



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:40 AM UTC

PDB ID : 1OIB / pdb_00001oib
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

<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

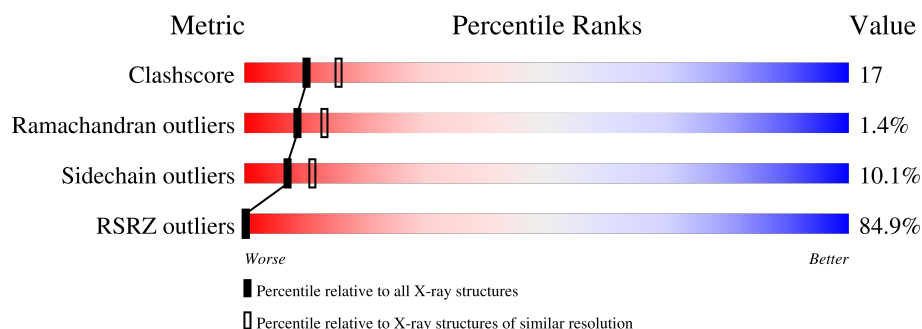
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	B	321	

2 Entry composition

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 mutation	UNP P06128
B	141	ASP	THR	engineered mutation	UNP P06128

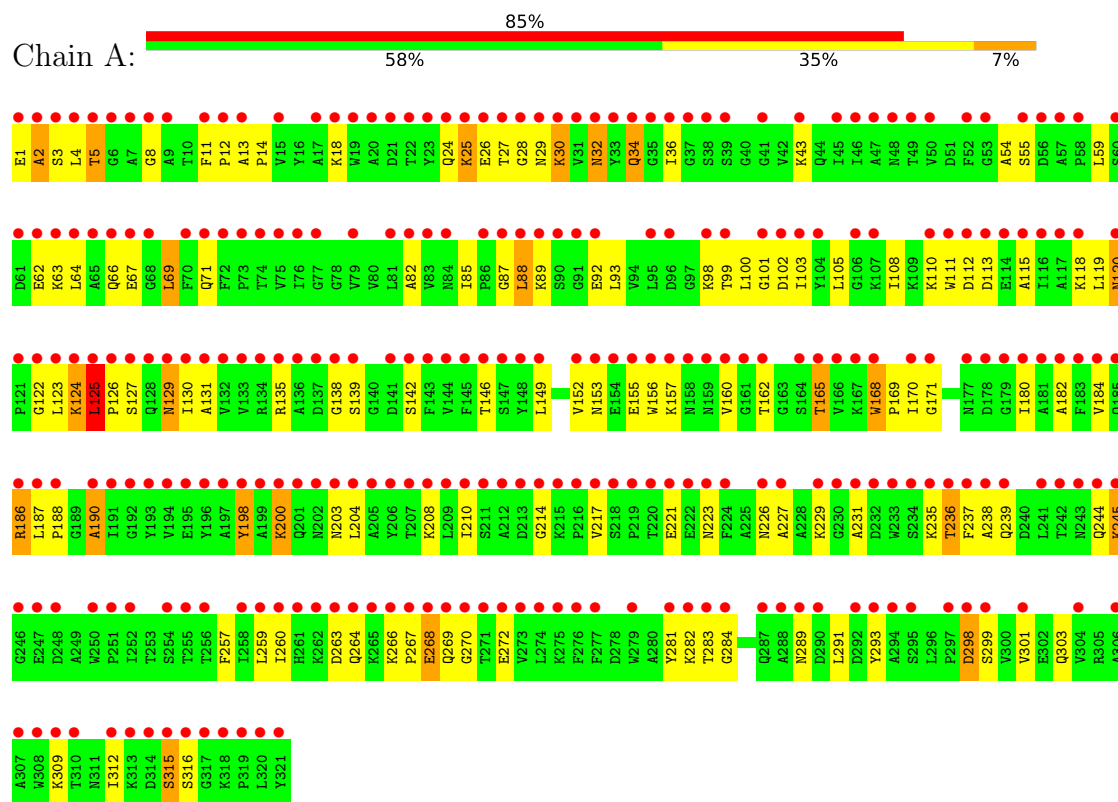
- Molecule 2 is water.

