



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BGX
Title : TAQ POLYMERASE IN COMPLEX WITH TP7, AN INHIBITORY FAB
Authors : Murali, R.; Sharkey, D.J.; Daiss, J.L.; Krishna Murthy, H.M.
Deposited on : 1998-06-02
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

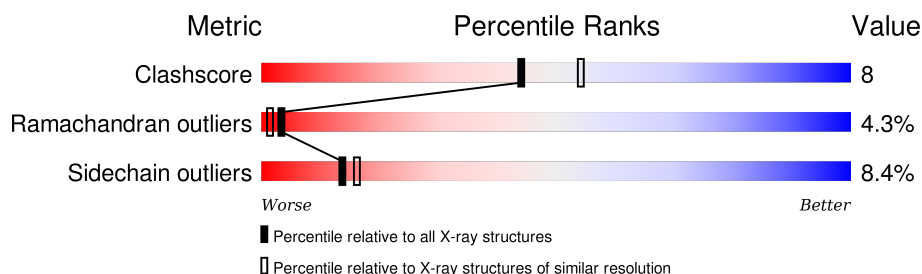
1 Overall quality at a glance

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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (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 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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	T	832	
2	L	210	
3	H	213	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10077 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 TAQ DNA POLYMERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	828	Total	C	N	O	S	0	0	0
			6570	4197	1166	1191	16			

- Molecule 2 is a protein called TP7 MAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	210	Total	C	N	O	S	0	0	0
			1613	1004	266	333	10			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	17	GLU	GLN	CONFLICT	GB 437099
L	21	MET	ILE	CONFLICT	GB 437099
L	?	-	SER	DELETION	GB 437099
L	?	-	ARG	DELETION	GB 437099
L	32	TYR	PHE	CONFLICT	GB 437099
L	33	MET	LEU	CONFLICT	GB 437099
L	34	TYR	HIS	CONFLICT	GB 437099
L	40	PRO	SER	CONFLICT	GB 437099
L	42	SER	ALA	CONFLICT	GB 437099
L	45	ARG	LYS	CONFLICT	GB 437099
L	47	LEU	TRP	CONFLICT	GB 437099
L	51	SER	THR	CONFLICT	GB 437099
L	52	THR	SER	CONFLICT	GB 437099
L	53	ASN	LYS	CONFLICT	GB 437099
L	56	SER	PRO	CONFLICT	GB 437099
L	60	VAL	ALA	CONFLICT	GB 437099
L	77	ARG	SER	CONFLICT	GB 437099
L	85	THR	SER	CONFLICT	GB 437099
L	87	TYR	PHE	CONFLICT	GB 437099
L	89	GLN	HIS	CONFLICT	GB 437099

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
L	93	THR	SER	CONFLICT	GB 437099

- Molecule 3 is a protein called TP7 MAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	209	Total	C	N	O	S	0	0	0
			1632	1046	259	322	5			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	15	TYR	SER	CONFLICT	GB 1513182
H	21	SER	THR	CONFLICT	GB 1513182
H	29	ILE	VAL	CONFLICT	GB 1513182
H	31A	ASP	GLU	CONFLICT	GB 1513182
H	48	MET	LEU	CONFLICT	GB 1513182
H	52	THR	ASN	CONFLICT	GB 1513182
H	55	THR	SER	CONFLICT	GB 1513182
H	57	ASP	SER	CONFLICT	GB 1513182
H	?	-	ASP	DELETION	GB 1513182
H	95	TYR	-	INSERTION	GB 1513182
H	96	TYR	-	INSERTION	GB 1513182
H	97	TYR	-	INSERTION	GB 1513182
H	98	GLY	-	INSERTION	GB 1513182
H	99	TYR	SER	CONFLICT	GB 1513182
H	101	TYR	-	INSERTION	GB 1513182
H	103	ASP	ALA	CONFLICT	GB 1513182
H	104	VAL	TYR	CONFLICT	GB 1513182
H	110	THR	LEU	CONFLICT	GB 1513182
H	111	LEU	VAL	CONFLICT	GB 1513182
H	115	SER	ALA	CONFLICT	GB 1513182
H	120	ALA	PRO	CONFLICT	GB 1513182
H	129	VAL	GLY	CONFLICT	GB 1513182
H	?	-	ALA	DELETION	GB 1513182
H	?	-	ALA	DELETION	GB 1513182
H	?	-	GLN	DELETION	GB 1513182
H	?	-	THR	DELETION	GB 1513182
H	?	-	ASN	DELETION	GB 1513182
H	?	-	MET	DELETION	GB 1513182
H	148	LEU	VAL	CONFLICT	GB 1513182
H	180	THR	PRO	CONFLICT	GB 1513182
H	187	GLN	GLU	CONFLICT	GB 1513182

