ALA	2.6
1	A	238	ALA	2.6
1	A	19	TRP	2.6
1	A	154	GLU	2.6
1	B	187	LEU	2.5
1	B	267	PRO	2.5
1	A	2	ALA	2.5
1	B	211	SER	2.5
1	B	138	GLY	2.5
1	B	208	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	283	THR	2.4
1	A	298	ASP	2.4
1	B	231	ALA	2.4
1	A	260	ILE	2.4
1	A	272	GLU	2.3
1	B	114	GLU	2.3
1	A	245	LYS	2.3
1	A	192	GLY	2.3
1	A	167	LYS	2.3
1	A	137	ASP	2.3
1	B	154	GLU	2.3
1	A	3	SER	2.3
1	A	138	GLY	2.3
1	A	210	ILE	2.3
1	A	244	GLN	2.3
1	B	7	ALA	2.3
1	A	234	SER	2.2
1	B	185	GLN	2.2
1	A	309	LYS	2.2
1	B	217	VAL	2.2
1	B	209	LEU	2.2
1	A	35	GLY	2.2
1	A	136	ALA	2.2
1	B	128	GLN	2.2
1	A	4	LEU	2.2
1	A	265	LYS	2.2
1	B	318	LYS	2.2
1	B	263	ASP	2.2
1	B	210	ILE	2.2
1	B	264	GLN	2.1
1	B	77	GLY	2.1
1	B	46	ILE	2.1
1	A	23	TYR	2.1
1	A	162	THR	2.1
1	A	46	ILE	2.1
1	B	198	TYR	2.1
1	B	165	THR	2.1
1	B	203	ASN	2.1
1	A	18	LYS	2.1
1	B	110	LYS	2.1
1	B	170	ILE	2.1
1	A	124	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	141	ASP	2.0
1	A	304	VAL	2.0
1	A	231	ALA	2.0
1	B	126	PRO	2.0
1	B	50	VAL	2.0
1	B	23	TYR	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 carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.