



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 2J0F / pdb_00002j0f
Title : Structural basis for non-competitive product inhibition in human thymidine phosphorylase: implication for drug design
Authors : El Omari, K.; Bronckaers, A.; Liekens, S.; Perez-Perez, M.J.; Balzarini, J.; Stammers, D.K.
Deposited on : 2006-08-02
Resolution : 2.31 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
Mogul : 2022.3.0, CSD as543be (2022)
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

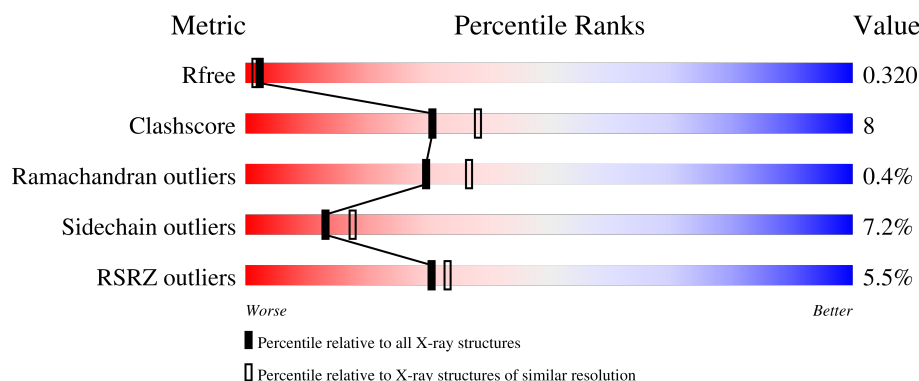
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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 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	482	2% 76% 14% 7%
1	B	482	5% 74% 16% 7%
1	C	482	4% 76% 14% 7%
1	D	482	9% 77% 14% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TDR	A	1480	-	X	-	-
2	TDR	B	1480	-	X	-	-
2	TDR	C	1480	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13513 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.

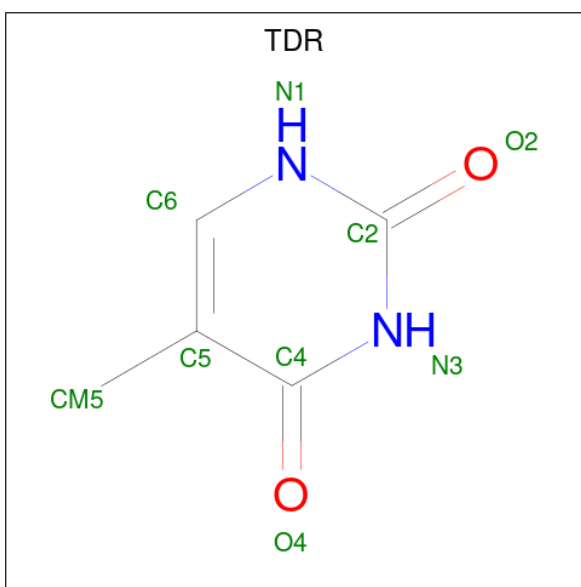
- Molecule 1 is a protein called THYMIDINE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	B	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	C	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	D	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ALA	GLY	conflict	UNP P19971
A	239	GLY	ALA	conflict	UNP P19971
A	471	LEU	SER	conflict	UNP P19971
B	238	ALA	GLY	conflict	UNP P19971
B	239	GLY	ALA	conflict	UNP P19971
B	471	LEU	SER	conflict	UNP P19971
C	238	ALA	GLY	conflict	UNP P19971
C	239	GLY	ALA	conflict	UNP P19971
C	471	LEU	SER	conflict	UNP P19971
D	238	ALA	GLY	conflict	UNP P19971
D	239	GLY	ALA	conflict	UNP P19971
D	471	LEU	SER	conflict	UNP P19971

- Molecule 2 is THYMINE (CCD ID: TDR) (formula: C₅H₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	5	2	2		
2	B	1	Total	C	N	O	0	0
			9	5	2	2		
2	C	1	Total	C	N	O	0	0
			9	5	2	2		

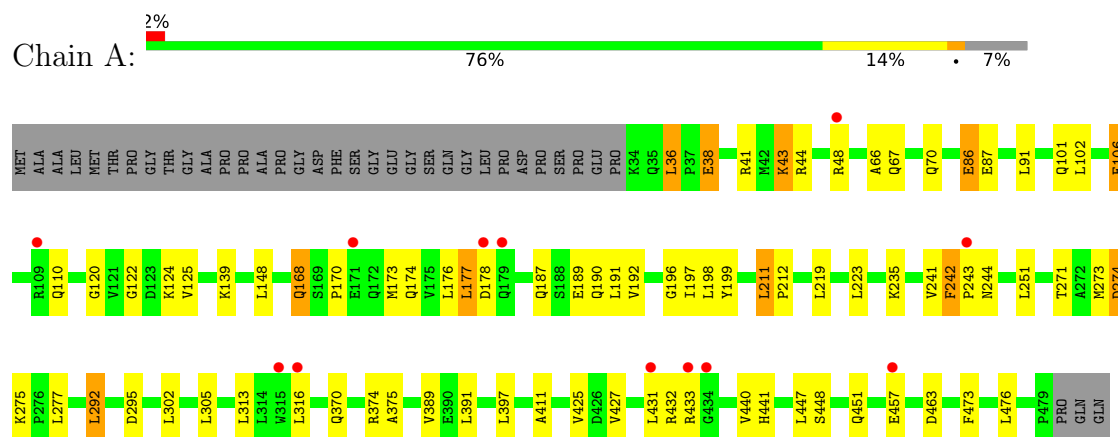
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	95	Total	O	0	0
			95	95		
3	C	169	Total	O	0	0
			169	169		
3	D	67	Total	O	0	0
			67	67		