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	188	SER	THR	CONFLICT	GB 1513182
H	189	ILE	VAL	CONFLICT	GB 1513182
H	207	GLU	VAL	CONFLICT	GB 1513182

- Molecule 4 is water.

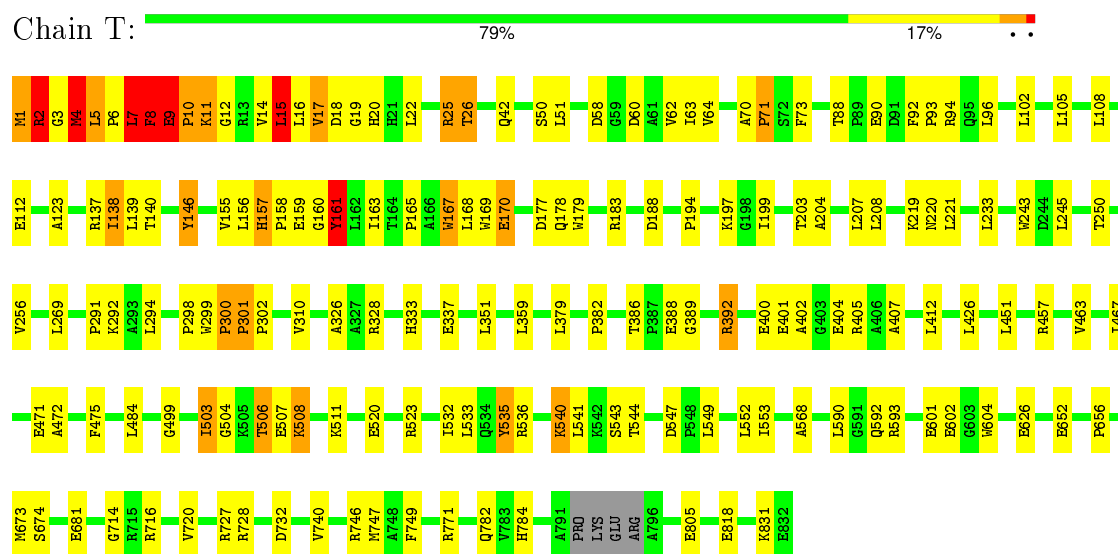
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	57	Total 57	O 57	0	0
4	L	71	Total 71	O 71	0	0
4	T	134	Total 134	O 134	0	0

3 Residue-property plots

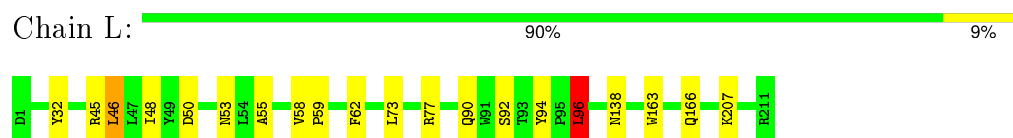
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

Note EDS was not executed.

