



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:10 PM UTC

PDB ID : 1QZQ / pdb_00001qzq
Title : human Tyrosyl DNA phosphodiesterase
Authors : Raymond, A.C.; Rideout, M.C.; Staker, B.; Hjerrild, K.; Burgin Jr., A.B.
Deposited on : 2003-09-17
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

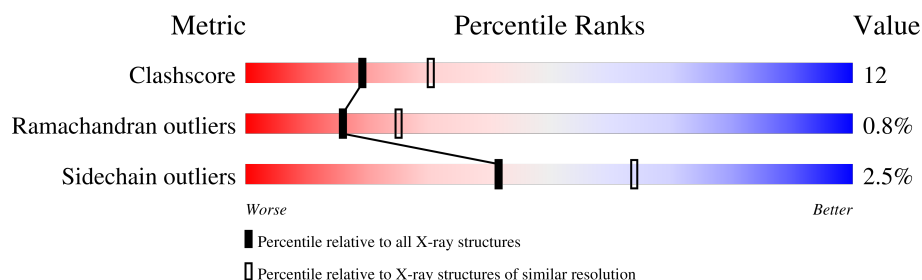
1 Overall quality at a glance

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)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	483	 67% 21% .. 9%
1	B	483	 65% 23% • 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7250 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 tyrosyl-DNA phosphodiesterase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	439	Total	C	N	O	S	0	0	0
			3517	2282	593	630	12			
1	B	437	Total	C	N	O	S	0	0	0
			3495	2270	589	623	13			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	MET	-	cloning artifact	UNP Q9NUW8
A	127	GLU	-	cloning artifact	UNP Q9NUW8
A	128	GLU	-	cloning artifact	UNP Q9NUW8
A	129	TYR	-	cloning artifact	UNP Q9NUW8
A	130	MET	-	cloning artifact	UNP Q9NUW8
A	131	PRO	-	cloning artifact	UNP Q9NUW8
A	132	THR	-	cloning artifact	UNP Q9NUW8
A	133	GLU	-	cloning artifact	UNP Q9NUW8
A	134	HIS	-	expression tag	UNP Q9NUW8
A	135	HIS	-	expression tag	UNP Q9NUW8
A	136	HIS	-	expression tag	UNP Q9NUW8
A	137	HIS	-	expression tag	UNP Q9NUW8
A	138	HIS	-	expression tag	UNP Q9NUW8
A	139	HIS	-	expression tag	UNP Q9NUW8
A	140	GLU	-	cloning artifact	UNP Q9NUW8
A	141	ASN	-	cloning artifact	UNP Q9NUW8
A	142	LEU	-	cloning artifact	UNP Q9NUW8
A	143	TYR	-	cloning artifact	UNP Q9NUW8
A	144	PHE	-	cloning artifact	UNP Q9NUW8
A	145	GLN	-	cloning artifact	UNP Q9NUW8
A	146	GLY	-	cloning artifact	UNP Q9NUW8
A	147	THR	-	cloning artifact	UNP Q9NUW8
A	148	SER	-	cloning artifact	UNP Q9NUW8
B	126	MET	-	cloning artifact	UNP Q9NUW8
B	127	GLU	-	cloning artifact	UNP Q9NUW8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	128	GLU	-	cloning artifact	UNP Q9NUW8
B	129	TYR	-	cloning artifact	UNP Q9NUW8
B	130	MET	-	cloning artifact	UNP Q9NUW8
B	131	PRO	-	cloning artifact	UNP Q9NUW8
B	132	THR	-	cloning artifact	UNP Q9NUW8
B	133	GLU	-	cloning artifact	UNP Q9NUW8
B	134	HIS	-	expression tag	UNP Q9NUW8
B	135	HIS	-	expression tag	UNP Q9NUW8
B	136	HIS	-	expression tag	UNP Q9NUW8
B	137	HIS	-	expression tag	UNP Q9NUW8
B	138	HIS	-	expression tag	UNP Q9NUW8
B	139	HIS	-	expression tag	UNP Q9NUW8
B	140	GLU	-	cloning artifact	UNP Q9NUW8
B	141	ASN	-	cloning artifact	UNP Q9NUW8
B	142	LEU	-	cloning artifact	UNP Q9NUW8
B	143	TYR	-	cloning artifact	UNP Q9NUW8
B	144	PHE	-	cloning artifact	UNP Q9NUW8
B	145	GLN	-	cloning artifact	UNP Q9NUW8
B	146	GLY	-	cloning artifact	UNP Q9NUW8
B	147	THR	-	cloning artifact	UNP Q9NUW8
B	148	SER	-	cloning artifact	UNP Q9NUW8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	138	Total	O	0	0
			138	138		
2	B	100	Total	O	0	0
			100	100		