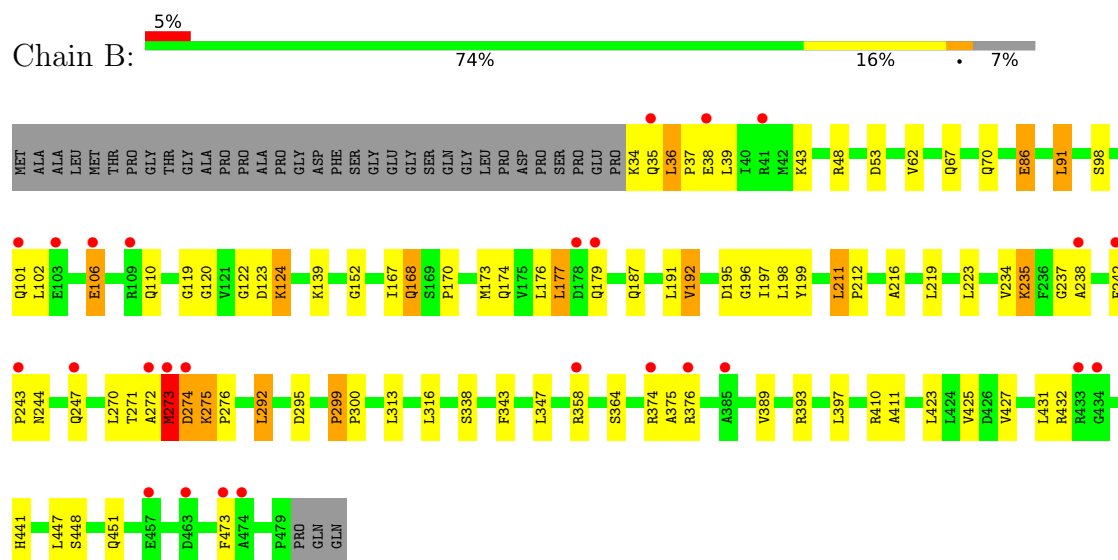
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

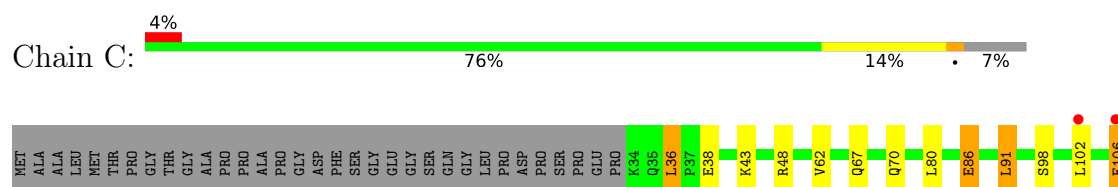
• Molecule 1: THYMIDINE PHOSPHORYLASE

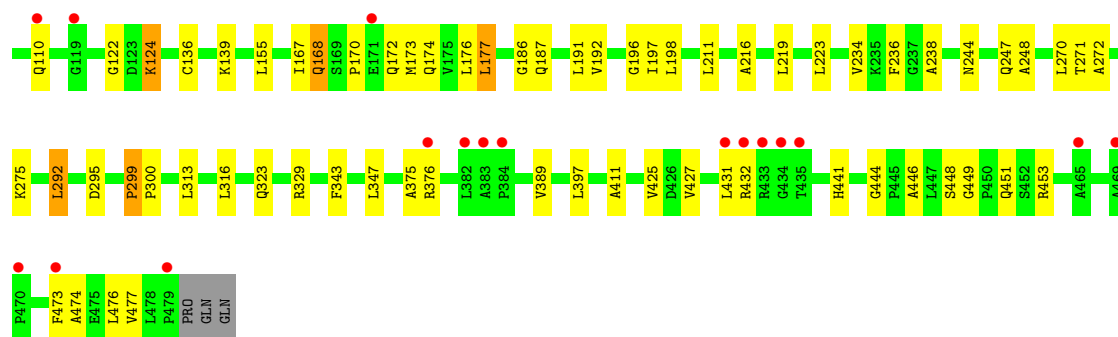


• Molecule 1: THYMIDINE PHOSPHORYLASE

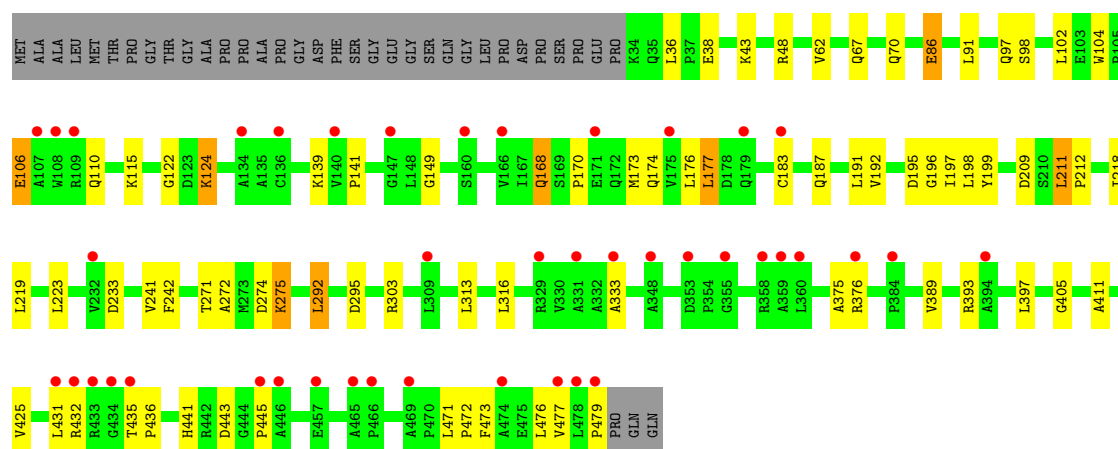
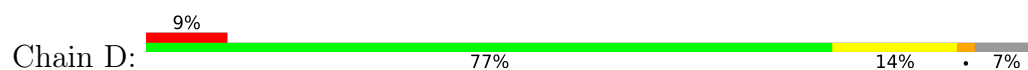