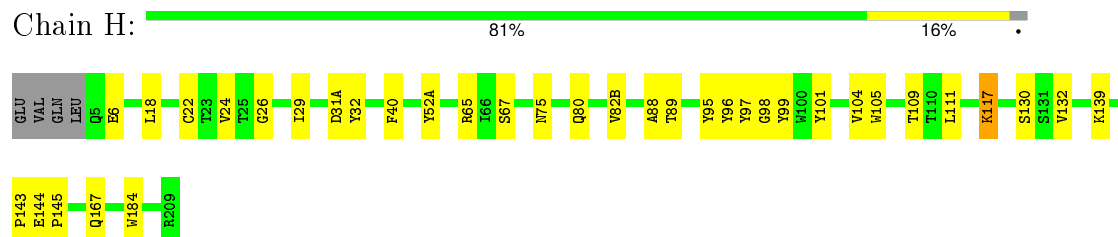
• Molecule 1: TAQ DNA POLYMERASE



• Molecule 2: TP7 MAB



• Molecule 3: TP7 MAB



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	76.60Å 89.10Å 89.30Å 100.70° 115.30° 95.30°	Depositor
Resolution (Å)	8.00 – 2.30	Depositor
% Data completeness (in resolution range)	82.0 (8.00-2.30)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.189 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10077	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	T	0.55	0/6712	0.73	8/9086 (0.1%)
2	L	0.54	0/1651	0.71	1/2245 (0.0%)
3	H	0.59	0/1682	0.77	3/2308 (0.1%)
All	All	0.55	0/10045	0.73	12/13639 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	2	ARG	NE-CZ-NH2	7.46	124.03	120.30
3	H	144	GLU	C-N-CD	-6.79	105.65	120.60
1	T	4	MET	CG-SD-CE	6.16	110.06	100.20
1	T	1	MET	CG-SD-CE	6.12	109.99	100.20
1	T	168	LEU	CA-CB-CG	6.10	129.33	115.30
1	T	300	PRO	C-N-CD	-6.07	107.24	120.60
1	T	15	LEU	CA-CB-CG	6.05	129.22	115.30
3	H	184	TRP	C-N-CD	-6.02	107.36	120.60
2	L	96	LEU	CA-CB-CG	5.97	129.04	115.30
1	T	161	TYR	N-CA-C	5.87	126.85	111.00
1	T	359	LEU	CA-CB-CG	5.73	128.47	115.30
3	H	98	GLY	N-CA-C	-5.62	99.05	113.10

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	T	6570	0	6640	143	1
2	L	1613	0	1535	9	0
3	H	1632	0	1568	6	0
4	H	57	0	0	1	0
4	L	71	0	0	0	0
4	T	134	0	0	1	0
All	All	10077	0	9743	156	1

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 8.