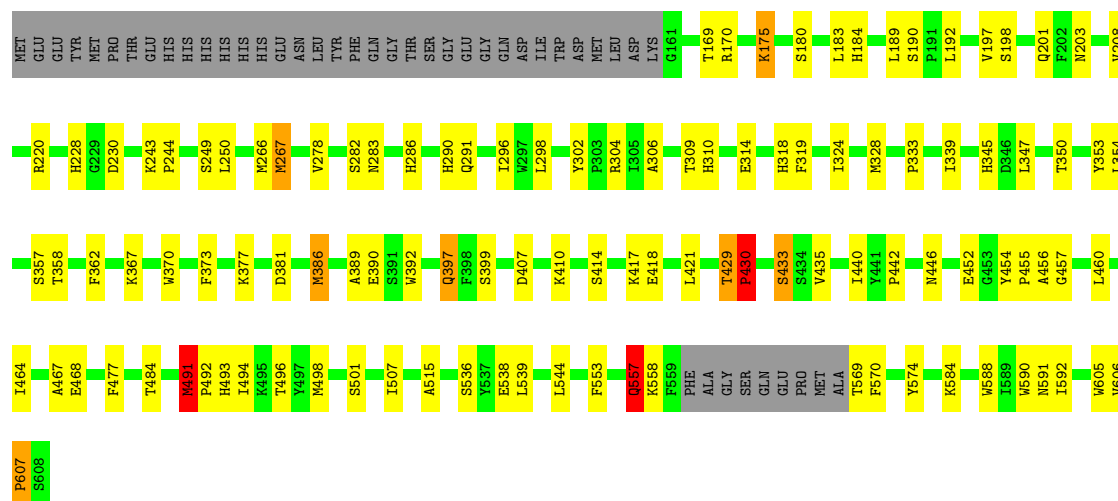
3 Residue-property plots

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. 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. 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.

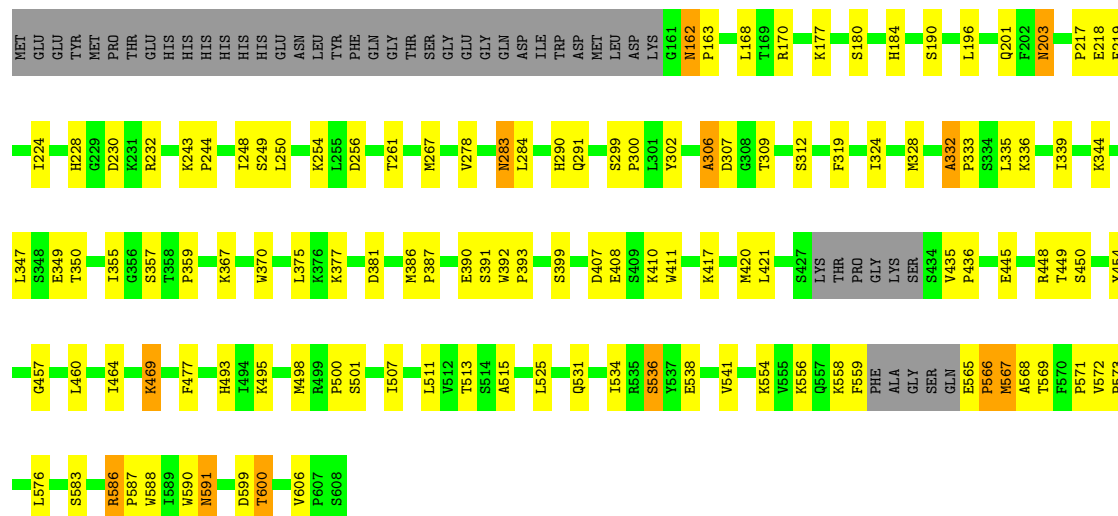
- Molecule 1: tyrosyl-DNA phosphodiesterase 1