• Molecule 1: THYMIDINE PHOSPHORYLASE





● Molecule 1: THYMIDINE PHOSPHORYLASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.08Å 76.09Å 99.58Å 90.00° 98.61° 90.00°	Depositor
Resolution (Å)	102.06 – 2.31 101.92 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (102.06-2.31) 99.3 (101.92-2.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.01 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.246 , 0.287 0.289 , 0.320	Depositor DCC
R_{free} test set	3368 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13513	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 45.03 % 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 1.4005e-04. 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

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

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	0.65	0/3305	0.96	0/4483
1	B	0.63	1/3305 (0.0%)	0.97	6/4483 (0.1%)
1	C	0.63	1/3305 (0.0%)	0.93	4/4483 (0.1%)
1	D	0.50	0/3305	0.90	2/4483 (0.0%)
All	All	0.60	2/13220 (0.0%)	0.94	12/17932 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	PRO	CA-C	6.72	1.56	1.52
1	C	299	PRO	CA-C	5.20	1.55	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	471	LEU	CA-C-N	6.27	127.68	119.84
1	D	471	LEU	C-N-CA	6.27	127.68	119.84
1	B	242	PHE	CA-C-N	6.11	125.81	119.82
1	B	242	PHE	C-N-CA	6.11	125.81	119.82
1	B	273	MET	N-CA-C	5.45	117.78	108.90
1	C	444	GLY	CA-C-N	5.13	126.26	119.84
1	C	444	GLY	C-N-CA	5.13	126.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	449	GLY	CA-C-N	5.13	124.75	119.05
1	C	449	GLY	C-N-CA	5.13	124.75	119.05
1	B	273	MET	N-CA-CB	-5.04	102.21	110.68
1	B	275	LYS	CA-C-N	-5.04	115.04	120.03
1	B	275	LYS	C-N-CA	-5.04	115.04	120.03

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	272	ALA	Peptide
1	B	273	MET	Peptide