All (156) 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:T:9:GLU:HG3	1:T:63:ILE:C	1.18	1.50
1:T:392:ARG:NH1	1:T:392:ARG:HB2	1.37	1.39
1:T:3:GLY:HA2	1:T:159:GLU:OE1	1.24	1.36
1:T:392:ARG:CB	1:T:392:ARG:HH11	1.41	1.31
1:T:9:GLU:CG	1:T:63:ILE:C	1.99	1.28
1:T:3:GLY:CA	1:T:159:GLU:OE1	1.86	1.22
1:T:9:GLU:CG	1:T:63:ILE:O	1.88	1.18
1:T:9:GLU:HG3	1:T:63:ILE:O	1.43	1.11
1:T:5:LEU:O	1:T:159:GLU:OE2	1.68	1.10
1:T:4:MET:CG	1:T:159:GLU:HB3	1.85	1.07
1:T:9:GLU:HA	1:T:9:GLU:OE1	1.49	1.06
1:T:9:GLU:HG2	1:T:64:VAL:HA	1.14	1.06
1:T:8:PHE:HA	1:T:17:VAL:HB	1.09	1.04
1:T:4:MET:HG3	1:T:159:GLU:HB3	1.38	1.04
1:T:389:GLY:CA	1:T:392:ARG:HH22	1.71	1.02
1:T:9:GLU:HG2	1:T:64:VAL:CA	1.91	1.00
1:T:389:GLY:HA2	1:T:392:ARG:HH22	1.27	0.95
1:T:8:PHE:O	1:T:8:PHE:HD1	1.50	0.93
2:L:46:LEU:HD13	2:L:46:LEU:C	1.89	0.92
1:T:1:MET:O	1:T:2:ARG:O	1.88	0.90
1:T:9:GLU:CG	1:T:64:VAL:N	2.36	0.87
1:T:389:GLY:N	1:T:392:ARG:NH2	2.23	0.86
1:T:9:GLU:CG	1:T:64:VAL:HA	2.04	0.86
1:T:389:GLY:HA2	1:T:392:ARG:NH2	1.92	0.84
1:T:4:MET:CG	1:T:159:GLU:CB	2.54	0.84
1:T:4:MET:O	1:T:5:LEU:HD23	1.78	0.84
1:T:9:GLU:HB3	1:T:62:VAL:CG1	2.08	0.83
1:T:4:MET:HG2	1:T:159:GLU:CB	2.09	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:8:PHE:CA	1:T:17:VAL:HB	2.03	0.83
1:T:9:GLU:HG3	1:T:64:VAL:N	1.94	0.83
1:T:9:GLU:HG3	1:T:63:ILE:CA	2.09	0.82
1:T:6:PRO:O	1:T:7:LEU:HD23	1.81	0.81
1:T:7:LEU:CD1	1:T:51:LEU:HD13	2.10	0.81
1:T:10:PRO:HB3	1:T:16:LEU:HG	1.65	0.79
1:T:4:MET:HG2	1:T:159:GLU:HB3	1.62	0.78
1:T:8:PHE:HD2	1:T:19:GLY:HA3	1.48	0.78
1:T:4:MET:N	1:T:159:GLU:OE1	2.16	0.78
2:L:46:LEU:O	2:L:46:LEU:HD13	1.83	0.78
1:T:389:GLY:CA	1:T:392:ARG:NH2	2.43	0.77
1:T:4:MET:HG3	1:T:159:GLU:CB	2.15	0.76
1:T:471:GLU:HG3	1:T:535:TYR:OH	1.84	0.76
1:T:4:MET:H	1:T:159:GLU:CD	1.88	0.76
1:T:9:GLU:HB3	1:T:62:VAL:HG13	1.70	0.73
1:T:389:GLY:HA2	1:T:392:ARG:HH12	1.54	0.72
1:T:8:PHE:O	1:T:9:GLU:HB2	1.86	0.72
2:L:46:LEU:CD1	2:L:46:LEU:C	2.55	0.71
1:T:7:LEU:HD12	1:T:51:LEU:HD13	1.72	0.71
1:T:9:GLU:CB	1:T:63:ILE:O	2.38	0.70
1:T:389:GLY:N	1:T:392:ARG:HH22	1.86	0.70
1:T:9:GLU:HG2	1:T:63:ILE:O	1.87	0.70
1:T:388:GLU:C	1:T:392:ARG:NH2	2.45	0.69
1:T:7:LEU:HD11	1:T:51:LEU:HD13	1.74	0.68