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

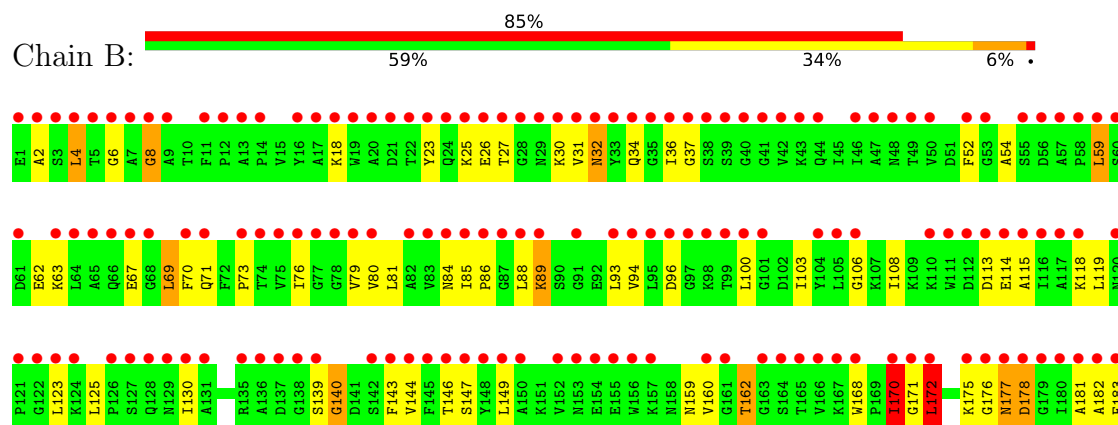
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: PHOSPHATE-BINDING PROTEIN



• Molecule 1: PHOSPHATE-BINDING PROTEIN





4 Data and refinement statistics

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 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.40) 79.6 (8.00-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.90Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.166 , (Not available) 0.304 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 91.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	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.*

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

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	0.75	0/2494	1.26	29/3385 (0.9%)
1	B	0.73	0/2494	1.27	32/3385 (0.9%)
All	All	0.74	0/4988	1.27	61/6770 (0.9%)

There are no bond length outliers.

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ASP	N-CA-C	9.27	125.06	110.32
1	A	200	LYS	N-CA-C	9.26	121.06	110.97
1	B	159	ASN	N-CA-C	8.08	123.25	113.23
1	B	257	PHE	N-CA-C	7.92	122.36	109.85
1	A	208	LYS	N-CA-C	-7.76	98.40	110.42
1	B	239	GLN	N-CA-C	7.74	121.56	108.02
1	A	8	GLY	N-CA-C	7.72	120.17	110.29
1	B	8	GLY	N-CA-C	7.49	120.09	110.20
1	B	139	SER	N-CA-C	7.35	120.45	108.55
1	B	178	ASP	N-CA-C	-7.08	103.50	111.07
1	A	168	TRP	CA-C-N	6.93	126.40	118.85
1	A	168	TRP	C-N-CA	6.93	126.40	118.85
1	B	32	ASN	N-CA-C	-6.89	99.08	110.17
1	A	298	ASP	N-CA-C	6.78	119.51	111.71
1	B	237	PHE	N-CA-C	6.64	124.95	110.80
1	B	266	LYS	CA-C-N	6.49	127.96	119.84
1	B	266	LYS	C-N-CA	6.49	127.96	119.84
1	B	168	TRP	CA-C-N	6.47	125.90	118.85
1	B	168	TRP	C-N-CA	6.47	125.90	118.85
1	A	25	LYS	N-CA-C	-6.46	103.36	111.11
1	B	224	PHE	N-CA-C	-6.43	104.20	111.14
1	A	2	ALA	N-CA-C	-6.42	100.06	110.20
1	B	187	LEU	N-CA-C	6.41	122.58	108.73
1	B	113	ASP	N-CA-C	-6.33	100.80	110.30
1	B	140	GLY	N-CA-C	-6.30	105.19	112.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLY	N-CA-C	6.24	120.03	112.48
1	A	316	SER	N-CA-C	6.21	120.63	111.87
1	A	120	ASN	CA-C-N	6.17	127.55	119.84
1	A	120	ASN	C-N-CA	6.17	127.55	119.84
1	B	170	ILE	CB-CA-C	-6.16	101.18	111.29
1	A	125	LEU	CA-C-N	6.16	126.07	119.85
1	A	125	LEU	C-N-CA	6.16	126.07	119.85
1	A	268	GLU	N-CA-C	-6.14	104.59	111.28
1	B	30	LYS	N-CA-C	6.11	118.37	108.41
1	A	284	GLY	N-CA-C	6.00	121.27	114.67
1	B	246	GLY	N-CA-C	-5.95	106.08	112.08
1	A	139	SER	N-CA-C	5.81	117.90	109.07
1	A	257	PHE	N-CA-C	5.78	118.97	109.72
1	A	266	LYS	CA-C-N	5.77	127.06	119.84
1	A	266	LYS	C-N-CA	5.77	127.06	119.84
1	A	28	GLY	N-CA-C	-5.77	107.28	115.30
1	A	26	GLU	N-CA-C	5.76	119.49	112.23
1	B	251	PRO	N-CA-C	5.73	121.37	113.98
1	B	172	LEU	N-CA-C	-5.67	101.30	110.32
1	A	186	ARG	N-CA-C	5.66	119.80	113.01
1	A	142	SER	N-CA-C	-5.58	105.28	111.36
1	B	149	LEU	N-CA-C	5.55	117.33	111.28
1	A	203	ASN	N-CA-C	5.42	118.68	111.30
1	A	155	GLU	N-CA-C	5.41	116.98	111.14
1	B	171	GLY	N-CA-C	5.39	118.79	111.72
1	A	190	ALA	N-CA-C	5.31	117.99	110.50
1	B	69	LEU	N-CA-C	5.26	116.66	109.18
1	A	69	LEU	N-CA-C	5.23	117.23	109.69
1	B	265	LYS	N-CA-C	-5.22	106.42	112.89
1	B	147	SER	N-CA-C	-5.15	105.67	111.28
1	B	203	ASN	N-CA-C	5.15	121.77	110.80
1	B	176	GLY	CA-C-O	-5.08	118.72	122.23
1	B	130	ILE	N-CA-C	-5.06	102.33	109.21
1	A	30	LYS	N-CA-C	5.05	116.62	108.34
1	B	215	LYS	CA-C-N	5.01	125.24	119.83
1	B	215	LYS	C-N-CA	5.01	125.24	119.83