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	3259	0	3361	69	1
1	B	3259	0	3361	61	2
1	C	3259	0	3361	53	0
1	D	3259	0	3361	51	1
2	A	9	0	6	0	0
2	B	9	0	6	0	0
2	C	9	0	6	0	0
3	A	119	0	0	14	0
3	B	95	0	0	6	0
3	C	169	0	0	9	0
3	D	67	0	0	15	0
All	All	13513	0	13462	219	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (219) 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:242:PHE:HZ	1:A:251:LEU:CD2	1.57	1.16
1:D:183:CYS:SG	3:D:2019:HOH:O	1.96	1.14
1:C:476:LEU:O	1:D:376:ARG:NH1	1.80	1.13
1:A:242:PHE:CZ	1:A:251:LEU:CD2	2.34	1.08
1:A:242:PHE:CZ	1:A:251:LEU:HD22	1.89	1.06
1:C:106:GLU:HB2	3:C:2033:HOH:O	1.56	1.02
1:A:242:PHE:HZ	1:A:251:LEU:HD22	1.22	0.96
1:D:141:PRO:HA	3:D:2019:HOH:O	1.63	0.95
1:A:242:PHE:CZ	1:A:251:LEU:HD23	2.03	0.93
1:C:168:GLN:HG2	1:C:176:LEU:HD11	1.52	0.91
1:D:168:GLN:HG2	1:D:176:LEU:HD11	1.54	0.90
1:A:433:ARG:NH1	1:B:358:ARG:HG2	1.88	0.88
1:A:168:GLN:HG2	1:A:176:LEU:HD11	1.55	0.88
1:D:199:TYR:HE2	3:D:2026:HOH:O	1.56	0.87
1:B:168:GLN:HG2	1:B:176:LEU:HD11	1.53	0.87
1:C:453:ARG:NH2	3:C:2166:HOH:O	2.06	0.87
1:D:187:GLN:HG3	1:D:196:GLY:CA	2.07	0.84
1:A:187:GLN:HG3	1:A:196:GLY:CA	2.09	0.83
1:B:187:GLN:HG3	1:B:196:GLY:CA	2.09	0.83
1:A:305:LEU:HB3	3:A:2075:HOH:O	1.81	0.81
1:C:238:ALA:HB1	3:C:2144:HOH:O	1.82	0.80
1:C:187:GLN:HG3	1:C:196:GLY:CA	2.12	0.80
1:D:104:TRP:HD1	3:D:2032:HOH:O	1.64	0.79
1:D:393:ARG:NH2	3:D:2055:HOH:O	2.18	0.77
1:A:67:GLN:HE22	1:C:411:ALA:H	1.32	0.77
1:B:274:ASP:O	1:B:275:LYS:HB2	1.84	0.76
1:C:329:ARG:NH2	3:C:2123:HOH:O	1.79	0.76
1:D:303:ARG:N	3:D:2045:HOH:O	2.21	0.74
1:A:187:GLN:HG3	1:A:196:GLY:HA2	1.70	0.73
1:D:187:GLN:HG3	1:D:196:GLY:HA2	1.69	0.73
1:A:411:ALA:H	1:C:67:GLN:HE22	1.37	0.72
1:D:274:ASP:O	1:D:275:LYS:HB2	1.91	0.71
1:B:187:GLN:HG3	1:B:196:GLY:HA2	1.73	0.69
1:A:48:ARG:HH21	1:A:86:GLU:HB3	1.57	0.69
1:C:187:GLN:HG3	1:C:196:GLY:HA2	1.74	0.68
1:D:233:ASP:OD1	3:D:2034:HOH:O	2.12	0.68
1:D:333:ALA:O	3:D:2047:HOH:O	2.12	0.68
1:B:411:ALA:H	1:D:67:GLN:HE22	1.41	0.68
1:D:218:ILE:HG12	3:D:2014:HOH:O	1.93	0.68
1:C:476:LEU:C	1:D:376:ARG:HH11	1.96	0.68
1:B:376:ARG:NH2	3:B:2069:HOH:O	2.26	0.68
1:D:115:LYS:NZ	3:D:2013:HOH:O	2.21	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HH21	1:C:86:GLU:HB3	1.61	0.66
1:C:106:GLU:H	1:C:106:GLU:CD	2.03	0.66
1:B:48:ARG:HH21	1:B:86:GLU:HB3	1.60	0.66
1:D:48:ARG:HH21	1:D:86:GLU:HB3	1.61	0.66
1:A:242:PHE:CE2	1:A:251:LEU:HD22	2.30	0.65
1:A:120:GLY:HA3	1:A:235:LYS:HD2	1.79	0.65
1:A:48:ARG:NH2	1:A:86:GLU:HB3	2.12	0.64
1:D:443:ASP:O	3:D:2063:HOH:O	2.15	0.64
1:A:48:ARG:HD2	3:A:2008:HOH:O	1.96	0.64
1:D:149:GLY:HA3	3:D:2020:HOH:O	1.97	0.63
1:A:370:GLN:HG3	3:A:2083:HOH:O	1.98	0.63
1:A:374:ARG:HD2	3:A:2085:HOH:O	1.97	0.63
1:A:274:ASP:O	1:A:391:LEU:HD12	1.98	0.63
1:C:323:GLN:HG3	3:C:2115:HOH:O	1.98	0.62
1:B:106:GLU:H	1:B:106:GLU:CD	2.09	0.61
1:C:271:THR:HG22	1:C:474:ALA:HA	1.83	0.61
1:D:67:GLN:H	1:D:70:GLN:HE21	1.47	0.61
1:B:48:ARG:NH2	1:B:86:GLU:HB3	2.16	0.60
1:D:479:PRO:HD3	3:D:2039:HOH:O	1.99	0.60
1:A:106:GLU:H	1:A:106:GLU:CD	2.09	0.60
1:D:106:GLU:H	1:D:106:GLU:CD	2.10	0.60
1:A:67:GLN:H	1:A:70:GLN:HE21	1.50	0.59
1:D:48:ARG:NH2	1:D:86:GLU:HB3	2.18	0.59
1:B:374:ARG:HD2	3:B:2066:HOH:O	2.02	0.58
1:B:271:THR:HA	1:B:473:PHE:O	2.03	0.58
1:A:44:ARG:HG2	1:C:80:LEU:HD21	1.84	0.58
1:A:170:PRO:HA	1:A:173:MET:HE3	1.86	0.57