1:T:8:PHE:C	1:T:8:PHE:HD1	1.97	0.68
1:T:4:MET:SD	1:T:159:GLU:C	2.73	0.67
1:T:9:GLU:CG	1:T:64:VAL:CA	2.66	0.67
1:T:4:MET:SD	1:T:160:GLY:HA3	2.35	0.66
1:T:3:GLY:HA2	1:T:157:HIS:CD2	2.31	0.66
1:T:10:PRO:HA	1:T:15:LEU:O	1.96	0.66
1:T:9:GLU:HB3	1:T:62:VAL:HG12	1.77	0.65
1:T:8:PHE:C	1:T:8:PHE:CD1	2.69	0.65
1:T:389:GLY:HA2	1:T:392:ARG:NH1	2.11	0.65
1:T:8:PHE:CD1	1:T:8:PHE:O	2.42	0.65
1:T:2:ARG:HH22	1:T:138:ILE:HG13	1.61	0.64
1:T:4:MET:HG2	1:T:159:GLU:HB2	1.79	0.63
1:T:388:GLU:O	1:T:392:ARG:CZ	2.47	0.62
1:T:9:GLU:OE1	1:T:9:GLU:CA	2.36	0.62
1:T:392:ARG:HH11	1:T:392:ARG:HB2	0.54	0.62
1:T:3:GLY:N	1:T:157:HIS:HD2	1.98	0.61
2:L:46:LEU:O	2:L:46:LEU:CD1	2.48	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:3:GLY:C	1:T:159:GLU:OE1	2.40	0.60
1:T:389:GLY:HA2	1:T:392:ARG:CZ	2.32	0.60
1:T:7:LEU:HD23	1:T:50:SER:HB3	1.85	0.59
1:T:392:ARG:HH11	1:T:392:ARG:CG	2.15	0.58
1:T:63:ILE:HG22	1:T:64:VAL:H	1.69	0.58
1:T:299:TRP:N	1:T:300:PRO:HD2	2.18	0.58
1:T:14:VAL:HG12	1:T:15:LEU:H	1.68	0.57
1:T:4:MET:SD	1:T:159:GLU:O	2.63	0.57
1:T:9:GLU:O	1:T:62:VAL:HG13	2.04	0.56
1:T:5:LEU:C	1:T:159:GLU:OE2	2.41	0.56
1:T:382:PRO:HB2	1:T:728:ARG:HH21	1.71	0.56
1:T:4:MET:SD	1:T:160:GLY:CA	2.94	0.55
1:T:451:LEU:HD13	1:T:549:LEU:HB3	1.86	0.55
1:T:388:GLU:C	1:T:392:ARG:CZ	2.75	0.55
2:L:46:LEU:HD21	2:L:55:ALA:HB1	1.89	0.55
1:T:379:LEU:HB3	1:T:426:LEU:HD22	1.90	0.54
1:T:9:GLU:HG2	1:T:64:VAL:N	2.11	0.54
1:T:183:ARG:HB3	1:T:245:LEU:HD13	1.89	0.54
1:T:3:GLY:CA	1:T:157:HIS:HD2	2.21	0.53
1:T:310:VAL:HG22	1:T:405:ARG:HH21	1.73	0.53
1:T:6:PRO:O	1:T:7:LEU:CD2	2.54	0.52
1:T:15:LEU:HD12	1:T:137:ARG:NH2	2.25	0.51
1:T:3:GLY:CA	1:T:157:HIS:CD2	2.93	0.51
1:T:9:GLU:OE2	1:T:63:ILE:HB	2.11	0.51
1:T:7:LEU:CD2	1:T:50:SER:HB3	2.40	0.51
1:T:7:LEU:O	1:T:8:PHE:HB3	2.10	0.51
1:T:5:LEU:O	1:T:159:GLU:HG2	2.10	0.51
1:T:70:ALA:HB3	1:T:71:PRO:HD3	1.92	0.51
1:T:463:VAL:O	1:T:467:ILE:HG13	2.10	0.51
1:T:747:MET:HA	1:T:747:MET:HE2	1.91	0.51
1:T:163:ILE:HG23	1:T:167:TRP:HB3	1.91	0.51
1:T:2:ARG:N	1:T:716:ARG:HB2	2.26	0.50
1:T:102:LEU:HD12	1:T:105:LEU:HD12	1.93	0.49
1:T:732:ASP:OD1	1:T:740:VAL:HG12	2.12	0.49
1:T:25:ARG:HD2	1:T:716:ARG:HH22	1.79	0.48
1:T:506:THR:HG23	3:H:26:GLY:HA3	1.96	0.48