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	87	0
1	B	2439	0	2414	79	0
2	A	19	0	0	2	0
2	B	18	0	0	1	0
All	All	4915	0	4828	166	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 17.

All (166) 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:B:265:LYS:HD3	1:B:266:LYS:HZ3	1.55	0.71
1:A:263:ASP:OD1	1:A:315:SER:HA	1.91	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:HB2	1:B:309:LYS:NZ	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:NZ	1:B:313:LYS:HB3	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:99:THR:O	1:A:103:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLN:O	1:A:267:PRO:HD3	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:B:143:PHE:C	1:B:143:PHE:CD1	2.90	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:5:THR:HB	1:A:32:ASN:HB3	1.95	0.49
1:A:187:LEU:HD12	1:A:188:PRO:HD2	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:H	1:A:245:LYS:CD	2.17	0.49
1:B:209:LEU:HD23	1:B:250:TRP:HH2	1.77	0.49
1:A:269:GLN:HE21	1:A:269:GLN:N	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:H	1:A:198:TYR:HD1	1.61	0.48
1:A:115:ALA:O	1:A:118:LYS:HE3	2.14	0.48
1:B:182:ALA:C	1:B:186:ARG:HD3	2.38	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:HB2	1:B:309:LYS:HZ2	1.79	0.46
1:A:98:LYS:HD3	1:A:153:ASN:ND2	2.29	0.46
1:A:221:GLU:OE2	1:A:289:ASN:O	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:C	1:A:238:ALA:H	2.24	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:84:ASN:HB2	1:B:184:VAL:O	2.16	0.45
1:B:291:LEU:HD12	1:B:291:LEU:HA	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:HD22	1:A:129:ASN:N	2.16	0.44
1:A:88:LEU:CD1	1:A:92:GLU:HB3	2.48	0.44
1:A:217:VAL:CG1	1:A:223:ASN:HD22	2.31	0.44
1:A:198:TYR:CD1	1:A:198:TYR:N	2.86	0.44
1:A:124:LYS:HB2	1:A:124:LYS:NZ	2.32	0.44
1:A:34:GLN:HB3	1:A:36:ILE:HG23	2.00	0.43
1:A:168:TRP:HA	1:A:169:PRO:HD3	1.81	0.43
1:B:23:TYR:CE1	1:B:27:THR:HG21	2.53	0.43
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:269:GLN:NE2	1:A:269:GLN:CA	2.81	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:HE21	1:A:239:GLN:HB3	1.60	0.43
1:B:318:LYS:HD3	1:B:318:LYS:C	2.44	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:211:SER:C	1:B:213:ASP:N	2.77	0.42
1:B:264:GLN:HG3	1:B:320:LEU:CD1	2.49	0.42
1:A:111:TRP:C	1:A:113:ASP:H	2.26	0.42
1:A:269:GLN:NE2	1:A:269:GLN:HA	2.34	0.42
1:B:265:LYS:C	1:B:267:PRO:HD3	2.44	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:88:LEU:C	1:B:89:LYS:HE3	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:GLN:O	1:A:270:GLY:C	2.62	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:HB2	1:B:309:LYS:HZ3	1.84	0.41
1:A:24:GLN:O	1:A:25:LYS:C	2.63	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: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:32:ASN:OD1	1:B:34:GLN:NE2	2.54	0.40
1:B:177:ASN:HD22	1:B:177:ASN:HA	1.59	0.40
1:B:54:ALA:HB1	2:B:422:HOH:O	2.20	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
1:B:73:PRO:HA	1:B:256:THR:O	2.21	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