1:C:48:ARG:NH2	1:C:86:GLU:HB3	2.19	0.57
1:C:323:GLN:CG	3:C:2115:HOH:O	2.52	0.57
1:A:190:GLN:HG2	3:A:2026:HOH:O	2.03	0.57
1:C:236:PHE:CZ	1:C:272:ALA:HB2	2.39	0.57
1:C:173:MET:CE	1:C:191:LEU:HD11	2.35	0.57
1:A:273:MET:HG2	3:A:2074:HOH:O	2.05	0.56
1:C:67:GLN:H	1:C:70:GLN:HE21	1.52	0.56
1:A:457:GLU:HA	1:B:179:GLN:HE22	1.70	0.56
1:C:477:VAL:HA	1:D:376:ARG:NH1	2.21	0.56
1:C:476:LEU:C	1:D:376:ARG:NH1	2.59	0.56
1:B:67:GLN:H	1:B:70:GLN:HE21	1.52	0.56
1:A:139:LYS:HB3	1:A:177:LEU:HD13	1.87	0.56
1:B:67:GLN:HE22	1:D:411:ALA:H	1.53	0.55
1:C:170:PRO:HA	1:C:173:MET:HE3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:GLN:NE2	1:C:411:ALA:H	2.03	0.55
1:D:303:ARG:HB2	3:D:2045:HOH:O	2.06	0.55
1:A:173:MET:CE	1:A:191:LEU:HD11	2.37	0.55
1:B:139:LYS:HB3	1:B:177:LEU:HD13	1.88	0.54
1:D:170:PRO:HA	1:D:173:MET:HE3	1.89	0.54
1:A:463:ASP:OD2	1:B:338:SER:HA	2.08	0.54
1:A:125:VAL:HG22	3:A:2075:HOH:O	2.07	0.54
1:C:106:GLU:CD	1:C:106:GLU:N	2.66	0.53
1:A:457:GLU:HG2	3:A:2117:HOH:O	2.08	0.53
1:D:271:THR:HA	1:D:473:PHE:HB3	1.89	0.53
1:B:120:GLY:HA3	1:B:235:LYS:HD2	1.90	0.53
1:D:376:ARG:HG3	1:D:443:ASP:OD1	2.09	0.53
1:B:275:LYS:HD2	1:B:427:VAL:HG21	1.90	0.52
1:B:120:GLY:HA2	1:B:273:MET:SD	2.50	0.51
1:D:274:ASP:O	1:D:275:LYS:CB	2.58	0.51
1:B:273:MET:HA	1:B:274:ASP:O	2.12	0.50
1:B:102:LEU:HD21	1:B:173:MET:CE	2.41	0.50
1:D:139:LYS:HB3	1:D:177:LEU:HD13	1.93	0.50
1:A:102:LEU:HD21	1:A:173:MET:CE	2.41	0.50
1:D:187:GLN:HG3	1:D:196:GLY:HA3	1.90	0.50
1:A:432:ARG:N	1:A:432:ARG:HD2	2.25	0.50
1:D:405:GLY:HA2	3:D:2025:HOH:O	2.12	0.50
1:B:432:ARG:N	1:B:432:ARG:HD2	2.26	0.50
1:B:170:PRO:HA	1:B:173:MET:HE3	1.94	0.49
1:C:244:ASN:HD22	1:C:247:GLN:H	1.60	0.49
1:A:189:GLU:HG3	3:A:2058:HOH:O	2.12	0.49
1:A:101:GLN:HB2	3:A:2027:HOH:O	2.12	0.49
1:C:136:CYS:SG	1:C:329:ARG:HG3	2.52	0.49
1:A:447:LEU:HB3	1:A:451:GLN:HG3	1.94	0.49
1:A:275:LYS:HD2	1:A:427:VAL:HG23	1.94	0.49
1:D:106:GLU:CD	1:D:106:GLU:N	2.71	0.49
1:D:173:MET:CE	1:D:191:LEU:HD11	2.42	0.49
1:B:273:MET:HB3	1:B:275:LYS:O	2.13	0.49
1:A:457:GLU:HA	1:B:179:GLN:NE2	2.28	0.48
1:B:36:LEU:HD22	1:B:70:GLN:HB3	1.94	0.48
1:A:120:GLY:CA	1:A:235:LYS:HD2	2.42	0.48
1:A:433:ARG:HH12	1:B:358:ARG:HG2	1.76	0.48
1:A:106:GLU:CD	1:A:106:GLU:N	2.71	0.48
1:C:139:LYS:HB3	1:C:177:LEU:HD13	1.95	0.48
1:A:271:THR:HA	1:A:473:PHE:O	2.15	0.47
1:B:106:GLU:CD	1:B:106:GLU:N	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:MET:CE	1:B:191:LEU:HD11	2.44	0.47
1:A:122:GLY:O	1:A:124:LYS:HE2	2.15	0.47
1:B:187:GLN:HG3	1:B:196:GLY:HA3	1.94	0.47
1:A:277:LEU:HD21	3:A:2075:HOH:O	2.15	0.47
1:B:234:VAL:O	1:B:270:LEU:HA	2.14	0.47
1:C:271:THR:HB	1:C:473:PHE:O	2.15	0.47
1:A:38:GLU:HG2	3:A:2004:HOH:O	2.15	0.46
1:B:410:ARG:HD2	3:B:2081:HOH:O	2.15	0.46
1:A:448:SER:OG	1:A:451:GLN:HG2	2.15	0.46
1:A:440:VAL:HG11	1:A:447:LEU:HD21	1.97	0.46
1:D:432:ARG:HD2	1:D:432:ARG:N	2.30	0.46
1:C:234:VAL:O	1:C:270:LEU:HA	2.16	0.46
1:C:275:LYS:HD2	1:C:427:VAL:HG21	1.98	0.46
1:B:276:PRO:HG2	1:B:423:LEU:HD11	1.98	0.46
1:A:211:LEU:HB3	1:A:212:PRO:CD	2.46	0.46
1:A:36:LEU:HD11	1:A:66:ALA:CB	2.46	0.46
1:B:292:LEU:O	1:B:295:ASP:HB2	2.16	0.45
1:C:292:LEU:O	1:C:295:ASP:HB2	2.16	0.45
1:D:272:ALA:H	1:D:473:PHE:CB	2.29	0.45
1:C:36:LEU:HD22	1:C:70:GLN:HB3	1.97	0.45
1:C:102:LEU:HD21	1:C:173:MET:CE	2.46	0.45
1:D:389:VAL:HG23	1:D:431:LEU:HD22	1.98	0.45