Chain A: 



- Molecule 1: tyrosyl-DNA phosphodiesterase 1

Chain B: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.02Å 105.13Å 194.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.54 – 2.40	Depositor
% Data completeness (in resolution range)	99.4 (48.54-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	CNX 2002	Depositor
R, R_{free}	0.185 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7250	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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	A	0.58	2/3633 (0.1%)	1.08	23/4934 (0.5%)
1	B	0.52	0/3610	1.04	23/4904 (0.5%)
All	All	0.55	2/7243 (0.0%)	1.06	46/9838 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	491	MET	SD-CE	-6.88	1.62	1.79
1	A	267	MET	SD-CE	-5.75	1.65	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	SER	N-CA-C	8.49	119.46	108.34
1	A	606	VAL	CA-C-N	8.45	130.40	119.84
1	A	606	VAL	C-N-CA	8.45	130.40	119.84
1	A	208	VAL	N-CA-C	8.38	118.47	110.42
1	A	515	ALA	N-CA-C	8.21	120.98	109.15
1	A	590	TRP	N-CA-C	7.75	120.62	111.71
1	A	197	VAL	N-CA-C	-7.68	105.68	111.90
1	A	433	SER	N-CA-C	7.54	120.95	108.96
1	B	493	HIS	N-CA-C	-7.51	103.68	114.12
1	A	493	HIS	N-CA-C	-7.11	104.24	114.12
1	B	312	SER	N-CA-C	-6.63	99.72	110.20
1	B	572	VAL	CA-C-N	6.39	126.07	119.56
1	B	572	VAL	C-N-CA	6.39	126.07	119.56
1	B	590	TRP	N-CA-C	6.35	120.29	112.54
1	A	536	SER	N-CA-C	6.24	119.31	110.14
1	B	606	VAL	CA-C-N	6.15	126.17	119.89
1	B	606	VAL	C-N-CA	6.15	126.17	119.89
1	B	283	ASN	N-CA-C	-6.04	102.56	110.53
1	A	494	ILE	N-CA-C	-6.00	103.52	110.05
1	A	370	TRP	N-CA-C	5.90	117.17	108.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	190	SER	CA-C-N	5.82	126.22	119.47
1	A	190	SER	C-N-CA	5.82	126.22	119.47
1	A	591	ASN	N-CA-C	5.78	120.72	111.81
1	B	180	SER	N-CA-C	-5.75	100.46	109.25
1	A	220	ARG	N-CA-C	5.69	119.84	113.01
1	B	299	SER	CA-C-N	-5.65	114.94	120.98
1	B	299	SER	C-N-CA	-5.65	114.94	120.98
1	B	515	ALA	N-CA-C	5.62	117.85	109.59
1	A	557	GLN	N-CA-C	5.56	118.67	109.94
1	B	190	SER	CA-C-N	5.54	125.16	119.56
1	B	190	SER	C-N-CA	5.54	125.16	119.56
1	B	332	ALA	CA-C-N	5.53	125.00	119.24
1	B	332	ALA	C-N-CA	5.53	125.00	119.24
1	A	477	PHE	N-CA-C	5.52	118.45	110.28
1	A	435	VAL	N-CA-C	5.43	114.93	108.96
1	B	591	ASN	N-CA-C	5.37	118.64	112.57
1	B	370	TRP	N-CA-C	5.30	117.03	109.14
1	A	362	PHE	N-CA-C	5.29	117.58	109.07
1	A	282	SER	N-CA-C	5.25	118.78	109.96
1	A	467	ALA	N-CA-C	5.10	116.53	111.07
1	B	460	LEU	CA-C-N	5.08	126.19	119.84
1	B	460	LEU	C-N-CA	5.08	126.19	119.84
1	A	286	HIS	N-CA-C	5.08	117.20	111.11
1	B	477	PHE	N-CA-C	5.04	117.75	110.28
1	B	336	LYS	N-CA-C	-5.02	105.94	111.71
1	A	570	PHE	N-CA-C	5.00	115.96	109.65