1:T:392:ARG:NH1	1:T:392:ARG:CG	2.75	0.47
1:T:157:HIS:ND1	1:T:158:PRO:HD2	2.29	0.47
1:T:5:LEU:O	1:T:159:GLU:CD	2.47	0.47
1:T:4:MET:SD	1:T:160:GLY:N	2.88	0.46
1:T:5:LEU:H	1:T:159:GLU:CD	2.18	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:25:ARG:HH11	1:T:716:ARG:NH2	2.13	0.46
3:H:67:SER:HB2	3:H:80:GLN:HB3	1.98	0.46
1:T:2:ARG:HG2	1:T:140:THR:O	2.15	0.46
1:T:8:PHE:CD2	1:T:19:GLY:HA3	2.39	0.46
1:T:732:ASP:OD1	1:T:740:VAL:CG1	2.64	0.46
1:T:92:PHE:H	1:T:93:PRO:HD2	1.81	0.46
1:T:590:LEU:HD23	1:T:593:ARG:HH21	1.80	0.46
1:T:523:ARG:HH21	1:T:533:LEU:HB3	1.81	0.45
1:T:11:LYS:HD2	1:T:12:GLY:H	1.81	0.45
1:T:9:GLU:CB	1:T:62:VAL:CG1	2.89	0.45
1:T:351:LEU:HD11	1:T:412:LEU:HD12	1.98	0.45
3:H:117:LYS:HB2	4:H:219:HOH:O	2.16	0.45
1:T:673:MET:HG2	1:T:674:SER:H	1.81	0.45
1:T:14:VAL:HG22	1:T:60:ASP:H	1.82	0.44
1:T:451:LEU:HD22	1:T:549:LEU:HD23	1.98	0.44
1:T:1:MET:C	1:T:2:ARG:O	2.53	0.44
1:T:17:VAL:HG12	1:T:18:ASP:H	1.82	0.44
1:T:503:ILE:HD12	1:T:504:GLY:H	1.83	0.44
3:H:18:LEU:HD11	3:H:111:LEU:HD21	1.99	0.44
1:T:25:ARG:HH11	1:T:716:ARG:HH22	1.66	0.44
3:H:65:ARG:HH21	3:H:82(B):VAL:HA	1.83	0.44
2:L:48:ILE:HD12	2:L:73:LEU:HD13	2.00	0.43
3:H:24:VAL:HG13	3:H:75:ASN:ND2	2.33	0.43
1:T:292:LYS:HE2	1:T:404:GLU:HB3	2.01	0.43
1:T:16:LEU:HB3	1:T:137:ARG:O	2.19	0.43
1:T:310:VAL:HG23	1:T:402:ALA:HB2	2.02	0.42
1:T:294:LEU:HD22	1:T:407:ALA:HB1	2.00	0.42
1:T:508:LYS:HD3	1:T:508:LYS:H	1.85	0.42
1:T:62:VAL:HB	1:T:108:LEU:HD22	2.01	0.42
1:T:326:ALA:HB3	1:T:333:HIS:HB2	2.02	0.42
1:T:472:ALA:HB1	4:T:889:HOH:O	2.20	0.42
1:T:2:ARG:NE	1:T:155:VAL:HG13	2.34	0.42
1:T:388:GLU:O	1:T:392:ARG:NH1	2.53	0.41
1:T:92:PHE:N	1:T:93:PRO:HD2	2.35	0.41
1:T:3:GLY:HA3	1:T:159:GLU:OE1	2.03	0.41
1:T:96:LEU:H	1:T:96:LEU:HD12	1.85	0.41
1:T:123:ALA:HB1	1:T:250:THR:HG22	2.02	0.41
1:T:5:LEU:O	1:T:159:GLU:CG	2.69	0.41
1:T:601:GLU:HG3	1:T:602:GLU:H	1.86	0.41
1:T:22:LEU:HD23	1:T:22:LEU:HA	1.95	0.41
1:T:484:LEU:H	2:L:59:PRO:HD3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:540:LYS:HA	1:T:544:THR:H	1.86	0.41
1:T:62:VAL:HG12	1:T:63:ILE:O	2.21	0.40
2:L:46:LEU:CD2	2:L:55:ALA:CB	2.98	0.40
1:T:6:PRO:HG3	1:T:26:THR:OG1	2.22	0.40
2:L:48:ILE:HD11	2:L:62:PHE:HB3	2.02	0.40