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%)	36	50
1	B	319/321 (99%)	293 (92%)	18 (6%)	8 (2%)	4	5
All	All	638/642 (99%)	587 (92%)	42 (7%)	9 (1%)	9	13

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%)	228 (90%)	24 (10%)	8	13
1	B	252/252 (100%)	225 (89%)	27 (11%)	6	10
All	All	504/504 (100%)	453 (90%)	51 (10%)	7	11

All (51) 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	32	ASN
1	A	34	GLN
1	A	55	SER
1	A	69	LEU
1	A	88	LEU
1	A	124	LYS
1	A	125	LEU
1	A	127	SER
1	A	129	ASN
1	A	157	LYS
1	A	160	VAL
1	A	162	THR

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Mol	Chain	Res	Type
1	A	165	THR
1	A	170	ILE
1	A	198	TYR
1	A	200	LYS
1	A	245	LYS
1	A	268	GLU
1	A	298	ASP
1	A	309	LYS
1	A	315	SER
1	B	4	LEU
1	B	25	LYS
1	B	26	GLU
1	B	59	LEU
1	B	62	GLU
1	B	80	VAL
1	B	89	LYS
1	B	93	LEU
1	B	100	LEU
1	B	160	VAL
1	B	162	THR
1	B	170	ILE
1	B	172	LEU
1	B	175	LYS
1	B	177	ASN
1	B	178	ASP
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	296	LEU
1	B	309	LYS
1	B	310	THR
1	B	313	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	44	GLN

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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	289	ASN
1	A	303	GLN
1	B	29	ASN
1	B	34	GLN
1	B	44	GLN
1	B	71	GLN
1	B	128	GLN
1	B	158	ASN
1	B	159	ASN
1	B	177	ASN
1	B	185	GLN
1	B	239	GLN
1	B	264	GLN
1	B	287	GLN
1	B	289	ASN
1	B	303	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](#)

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

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	321/321 (100%)	3.28	272 (84%) 0 0	3, 16, 36, 58	0
1	B	321/321 (100%)	3.19	273 (85%) 0 0	3, 16, 37, 57	0
All	All	642/642 (100%)	3.24	545 (84%) 0 0	3, 16, 37, 58	0

All (545) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	SER	10.3
1	B	87	GLY	9.3
1	B	236	THR	9.3
1	A	246	GLY	8.9
1	B	182	ALA	8.5
1	A	232	ASP	8.4
1	A	230	GLY	7.6
1	A	201	GLN	7.6
1	B	272	GLU	7.5
1	B	211	SER	7.0
1	A	220	THR	6.9
1	B	237	PHE	6.9
1	A	211	SER	6.9
1	A	301	VAL	6.6
1	A	129	ASN	6.6
1	A	192	GLY	6.6
1	B	231	ALA	6.5
1	A	237	PHE	6.4
1	B	89	LYS	6.3
1	B	129	ASN	6.3
1	A	39	SER	6.3
1	B	27	THR	6.2
1	B	220	THR	6.2
1	A	48	ASN	6.2