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	3517	0	3463	80	0
1	B	3495	0	3430	82	0
2	A	138	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	100	0	0	0	0
All	All	7250	0	6893	162	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 12.

All (162) 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:A:201:GLN:HE22	1:A:267:MET:HE3	1.18	1.02
1:A:442:PRO:HB3	1:A:491:MET:HE2	1.40	1.01
1:A:386:MET:HE2	1:A:389:ALA:HA	1.43	1.00
1:A:557:GLN:HE21	1:A:558:LYS:H	1.08	0.92
1:A:201:GLN:HE22	1:A:267:MET:CE	1.83	0.91
1:B:261:THR:H	1:B:536:SER:HB3	1.41	0.85
1:B:261:THR:O	1:B:536:SER:HB2	1.77	0.84
1:A:386:MET:HE2	1:A:389:ALA:CA	2.10	0.81
1:B:450:SER:O	1:B:600:THR:HG21	1.81	0.80
1:B:228:HIS:HD2	1:B:230:ASP:H	1.28	0.79
1:B:162:ASN:HD22	1:B:162:ASN:N	1.82	0.78
1:A:442:PRO:HB3	1:A:491:MET:CE	2.15	0.75
1:A:306:ALA:HB3	1:A:309:THR:OG1	1.87	0.74
1:A:446:ASN:HB3	1:A:491:MET:HE1	1.68	0.74
1:A:414:SER:O	1:A:418:GLU:HG2	1.88	0.73
1:B:196:LEU:HD23	1:B:219:PHE:HB3	1.70	0.73
1:A:417:LYS:O	1:A:421:LEU:HG	1.90	0.71
1:A:429:THR:H	1:A:430:PRO:CD	2.02	0.71
1:A:386:MET:HE3	1:A:392:TRP:CG	2.26	0.71
1:B:243:LYS:HB3	1:B:244:PRO:HD3	1.73	0.70
1:A:228:HIS:HD2	1:A:230:ASP:H	1.39	0.70
1:B:162:ASN:HD22	1:B:162:ASN:H	1.38	0.70
1:A:201:GLN:NE2	1:A:267:MET:HE3	2.01	0.68
1:A:557:GLN:HE21	1:A:558:LYS:N	1.89	0.68
1:B:386:MET:HB2	1:B:387:PRO:HD2	1.76	0.68
1:B:203:ASN:OD1	1:B:283:ASN:HA	1.93	0.67
1:B:559:PHE:CE1	1:B:571:PRO:HB2	2.30	0.67
1:A:386:MET:HE3	1:A:392:TRP:CD1	2.30	0.66
1:A:390:GLU:HB2	1:A:433:SER:HA	1.78	0.66
1:A:386:MET:HE2	1:A:389:ALA:CB	2.25	0.66
1:A:464:ILE:O	1:A:468:GLU:HG2	1.97	0.65
1:A:386:MET:CE	1:A:389:ALA:HA	2.25	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:THR:HA	1:B:600:THR:HG22	1.80	0.63
1:A:407:ASP:OD1	1:A:410:LYS:HE2	2.00	0.62
1:B:375:LEU:CD2	1:B:420:MET:HE2	2.30	0.62
1:B:170:ARG:HD3	1:B:184:HIS:HB2	1.83	0.61
1:A:201:GLN:OE1	1:A:267:MET:HG2	2.00	0.61
1:B:163:PRO:HG3	1:B:567:MET:HA	1.80	0.61
1:A:429:THR:H	1:A:430:PRO:HD2	1.64	0.61
1:A:484:THR:HA	1:A:558:LYS:HB2	1.82	0.61
1:A:249:SER:C	1:A:250:LEU:HD12	2.26	0.60