1:B:447:LEU:HB3	1:B:451:GLN:HG3	1.99	0.45
1:C:389:VAL:HG23	1:C:431:LEU:HD22	1.98	0.45
1:D:102:LEU:HD21	1:D:173:MET:CE	2.46	0.45
1:B:152:GLY:HA3	3:B:2054:HOH:O	2.17	0.45
1:C:122:GLY:O	1:C:124:LYS:HE2	2.16	0.45
1:A:425:VAL:HG11	1:A:431:LEU:HD13	1.99	0.45
1:B:375:ALA:HB3	1:B:441:HIS:HB3	2.00	0.44
1:B:376:ARG:NH2	3:B:2071:HOH:O	2.50	0.44
1:C:375:ALA:HB3	1:C:441:HIS:HB3	1.99	0.44
1:B:122:GLY:O	1:B:124:LYS:HE2	2.18	0.44
1:B:211:LEU:HB3	1:B:212:PRO:CD	2.47	0.44
1:C:62:VAL:HG21	1:C:98:SER:HB2	1.99	0.44
1:A:187:GLN:HG3	1:A:196:GLY:HA3	1.93	0.44
1:B:119:GLY:O	1:B:235:LYS:HD2	2.18	0.44
1:C:432:ARG:N	1:C:432:ARG:HD2	2.32	0.44
1:A:139:LYS:HB3	1:A:177:LEU:CD1	2.48	0.44
1:A:375:ALA:HB3	1:A:441:HIS:HB3	2.00	0.44
1:A:389:VAL:HG23	1:A:431:LEU:HD22	1.99	0.44
1:C:299:PRO:HA	1:C:300:PRO:HD3	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLN:HB3	1:B:37:PRO:HD2	2.00	0.43
1:A:211:LEU:HB3	1:A:212:PRO:HD3	2.00	0.43
1:B:34:LYS:HD2	1:B:53:ASP:OD1	2.19	0.43
1:B:39:LEU:HD22	1:B:53:ASP:HB3	2.01	0.43
1:D:122:GLY:O	1:D:124:LYS:HE2	2.18	0.43
1:A:148:LEU:HD13	1:A:199:TYR:CE1	2.54	0.43
1:B:120:GLY:CA	1:B:235:LYS:HD2	2.48	0.43
1:D:211:LEU:HB3	1:D:212:PRO:CD	2.49	0.43
1:C:173:MET:HE2	1:C:191:LEU:HD11	2.01	0.43
1:D:209:ASP:HB2	1:D:242:PHE:CE2	2.53	0.43
1:B:343:PHE:O	1:B:347:LEU:HG	2.19	0.42
1:C:155:LEU:HD11	1:C:186:GLY:HA2	2.01	0.42
1:D:375:ALA:HB3	1:D:441:HIS:HB3	2.01	0.42
1:B:91:LEU:HD13	1:B:216:ALA:CB	2.49	0.42
1:A:302:LEU:HD12	3:A:2075:HOH:O	2.20	0.42
1:C:425:VAL:HG11	1:C:431:LEU:HD13	2.00	0.42
1:B:62:VAL:HG21	1:B:98:SER:HB2	2.02	0.42
1:B:195:ASP:O	1:B:199:TYR:HB2	2.19	0.42
1:D:292:LEU:O	1:D:295:ASP:HB2	2.19	0.42
1:C:248:ALA:HB1	1:C:270:LEU:HD21	2.00	0.42
1:A:41:ARG:HD2	3:A:2004:HOH:O	2.20	0.42
1:B:139:LYS:HB3	1:B:177:LEU:CD1	2.50	0.42
1:B:123:ASP:CG	1:B:235:LYS:HZ1	2.25	0.42
1:C:343:PHE:O	1:C:347:LEU:HG	2.19	0.42
1:B:237:GLY:H	1:B:243:PRO:HA	1.84	0.41
1:B:448:SER:OG	1:B:451:GLN:HG2	2.20	0.41
1:B:119:GLY:O	1:B:235:LYS:HG3	2.20	0.41
1:B:425:VAL:HG11	1:B:431:LEU:HD13	2.03	0.41
1:B:389:VAL:HG23	1:B:431:LEU:HD22	2.03	0.41
1:C:292:LEU:HD13	3:C:2104:HOH:O	2.21	0.41
1:A:43:LYS:HE3	1:A:43:LYS:HA	2.01	0.41
1:A:43:LYS:NZ	1:A:87:GLU:OE2	2.53	0.41
1:A:102:LEU:HD21	1:A:173:MET:HE3	2.03	0.41
1:A:242:PHE:C	1:A:244:ASN:H	2.27	0.41
1:B:299:PRO:HA	1:B:300:PRO:HD3	1.96	0.41
1:A:274:ASP:O	1:A:391:LEU:CD1	2.66	0.41
1:B:102:LEU:HD21	1:B:173:MET:HE1	2.02	0.41
1:C:244:ASN:ND2	1:C:247:GLN:H	2.18	0.41
1:C:329:ARG:HD3	3:C:2116:HOH:O	2.20	0.41
1:A:102:LEU:HD21	1:A:173:MET:HE1	2.01	0.41
1:A:292:LEU:O	1:A:295:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLN:HB2	3:B:2018:HOH:O	2.21	0.41
1:C:376:ARG:NH2	3:C:2142:HOH:O	2.54	0.41
1:D:139:LYS:HB3	1:D:177:LEU:CD1	2.50	0.41
1:D:195:ASP:O	1:D:199:TYR:HB2	2.21	0.41
1:D:425:VAL:HG11	1:D:431:LEU:HD13	2.02	0.41
1:D:62:VAL:HG21	1:D:98:SER:HB2	2.02	0.40
1:A:36:LEU:HD11	1:A:66:ALA:HB2	2.02	0.40
1:C:172:GLN:O	1:C:176:LEU:HG	2.21	0.40
1:D:435:THR:HA	1:D:436:PRO:HD3	1.98	0.40
1:C:448:SER:OG	1:C:451:GLN:HG2	2.21	0.40
1:A:36:LEU:CD1	1:A:66:ALA:HA	2.51	0.40
1:B:191:LEU:O	1:B:192:VAL:C	2.64	0.40
1:C:91:LEU:HD13	1:C:216:ALA:CB	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:ASP:OD2	1:B:393:ARG:NH2[1_556]	2.11	0.09
1:B:364:SER:OG	1:D:97:GLN:O[2_544]	2.18	0.02