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Mol	Chain	Res	Type	RSRZ
1	B	106	GLY	6.2
1	B	37	GLY	6.1
1	A	236	THR	6.1
1	A	182	ALA	6.1
1	A	315	SER	6.1
1	A	25	LYS	6.0
1	A	87	GLY	6.0
1	A	37	GLY	5.9
1	B	187	LEU	5.9
1	A	235	LYS	5.9
1	B	230	GLY	5.9
1	B	271	THR	5.8
1	B	215	LYS	5.8
1	B	46	ILE	5.7
1	B	206	TYR	5.7
1	B	217	VAL	5.7
1	A	158	ASN	5.7
1	A	5	THR	5.6
1	A	35	GLY	5.6
1	B	315	SER	5.4
1	B	284	GLY	5.4
1	B	238	ALA	5.3
1	B	263	ASP	5.3
1	B	49	THR	5.3
1	A	32	ASN	5.2
1	B	181	ALA	5.2
1	A	142	SER	5.2
1	A	146	THR	5.1
1	B	232	ASP	5.1
1	B	265	LYS	5.1
1	A	137	ASP	5.0
1	A	254	SER	5.0
1	B	139	SER	5.0
1	A	162	THR	5.0
1	B	39	SER	5.0
1	B	4	LEU	5.0
1	B	250	TRP	4.9
1	A	316	SER	4.9
1	A	267	PRO	4.9
1	A	31	VAL	4.9
1	A	67	GLU	4.9
1	B	35	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
1	B	282	LYS	4.8
1	A	126	PRO	4.8
1	B	222	GLU	4.8
1	B	233	TRP	4.8
1	A	18	LYS	4.7
1	A	265	LYS	4.7
1	A	247	GLU	4.7
1	A	36	ILE	4.7
1	A	282	LYS	4.7
1	A	178	ASP	4.7
1	B	171	GLY	4.7
1	B	202	ASN	4.7
1	B	114	GLU	4.7
1	B	223	ASN	4.6
1	A	106	GLY	4.6
1	A	166	VAL	4.6
1	A	222	GLU	4.6
1	B	155	GLU	4.6
1	A	155	GLU	4.6
1	B	32	ASN	4.6
1	A	46	ILE	4.6
1	A	20	ALA	4.6
1	B	306	ALA	4.6
1	B	185	GLN	4.5
1	A	160	VAL	4.5
1	A	244	GLN	4.5
1	B	142	SER	4.5
1	A	112	ASP	4.4
1	B	283	THR	4.4
1	B	29	ASN	4.3
1	B	13	ALA	4.3
1	A	68	GLY	4.3
1	A	210	ILE	4.3
1	A	136	ALA	4.3
1	A	241	LEU	4.3
1	A	127	SER	4.3
1	A	50	VAL	4.3
1	A	231	ALA	4.3
1	B	288	ALA	4.3
1	B	101	GLY	4.3
1	B	301	VAL	4.3
1	A	58	PRO	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	185	GLN	4.2
1	B	128	GLN	4.2
1	A	271	THR	4.2
1	B	50	VAL	4.2
1	B	313	LYS	4.2
1	B	36	ILE	4.2
1	A	320	LEU	4.2
1	B	121	PRO	4.2
1	B	66	GLN	4.2
1	A	53	GLY	4.2
1	A	170	ILE	4.2
1	A	115	ALA	4.2
1	B	266	LYS	4.2
1	B	269	GLN	4.2
1	A	284	GLY	4.2
1	A	64	LEU	4.1
1	A	183	PHE	4.1
1	A	243	ASN	4.1
1	B	3	SER	4.1
1	B	78	GLY	4.1
1	A	95	LEU	4.1
1	A	19	TRP	4.1
1	A	223	ASN	4.1
1	B	297	PRO	4.1
1	A	272	GLU	4.1
1	A	234	SER	4.1
1	B	309	LYS	4.1
1	B	267	PRO	4.0
1	A	195	GLU	4.0
1	A	122	GLY	4.0
1	A	317	GLY	4.0
1	B	192	GLY	4.0
1	A	49	THR	4.0
1	A	86	PRO	4.0
1	B	264	GLN	4.0
1	A	124	LYS	4.0
1	A	66	GLN	4.0
1	A	11	PHE	4.0
1	B	247	GLU	4.0
1	A	181	ALA	4.0
1	A	314	ASP	4.0
1	B	198	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	250	TRP	3.9