1:A:189:LEU:HD21	1:A:267:MET:HE1	1.83	0.60
1:A:189:LEU:HD21	1:A:267:MET:CE	2.31	0.60
1:A:397:GLN:HB3	1:A:440:ILE:HB	1.84	0.59
1:A:557:GLN:NE2	1:A:558:LYS:H	1.91	0.59
1:B:586:ARG:HG3	1:B:587:PRO:HD2	1.85	0.59
1:B:267:MET:HB2	1:B:278:VAL:HB	1.84	0.58
1:A:357:SER:HB2	1:A:538:GLU:HB2	1.86	0.58
1:B:565:GLU:O	1:B:569:THR:HG23	2.04	0.58
1:B:454:TYR:CD2	1:B:599:ASP:HB3	2.39	0.57
1:B:228:HIS:CD2	1:B:230:ASP:H	2.17	0.57
1:B:218:GLU:OE2	1:B:218:GLU:N	2.28	0.57
1:B:319:PHE:CG	1:B:350:THR:HG21	2.39	0.57
1:A:354:LEU:HD11	1:A:539:LEU:HD11	1.86	0.57
1:B:261:THR:O	1:B:536:SER:CB	2.52	0.56
1:A:491:MET:HE3	1:A:492:PRO:HD2	1.86	0.55
1:A:442:PRO:CB	1:A:491:MET:HE2	2.24	0.55
1:A:592:ILE:C	1:A:607:PRO:HG2	2.32	0.55
1:B:417:LYS:O	1:B:421:LEU:HG	2.06	0.55
1:A:429:THR:N	1:A:430:PRO:CD	2.67	0.54
1:B:357:SER:HB2	1:B:538:GLU:HB2	1.87	0.54
1:A:397:GLN:HG2	1:A:574:TYR:CE1	2.42	0.54
1:A:457:GLY:HA3	1:A:588:TRP:CZ2	2.42	0.54
1:B:307:ASP:OD1	1:B:344:LYS:HE2	2.07	0.54
1:A:198:SER:HB2	2:A:688:HOH:O	2.07	0.54
1:A:319:PHE:CG	1:A:350:THR:HG21	2.42	0.54
1:B:407:ASP:OD2	1:B:410:LYS:HG2	2.07	0.54
1:B:228:HIS:HD2	1:B:230:ASP:N	2.02	0.53
1:A:169:THR:HG22	1:A:296:ILE:HD11	1.91	0.53
1:A:397:GLN:CB	1:A:440:ILE:HB	2.38	0.52
1:B:218:GLU:H	1:B:218:GLU:CD	2.16	0.52
1:A:228:HIS:HD2	1:A:230:ASP:N	2.03	0.52
1:A:243:LYS:HB3	1:A:244:PRO:HD3	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:ASN:N	1:B:162:ASN:ND2	2.55	0.51
1:A:203:ASN:OD1	1:A:283:ASN:HA	2.11	0.51
1:A:304:ARG:HD3	1:A:345:HIS:CE1	2.46	0.51
1:B:464:ILE:HG22	1:B:591:ASN:HD21	1.76	0.51
1:B:498:MET:HE1	1:B:576:LEU:HD11	1.92	0.51
1:B:224:ILE:HB	1:B:248:ILE:HG12	1.92	0.51
1:B:500:PRO:HA	1:B:507:ILE:HG22	1.92	0.51
1:B:469:LYS:HB2	1:B:469:LYS:NZ	2.26	0.51
1:A:353:TYR:CE1	1:A:544:LEU:HD12	2.45	0.50
1:B:201:GLN:OE1	1:B:267:MET:HG2	2.13	0.49
1:B:249:SER:C	1:B:250:LEU:HD12	2.37	0.49
1:B:162:ASN:HB2	1:B:163:PRO:HD2	1.93	0.49
1:B:232:ARG:HB2	1:B:232:ARG:NH1	2.28	0.49
1:B:250:LEU:HD12	1:B:250:LEU:N	2.28	0.49
1:B:302:TYR:CD1	1:B:347:LEU:HA	2.48	0.48
1:B:168:LEU:HD21	1:B:573:PRO:HB3	1.95	0.48
1:B:261:THR:N	1:B:536:SER:HB3	2.20	0.48