All (1) 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:T:177:ASP:OD2	1:T:604:TRP:NE1[1_655]	1.68	0.52

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	T	824/832 (99%)	695 (84%)	95 (12%)	34 (4%)	3	1
2	L	208/210 (99%)	181 (87%)	21 (10%)	6 (3%)	6	3
3	H	207/213 (97%)	179 (86%)	15 (7%)	13 (6%)	2	0
All	All	1239/1255 (99%)	1055 (85%)	131 (11%)	53 (4%)	3	1

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	T	2	ARG
1	T	7	LEU
1	T	9	GLU
1	T	11	LYS
1	T	58	ASP
1	T	139	LEU
1	T	161	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	301	PRO
1	T	302	PRO
1	T	568	ALA
2	L	32	TYR
3	H	89	THR
3	H	97	TYR
3	H	109	THR
1	T	203	THR
1	T	208	LEU
1	T	256	VAL
2	L	58	VAL
2	L	96	LEU
1	T	4	MET
1	T	71	PRO
1	T	146	TYR
1	T	204	ALA
1	T	298	PRO
1	T	541	LEU
1	T	784	HIS
2	L	138	ASN
3	H	88	ALA
1	T	8	PHE
1	T	10	PRO
1	T	219	LYS
1	T	291	PRO
1	T	543	SER
1	T	714	GLY
2	L	50	ASP
2	L	92	SER
3	H	130	SER
3	H	143	PRO
3	H	145	PRO
1	T	138	ILE
1	T	170	GLU
1	T	221	LEU
3	H	32	TYR
3	H	104	VAL
3	H	132	VAL
1	T	194	PRO
1	T	197	LYS
1	T	199	ILE
1	T	499	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	831	LYS
3	H	105	TRP
3	H	29	ILE
3	H	40	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	T	672/683 (98%)	605 (90%)	67 (10%)	9	11
2	L	184/185 (100%)	174 (95%)	10 (5%)	27	36
3	H	187/191 (98%)	176 (94%)	11 (6%)	24	32
All	All	1043/1059 (98%)	955 (92%)	88 (8%)	14	16

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	T	2	ARG
1	T	5	LEU
1	T	7	LEU
1	T	8	PHE
1	T	9	GLU
1	T	15	LEU
1	T	17	VAL
1	T	20	HIS
1	T	25	ARG
1	T	26	THR
1	T	42	GLN
1	T	73	PHE
1	T	88	THR
1	T	90	GLU
1	T	94	ARG
1	T	112	GLU
1	T	146	TYR
1	T	156	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	157	HIS
1	T	161	TYR
1	T	165	PRO
1	T	167	TRP
1	T	169	TRP
1	T	170	GLU
1	T	178	GLN
1	T	179	TRP
1	T	188	ASP
1	T	207	LEU
1	T	220	ASN
1	T	233	LEU
1	T	243	TRP
1	T	269	LEU
1	T	301	PRO
1	T	328	ARG
1	T	337	GLU
1	T	386	THR
1	T	392	ARG
1	T	400	GLU
1	T	401	GLU
1	T	457	ARG
1	T	475	PHE
1	T	503	ILE
1	T	506	THR
1	T	507	GLU
1	T	508	LYS
1	T	511	LYS
1	T	520	GLU
1	T	532	ILE
1	T	535	TYR
1	T	536	ARG
1	T	540	LYS
1	T	547	ASP
1	T	552	LEU
1	T	553	ILE
1	T	592	GLN
1	T	626	GLU
1	T	652	GLU
1	T	656	PRO
1	T	681	GLU
1	T	720	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	T	727	ARG
1	T	746	ARG
1	T	749	PHE
1	T	771	ARG
1	T	782	GLN
1	T	805	GLU
1	T	818	GLU
2	L	45	ARG
2	L	46	LEU
2	L	53	ASN
2	L	77	ARG
2	L	90	GLN
2	L	94	TYR
2	L	96	LEU
2	L	163	TRP
2	L	166	GLN
2	L	207	LYS
3	H	6	GLU
3	H	22	CYS
3	H	31(A)	ASP
3	H	52(A)	TYR
3	H	95	TYR
3	H	96	TYR
3	H	99	TYR
3	H	101	TYR
3	H	117	LYS
3	H	139	LYS
3	H	167	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	T	157	HIS
1	T	384	ASN
1	T	690	GLN
1	T	782	GLN
2	L	53	ASN
2	L	90	GLN
2	L	190	ASN
3	H	16	GLN
3	H	39	GLN
3	H	192	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.