1	A	288	ALA	3.9
1	A	33	TYR	3.9
1	A	214	GLY	3.9
1	B	318	LYS	3.9
1	B	168	TRP	3.9
1	A	293	TYR	3.9
1	B	2	ALA	3.9
1	B	65	ALA	3.9
1	A	248	ASP	3.9
1	A	60	SER	3.9
1	A	15	VAL	3.9
1	B	294	ALA	3.8
1	A	41	GLY	3.8
1	A	91	GLY	3.8
1	B	18	LYS	3.8
1	B	208	LYS	3.8
1	B	299	SER	3.8
1	B	19	TRP	3.8
1	A	113	ASP	3.8
1	A	213	ASP	3.8
1	A	144	VAL	3.8
1	A	233	TRP	3.8
1	B	110	LYS	3.8
1	A	226	ASN	3.8
1	B	76	ILE	3.8
1	A	304	VAL	3.8
1	A	206	TYR	3.8
1	B	38	SER	3.7
1	A	279	TRP	3.7
1	B	188	PRO	3.7
1	A	135	ARG	3.7
1	B	31	VAL	3.7
1	B	166	VAL	3.7
1	A	82	ALA	3.7
1	A	229	LYS	3.7
1	B	157	LYS	3.7
1	A	212	ALA	3.7
1	A	114	GLU	3.7
1	B	209	LEU	3.7
1	B	6	GLY	3.7
1	B	95	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	98	LYS	3.7
1	A	294	ALA	3.6
1	B	199	ALA	3.6
1	A	143	PHE	3.6
1	A	92	GLU	3.6
1	A	199	ALA	3.6
1	A	198	TYR	3.6
1	B	150	ALA	3.6
1	B	77	GLY	3.6
1	B	67	GLU	3.6
1	A	215	LYS	3.6
1	A	128	GLN	3.6
1	A	204	LEU	3.6
1	B	228	ALA	3.6
1	B	180	ILE	3.6
1	A	84	ASN	3.6
1	B	248	ASP	3.6
1	A	200	LYS	3.5
1	A	149	LEU	3.5
1	B	7	ALA	3.5
1	A	251	PRO	3.5
1	B	116	ILE	3.5
1	A	157	LYS	3.5
1	A	75	VAL	3.5
1	B	148	TYR	3.5
1	B	320	LEU	3.5
1	A	312	ILE	3.5
1	A	89	LYS	3.5
1	A	101	GLY	3.5
1	B	285	ALA	3.5
1	B	138	GLY	3.5
1	A	276	PHE	3.5
1	A	1	GLU	3.4
1	B	152	VAL	3.4
1	A	227	ALA	3.4
1	B	210	ILE	3.4
1	B	218	SER	3.4
1	A	186	ARG	3.4
1	B	84	ASN	3.4
1	A	297	PRO	3.4
1	B	246	GLY	3.4
1	A	193	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	145	PHE	3.4
1	B	314	ASP	3.4
1	A	27	THR	3.4
1	A	209	LEU	3.4
1	A	295	SER	3.4
1	A	104	TYR	3.4
1	A	281	TYR	3.4
1	A	120	ASN	3.4
1	A	38	SER	3.4
1	B	104	TYR	3.3
1	B	214	GLY	3.3
1	B	137	ASP	3.3
1	A	239	GLN	3.3
1	A	154	GLU	3.3
1	A	103	ILE	3.3
1	A	167	LYS	3.3
1	A	159	ASN	3.3
1	A	202	ASN	3.3
1	B	88	LEU	3.3
1	A	184	VAL	3.3
1	B	115	ALA	3.3
1	A	29	ASN	3.3
1	B	58	PRO	3.3
1	B	26	GLU	3.3
1	A	47	ALA	3.3
1	A	307	ALA	3.3
1	A	287	GLN	3.2
1	B	52	PHE	3.2
1	B	186	ARG	3.2
1	A	88	LEU	3.2
1	B	279	TRP	3.2
1	A	65	ALA	3.2
1	B	86	PRO	3.2
1	B	219	PRO	3.2
1	B	311	ASN	3.2
1	A	77	GLY	3.2
1	A	217	VAL	3.2
1	B	207	THR	3.2
1	B	255	THR	3.2
1	A	13	ALA	3.2
1	A	277	PHE	3.2
1	A	21	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	43	LYS	3.2
1	A	196	TYR	3.2
1	B	83	VAL	3.2
1	A	180	ILE	3.2
1	B	276	PHE	3.1
1	A	263	ASP	3.1
1	B	307	ALA	3.1