1:B:300:PRO:HG3	1:B:349:GLU:HG2	1.94	0.48
1:B:399:SER:OG	1:B:495:LYS:HE3	2.14	0.48
1:A:367:LYS:HE2	1:A:373:PHE:CE2	2.48	0.47
1:A:397:GLN:HG3	1:A:496:THR:OG1	2.15	0.47
1:B:390:GLU:O	1:B:435:VAL:HG22	2.13	0.47
1:B:232:ARG:HB2	1:B:232:ARG:HH11	1.80	0.47
1:A:170:ARG:HD3	1:A:184:HIS:HB2	1.97	0.46
1:B:469:LYS:HB2	1:B:469:LYS:HZ2	1.80	0.46
1:A:309:THR:HG22	1:A:310:HIS:N	2.31	0.46
1:A:429:THR:N	1:A:430:PRO:HD2	2.30	0.46
1:B:464:ILE:HG22	1:B:591:ASN:ND2	2.31	0.46
1:B:392:TRP:CD2	1:B:501:SER:HA	2.51	0.46
1:A:421:LEU:HD12	1:A:421:LEU:C	2.40	0.45
1:B:359:PRO:HG3	1:B:536:SER:HA	1.97	0.45
1:A:392:TRP:CD2	1:A:501:SER:HA	2.52	0.45
1:A:507:ILE:HG12	1:A:553:PHE:HB2	1.98	0.45
1:A:290:HIS:CD2	1:A:291:GLN:HG3	2.52	0.45
1:B:498:MET:HE3	1:B:507:ILE:HG21	1.97	0.45
1:B:525:LEU:HA	1:B:531:GLN:O	2.17	0.44
1:A:228:HIS:CD2	1:A:230:ASP:H	2.28	0.44
1:A:175:LYS:HB3	1:A:175:LYS:NZ	2.33	0.44
1:B:168:LEU:HG	1:B:559:PHE:CZ	2.52	0.44
1:B:203:ASN:ND2	1:B:284:LEU:HG	2.33	0.44
1:B:290:HIS:CD2	1:B:291:GLN:HG3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:GLU:OE2	1:B:448:ARG:NH2	2.50	0.44
1:A:169:THR:HA	1:A:183:LEU:O	2.18	0.44
1:A:302:TYR:CD1	1:A:347:LEU:HA	2.52	0.44
1:B:306:ALA:O	1:B:309:THR:HB	2.17	0.44
1:B:359:PRO:HA	1:B:534:ILE:O	2.17	0.43
1:B:556:LYS:C	1:B:558:LYS:H	2.26	0.43
1:A:454:TYR:N	1:A:455:PRO:CD	2.82	0.43
1:B:498:MET:HE3	1:B:507:ILE:CG2	2.48	0.43
1:B:435:VAL:HA	1:B:436:PRO:HD3	1.91	0.43
1:B:554:LYS:O	1:B:569:THR:HA	2.18	0.43
1:A:452:GLU:HB2	1:A:456:ALA:HB2	2.00	0.43
1:A:377:LYS:HE2	1:A:381:ASP:OD2	2.19	0.43
1:A:454:TYR:HB3	1:A:605:TRP:CE3	2.53	0.43
1:B:254:LYS:HD2	1:B:256:ASP:OD1	2.19	0.43
1:B:391:SER:O	1:B:393:PRO:HD3	2.19	0.43
1:B:566:PRO:HG2	1:B:567:MET:H	1.84	0.43
1:B:328:MET:SD	1:B:339:ILE:HD13	2.58	0.43
1:B:344:LYS:HD2	1:B:344:LYS:HA	1.84	0.42
1:B:566:PRO:C	1:B:568:ALA:H	2.27	0.42
1:A:324:ILE:O	1:A:328:MET:HG2	2.18	0.42
1:A:333:PRO:HD2	2:A:629:HOH:O	2.18	0.42
1:A:175:LYS:H	1:A:175:LYS:HG2	1.55	0.42
1:B:457:GLY:HA3	1:B:588:TRP:CZ2	2.54	0.42
1:B:565:GLU:HG3	1:B:568:ALA:HB3	2.01	0.42
1:B:511:LEU:HD12	1:B:541:VAL:O	2.20	0.42
1:A:457:GLY:HA3	1:A:588:TRP:CE2	2.55	0.41