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	444/482 (92%)	435 (98%)	8 (2%)	1 (0%)	43	53
1	B	444/482 (92%)	434 (98%)	8 (2%)	2 (0%)	24	30
1	C	444/482 (92%)	433 (98%)	10 (2%)	1 (0%)	43	53
1	D	444/482 (92%)	434 (98%)	7 (2%)	3 (1%)	18	22
All	All	1776/1928 (92%)	1736 (98%)	33 (2%)	7 (0%)	30	37

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	275	LYS
1	B	274	ASP
1	A	243	PRO
1	B	238	ALA
1	C	446	ALA
1	D	472	PRO
1	D	445	PRO

5.3.2 Protein sidechains [i](#)

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	333/359 (93%)	309 (93%)	24 (7%)	13	17
1	B	333/359 (93%)	307 (92%)	26 (8%)	11	15
1	C	333/359 (93%)	311 (93%)	22 (7%)	15	21
1	D	333/359 (93%)	309 (93%)	24 (7%)	13	17
All	All	1332/1436 (93%)	1236 (93%)	96 (7%)	13	17

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	38	GLU
1	A	43	LYS
1	A	86	GLU
1	A	91	LEU
1	A	106	GLU
1	A	110	GLN
1	A	168	GLN
1	A	174	GLN
1	A	177	LEU
1	A	192	VAL
1	A	197	ILE
1	A	198	LEU

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Mol	Chain	Res	Type
1	A	211	LEU
1	A	219	LEU
1	A	223	LEU
1	A	241	VAL
1	A	242	PHE
1	A	274	ASP
1	A	292	LEU
1	A	313	LEU
1	A	316	LEU
1	A	397	LEU
1	A	476	LEU
1	B	36	LEU
1	B	38	GLU
1	B	43	LYS
1	B	86	GLU
1	B	91	LEU
1	B	106	GLU
1	B	110	GLN
1	B	124	LYS
1	B	167	ILE
1	B	168	GLN
1	B	174	GLN
1	B	177	LEU
1	B	192	VAL
1	B	197	ILE
1	B	198	LEU
1	B	211	LEU
1	B	219	LEU
1	B	223	LEU
1	B	235	LYS
1	B	244	ASN
1	B	247	GLN
1	B	273	MET
1	B	292	LEU
1	B	313	LEU
1	B	316	LEU
1	B	397	LEU
1	C	36	LEU
1	C	38	GLU
1	C	43	LYS
1	C	86	GLU
1	C	91	LEU

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Mol	Chain	Res	Type
1	C	106	GLU
1	C	110	GLN
1	C	124	LYS
1	C	167	ILE
1	C	168	GLN
1	C	174	GLN
1	C	177	LEU
1	C	192	VAL
1	C	197	ILE
1	C	198	LEU
1	C	211	LEU
1	C	219	LEU
1	C	223	LEU
1	C	292	LEU
1	C	313	LEU
1	C	316	LEU
1	C	397	LEU
1	D	36	LEU
1	D	38	GLU
1	D	43	LYS
1	D	86	GLU
1	D	91	LEU
1	D	106	GLU
1	D	110	GLN
1	D	124	LYS
1	D	168	GLN
1	D	174	GLN
1	D	177	LEU
1	D	192	VAL
1	D	197	ILE
1	D	198	LEU
1	D	211	LEU
1	D	219	LEU
1	D	223	LEU
1	D	241	VAL
1	D	292	LEU
1	D	313	LEU
1	D	316	LEU
1	D	397	LEU
1	D	476	LEU
1	D	477	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	70	GLN
1	A	100	GLN
1	A	101	GLN
1	A	111	GLN
1	A	168	GLN
1	A	174	GLN
1	A	190	GLN
1	B	67	GLN
1	B	70	GLN
1	B	100	GLN
1	B	101	GLN
1	B	174	GLN
1	B	179	GLN
1	B	190	GLN
1	B	245	GLN
1	C	67	GLN
1	C	70	GLN
1	C	100	GLN
1	C	101	GLN
1	C	111	GLN
1	C	174	GLN
1	C	190	GLN
1	C	244	ASN
1	C	245	GLN
1	C	247	GLN
1	C	451	GLN
1	D	67	GLN
1	D	70	GLN
1	D	100	GLN
1	D	101	GLN
1	D	111	GLN
1	D	150	HIS
1	D	174	GLN
1	D	190	GLN
1	D	245	GLN
1	D	247	GLN
1	D	283	HIS
1	D	378	GLN
1	D	451	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](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TDR	C	1480	-	9,9,9	3.37	5 (55%)	12,12,12	3.33	7 (58%)
2	TDR	B	1480	-	9,9,9	3.46	5 (55%)	12,12,12	3.24	6 (50%)
2	TDR	A	1480	-	9,9,9	3.50	5 (55%)	12,12,12	3.07	7 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TDR	C	1480	-	-	-	0/1/1/1
2	TDR	B	1480	-	-	-	0/1/1/1
2	TDR	A	1480	-	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1480	TDR	O4-C4	6.54	1.36	1.23
2	B	1480	TDR	O2-C2	5.97	1.36	1.23
2	B	1480	TDR	O4-C4	5.72	1.34	1.23
2	C	1480	TDR	O2-C2	5.50	1.35	1.23
2	C	1480	TDR	O4-C4	5.46	1.33	1.23
2	A	1480	TDR	O2-C2	5.42	1.34	1.23
2	A	1480	TDR	C6-C5	3.91	1.39	1.34
2	B	1480	TDR	C6-C5	3.84	1.39	1.34
2	C	1480	TDR	C6-C5	3.63	1.39	1.34
2	B	1480	TDR	C4-C5	-3.53	1.39	1.44
2	C	1480	TDR	C4-C5	-3.33	1.39	1.44
2	C	1480	TDR	C4-N3	-2.91	1.33	1.38
2	A	1480	TDR	C4-C5	-2.80	1.40	1.44
2	A	1480	TDR	C4-N3	-2.32	1.34	1.38
2	B	1480	TDR	C4-N3	-2.25	1.34	1.38