1	A	118	LYS	3.1
1	B	167	LYS	3.1
1	A	8	GLY	3.1
1	A	270	GLY	3.1
1	B	161	GLY	3.1
1	A	255	THR	3.1
1	B	170	ILE	3.1
1	B	260	ILE	3.1
1	A	71	GLN	3.1
1	B	47	ALA	3.1
1	B	239	GLN	3.1
1	A	63	LYS	3.1
1	B	60	SER	3.1
1	A	273	VAL	3.1
1	B	75	VAL	3.1
1	A	165	THR	3.1
1	A	283	THR	3.1
1	B	33	TYR	3.1
1	A	57	ALA	3.1
1	A	275	LYS	3.1
1	B	221	GLU	3.1
1	B	11	PHE	3.1
1	B	113	ASP	3.1
1	B	143	PHE	3.1
1	A	55	SER	3.1
1	B	203	ASN	3.1
1	B	226	ASN	3.1
1	A	79	VAL	3.1
1	B	304	VAL	3.1
1	A	2	ALA	3.0
1	A	148	TYR	3.0
1	B	9	ALA	3.0
1	B	280	ALA	3.0
1	B	195	GLU	3.0
1	A	141	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	240	ASP	3.0
1	B	156	TRP	3.0
1	B	176	GLY	3.0
1	A	132	VAL	3.0
1	B	136	ALA	3.0
1	B	227	ALA	3.0
1	B	154	GLU	3.0
1	B	64	LEU	3.0
1	A	3	SER	3.0
1	A	245	LYS	3.0
1	A	111	TRP	3.0
1	B	200	LYS	3.0
1	B	254	SER	3.0
1	B	243	ASN	3.0
1	B	258	ILE	3.0
1	B	5	THR	3.0
1	B	308	TRP	3.0
1	A	238	ALA	3.0
1	B	145	PHE	3.0
1	B	48	ASN	3.0
1	A	138	GLY	3.0
1	A	76	ILE	2.9
1	B	277	PHE	2.9
1	A	90	SER	2.9
1	A	12	PRO	2.9
1	A	318	LYS	2.9
1	A	259	LEU	2.9
1	B	281	TYR	2.9
1	A	292	ASP	2.9
1	B	40	GLY	2.9
1	B	120	ASN	2.9
1	B	99	THR	2.9
1	B	17	ALA	2.9
1	B	126	PRO	2.9
1	B	23	TYR	2.9
1	B	112	ASP	2.9
1	A	268	GLU	2.9
1	A	152	VAL	2.9
1	B	61	ASP	2.9
1	B	213	ASP	2.9
1	B	34	GLN	2.9
1	A	28	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	171	GLY	2.9
1	A	147	SER	2.8
1	A	203	ASN	2.8
1	B	164	SER	2.8
1	B	194	VAL	2.8
1	B	82	ALA	2.8
1	A	81	LEU	2.8
1	B	172	LEU	2.8
1	B	268	GLU	2.8
1	A	262	LYS	2.8
1	A	309	LYS	2.8
1	B	124	LYS	2.8
1	B	42	VAL	2.8
1	B	94	VAL	2.8
1	B	73	PRO	2.8
1	B	302	GLU	2.8
1	B	303	GLN	2.8
1	B	43	LYS	2.8
1	A	23	TYR	2.8
1	B	28	GLY	2.8
1	B	147	SER	2.8
1	B	12	PRO	2.8
1	B	79	VAL	2.8
1	B	190	ALA	2.8
1	A	264	GLN	2.8
1	A	56	ASP	2.8
1	A	102	ASP	2.8
1	A	298	ASP	2.8
1	A	52	PHE	2.8
1	A	261	HIS	2.8
1	B	53	GLY	2.8
1	A	299	SER	2.8
1	A	242	THR	2.8
1	A	306	ALA	2.8
1	B	1	GLU	2.8
1	B	135	ARG	2.8
1	B	179	GLY	2.7
1	A	168	TRP	2.7
1	B	111	TRP	2.7
1	A	121	PRO	2.7
1	B	293	TYR	2.7
1	A	205	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	110	LYS	2.7
1	B	57	ALA	2.7
1	A	133	VAL	2.7
1	B	273	VAL	2.7
1	B	117	ALA	2.7
1	B	131	ALA	2.7
1	B	225	ALA	2.7
1	B	24	GLN	2.7
1	B	21	ASP	2.7
1	B	163	GLY	2.7
1	A	188	PRO	2.7
1	A	9	ALA	2.7
1	B	70	PHE	2.6
1	B	98	LYS	2.6