1:A:605:TRP:NE1	1:A:607:PRO:HG3	2.35	0.41
1:A:498:MET:HE3	1:A:507:ILE:HG21	2.02	0.41
1:A:192:LEU:HD12	1:A:192:LEU:N	2.35	0.41
1:A:250:LEU:HD12	1:A:250:LEU:N	2.36	0.41
1:A:192:LEU:HD12	1:A:192:LEU:H	1.84	0.41
1:A:180:SER:O	1:A:180:SER:OG	2.36	0.41
1:B:332:ALA:HA	1:B:333:PRO:HD3	1.88	0.41
1:A:314:GLU:OE2	1:A:318:HIS:HA	2.20	0.41
1:A:399:SER:HB2	1:A:460:LEU:HD23	2.03	0.41
1:B:377:LYS:HE2	1:B:381:ASP:OD2	2.20	0.41
1:B:335:LEU:HA	1:B:335:LEU:HD23	1.79	0.41
1:B:393:PRO:HB3	1:B:436:PRO:HB2	2.03	0.41
1:A:498:MET:HE3	1:A:507:ILE:CG2	2.51	0.41
1:A:266:MET:HA	1:A:278:VAL:O	2.21	0.41
1:B:495:LYS:HB2	1:B:513:THR:O	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:TYR:CD2	1:A:347:LEU:HG	2.56	0.41
1:B:324:ILE:HG23	1:B:339:ILE:HG23	2.03	0.41
1:B:565:GLU:O	1:B:565:GLU:HG3	2.20	0.41
1:B:583:SER:O	1:B:586:ARG:NH2	2.55	0.40
1:B:355:ILE:HD12	1:B:511:LEU:HD13	2.03	0.40
1:B:454:TYR:CE2	1:B:599:ASP:HB3	2.57	0.40
1:A:328:MET:SD	1:A:339:ILE:HD13	2.61	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/483 (90%)	416 (96%)	16 (4%)	3 (1%)	18	28
1	B	431/483 (89%)	409 (95%)	18 (4%)	4 (1%)	14	22
All	All	866/966 (90%)	825 (95%)	34 (4%)	7 (1%)	16	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	607	PRO
1	B	306	ALA
1	B	567	MET
1	A	430	PRO
1	A	429	THR
1	B	411	TRP
1	B	566	PRO

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	383/421 (91%)	373 (97%)	10 (3%)	40	63
1	B	378/421 (90%)	369 (98%)	9 (2%)	43	65
All	All	761/842 (90%)	742 (98%)	19 (2%)	42	64

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LYS
1	A	298	LEU
1	A	358	THR
1	A	386	MET
1	A	397	GLN
1	A	430	PRO
1	A	491	MET
1	A	557	GLN
1	A	569	THR
1	A	584	LYS
1	B	162	ASN
1	B	177	LYS
1	B	203	ASN
1	B	217	PRO
1	B	367	LYS
1	B	408	GLU
1	B	469	LYS
1	B	586	ARG
1	B	600	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	201	GLN
1	A	228	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	291	GLN
1	A	318	HIS
1	A	363	GLN
1	A	388	ASN
1	A	471	ASN
1	A	557	GLN
1	B	162	ASN
1	B	184	HIS
1	B	228	HIS
1	B	290	HIS
1	B	363	GLN
1	B	471	ASN
1	B	531	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.