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1480	TDR	C5-C4-N3	6.66	121.11	115.32
2	B	1480	TDR	C5-C4-N3	6.56	121.02	115.32
2	A	1480	TDR	N1-C2-N3	5.76	121.24	115.17
2	C	1480	TDR	N1-C2-N3	5.22	120.67	115.17
2	A	1480	TDR	C5-C4-N3	4.88	119.56	115.32
2	B	1480	TDR	N1-C2-N3	4.80	120.23	115.17
2	C	1480	TDR	C4-N3-C2	-4.76	119.81	126.37
2	B	1480	TDR	C4-N3-C2	-4.62	120.00	126.37
2	A	1480	TDR	C4-N3-C2	-4.38	120.33	126.37
2	B	1480	TDR	O4-C4-C5	-3.83	120.53	124.92
2	C	1480	TDR	O4-C4-C5	-3.37	121.06	124.92
2	A	1480	TDR	C5-C6-N1	-3.08	119.11	122.42
2	B	1480	TDR	C5-C6-N1	-2.80	119.40	122.42
2	C	1480	TDR	C5-C6-N1	-2.74	119.47	122.42
2	A	1480	TDR	CM5-C5-C6	-2.47	120.69	123.23
2	A	1480	TDR	O4-C4-C5	-2.40	122.17	124.92
2	C	1480	TDR	CM5-C5-C4	2.30	121.24	118.78
2	A	1480	TDR	O2-C2-N3	-2.24	117.88	121.86
2	C	1480	TDR	O2-C2-N1	-2.08	120.64	122.79
2	B	1480	TDR	CM5-C5-C4	2.02	120.93	118.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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(Å ²)	Q<0.9
1	A	446/482 (92%)	0.39	12 (2%) 56 59	3, 9, 28, 46	2 (0%)
1	B	446/482 (92%)	0.58	26 (5%) 29 31	4, 10, 28, 46	2 (0%)
1	C	446/482 (92%)	0.43	19 (4%) 40 42	4, 9, 27, 46	2 (0%)
1	D	446/482 (92%)	0.94	42 (9%) 14 16	4, 10, 30, 51	2 (0%)
All	All	1784/1928 (92%)	0.58	99 (5%) 30 33	3, 10, 28, 51	8 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	479	PRO	6.3
1	B	274	ASP	5.3
1	B	272	ALA	4.9
1	B	273	MET	4.6
1	D	477	VAL	4.6
1	C	383	ALA	4.4
1	C	469	ALA	4.4
1	D	107	ALA	4.3
1	A	243	PRO	4.3
1	C	465	ALA	4.1
1	C	473	PHE	3.8
1	B	179	GLN	3.8
1	D	478	LEU	3.7
1	C	376	ARG	3.7
1	B	109	ARG	3.6
1	B	38	GLU	3.6
1	B	457	GLU	3.5
1	D	465	ALA	3.4
1	A	457	GLU	3.4
1	B	178	ASP	3.2
1	B	376	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	238	ALA	3.1
1	A	109	ARG	3.1
1	A	434	GLY	3.1
1	D	431	LEU	3.1
1	C	434	GLY	3.1
1	D	446	ALA	3.1
1	D	474	ALA	3.0
1	C	479	PRO	3.0
1	D	140	VAL	3.0
1	D	175	VAL	3.0
1	B	433	ARG	2.8
1	D	348	ALA	2.7
1	C	435	THR	2.7
1	B	358	ARG	2.7
1	A	315	TRP	2.7
1	D	147	GLY	2.7
1	C	431	LEU	2.7
1	D	469	ALA	2.6
1	D	466	PRO	2.6
1	A	171	GLU	2.6
1	D	445	PRO	2.6
1	C	432	ARG	2.6
1	A	179	GLN	2.5
1	B	385	ALA	2.5
1	D	360	LEU	2.5
1	C	106	GLU	2.5
1	B	101	GLN	2.5
1	C	119	GLY	2.5
1	B	41	ARG	2.4
1	A	316	LEU	2.4
1	D	359	ALA	2.4
1	B	473	PHE	2.4
1	A	48	ARG	2.4
1	B	35	GLN	2.4
1	C	110	GLN	2.4
1	C	470	PRO	2.4
1	D	353	ASP	2.4
1	D	134	ALA	2.4
1	D	333	ALA	2.4
1	D	355	GLY	2.3
1	D	394	ALA	2.3
1	C	384	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	376	ARG	2.3
1	C	171	GLU	2.3
1	D	384	PRO	2.3
1	D	433	ARG	2.3
1	D	435	THR	2.3
1	D	179	GLN	2.3
1	B	242	PHE	2.2
1	C	382	LEU	2.2
1	D	183	CYS	2.2
1	D	108	TRP	2.2
1	D	329	ARG	2.2
1	D	358	ARG	2.2
1	B	474	ALA	2.2
1	D	331	ALA	2.2
1	D	309	LEU	2.2
1	A	433	ARG	2.2
1	A	178	ASP	2.2
1	B	106	GLU	2.2
1	B	247	GLN	2.2
1	D	232	VAL	2.1
1	D	109	ARG	2.1
1	A	431	LEU	2.1
1	B	463	ASP	2.1
1	B	243	PRO	2.1
1	D	166	VAL	2.1
1	D	434	GLY	2.1
1	B	103	GLU	2.1
1	D	457	GLU	2.1
1	D	160	SER	2.0
1	D	136	CYS	2.0
1	D	171	GLU	2.0
1	D	432	ARG	2.0
1	B	434	GLY	2.0
1	C	102	LEU	2.0
1	B	374	ARG	2.0
1	C	433	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TDR	C	1480	9/9	0.91	0.08	2,2,2,2	0
2	TDR	B	1480	9/9	0.94	0.07	2,3,3,4	0
2	TDR	A	1480	9/9	0.94	0.06	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.