1	A	289	ASN	2.6
1	A	4	LEU	2.6
1	B	193	TYR	2.6
1	A	6	GLY	2.6
1	A	290	ASP	2.6
1	B	8	GLY	2.6
1	B	292	ASP	2.6
1	A	130	ILE	2.6
1	B	127	SER	2.6
1	A	34	GLN	2.6
1	B	212	ALA	2.6
1	B	196	TYR	2.6
1	B	261	HIS	2.6
1	B	41	GLY	2.6
1	A	62	GLU	2.6
1	A	7	ALA	2.6
1	B	22	THR	2.6
1	B	197	ALA	2.6
1	A	308	TRP	2.5
1	A	61	ASP	2.5
1	B	251	PRO	2.5
1	A	45	ILE	2.5
1	A	187	LEU	2.5
1	A	30	LYS	2.5
1	A	107	LYS	2.5
1	A	258	ILE	2.5
1	B	93	LEU	2.5
1	B	291	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	24	GLN	2.5
1	B	118	LYS	2.5
1	A	96	ASP	2.5
1	A	260	ILE	2.5
1	B	123	LEU	2.5
1	B	183	PHE	2.5
1	B	241	LEU	2.5
1	A	266	LYS	2.5
1	A	194	VAL	2.5
1	B	300	VAL	2.5
1	B	321	TYR	2.5
1	A	252	ILE	2.5
1	B	25	LYS	2.5
1	B	149	LEU	2.5
1	A	177	ASN	2.5
1	B	177	ASN	2.5
1	A	17	ALA	2.5
1	A	256	THR	2.5
1	B	16	TYR	2.4
1	B	85	ILE	2.4
1	A	123	LEU	2.4
1	B	100	LEU	2.4
1	A	83	VAL	2.4
1	A	207	THR	2.4
1	A	310	THR	2.4
1	A	216	PRO	2.4
1	A	221	GLU	2.4
1	B	63	LYS	2.4
1	B	91	GLY	2.4
1	B	275	LYS	2.4
1	A	197	ALA	2.4
1	A	26	GLU	2.4
1	A	139	SER	2.4
1	A	218	SER	2.4
1	A	313	LYS	2.4
1	A	153	ASN	2.4
1	A	22	THR	2.4
1	B	165	THR	2.4
1	A	319	PRO	2.4
1	B	216	PRO	2.4
1	A	164	SER	2.4
1	B	146	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	125	LEU	2.3
1	B	191	ILE	2.3
1	B	178	ASP	2.3
1	B	259	LEU	2.3
1	B	144	VAL	2.3
1	B	242	THR	2.3
1	B	122	GLY	2.3
1	A	116	ILE	2.3
1	A	274	LEU	2.3
1	B	105	LEU	2.3
1	B	130	ILE	2.3
1	A	321	TYR	2.3
1	B	153	ASN	2.3
1	B	14	PRO	2.3
1	A	74	THR	2.3
1	A	99	THR	2.3
1	B	245	LYS	2.3
1	A	70	PHE	2.3
1	B	80	VAL	2.3
1	B	319	PRO	2.3
1	B	204	LEU	2.2
1	B	286	LYS	2.2
1	B	96	ASP	2.2
1	A	117	ALA	2.2
1	B	287	GLN	2.2
1	A	179	GLY	2.2
1	B	97	GLY	2.2
1	B	175	LYS	2.2
1	B	56	ASP	2.2
1	B	290	ASP	2.2
1	B	224	PHE	2.2
1	A	190	ALA	2.2
1	B	20	ALA	2.2
1	B	30	LYS	2.2
1	B	71	GLN	2.2
1	B	74	THR	2.2
1	B	244	GLN	2.2
1	B	189	GLY	2.2
1	A	134	ARG	2.2
1	A	224	PHE	2.2
1	B	289	ASN	2.2
1	A	156	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	44	GLN	2.1
1	B	68	GLY	2.1
1	B	296	LEU	2.1
1	B	262	LYS	2.1
1	A	72	PHE	2.1
1	A	73	PRO	2.1
1	A	219	PRO	2.1
1	B	160	VAL	2.1
1	A	131	ALA	2.1
1	A	161	GLY	2.1
1	A	191	ILE	2.1
1	B	229	LYS	2.1
1	B	59	LEU	2.1
1	B	55	SER	2.0
1	A	269	GLN	2.0
1	A	208	LYS	2.0
1	B	256	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.