



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 26, 2014 – 10:04 PM GMT

PDB ID : 2J0F
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 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/ValidationPDFNotes.html>

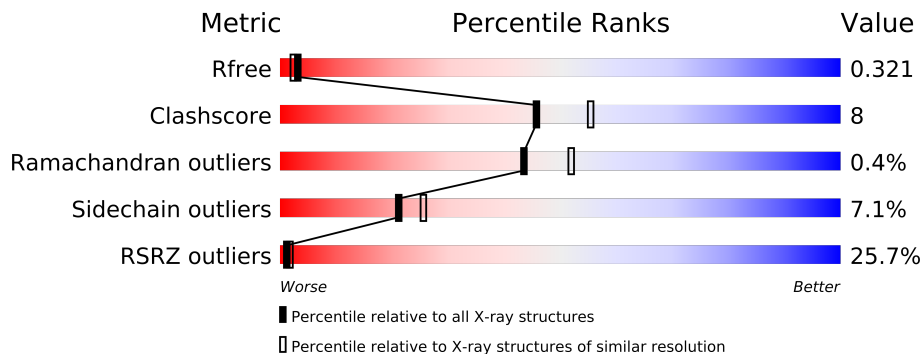
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3293 (2.34-2.30)
Clashscore	79885	4097 (2.34-2.30)
Ramachandran outliers	78287	4055 (2.34-2.30)
Sidechain outliers	78261	4054 (2.34-2.30)
RSRZ outliers	66119	3294 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	482	
1	B	482	
1	C	482	
1	D	482	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13513 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

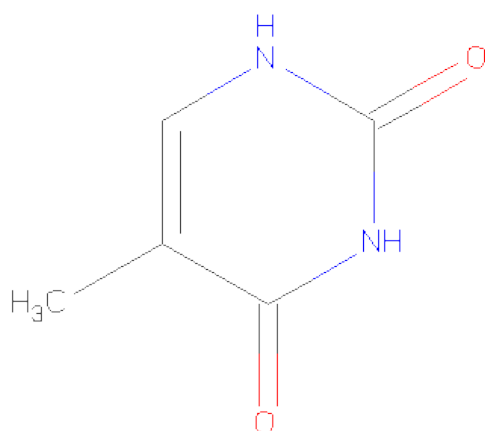
- Molecule 1 is a protein called THYMIDINE PHOSPHORYLASE.

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

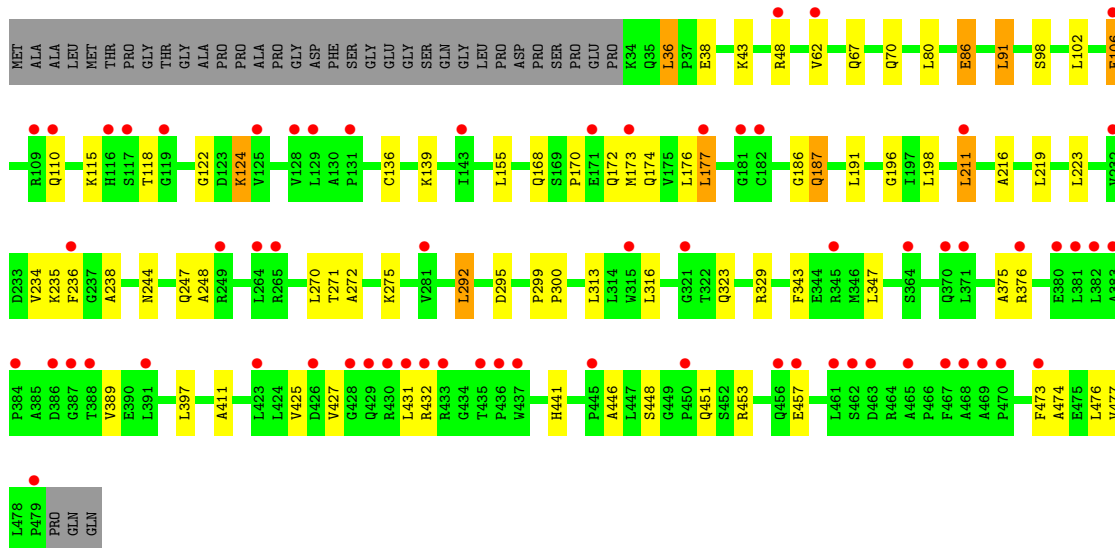
- Molecule 2 is THYMINE (three-letter code: TDR) (formula: C₅H₆N₂O₂).



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		

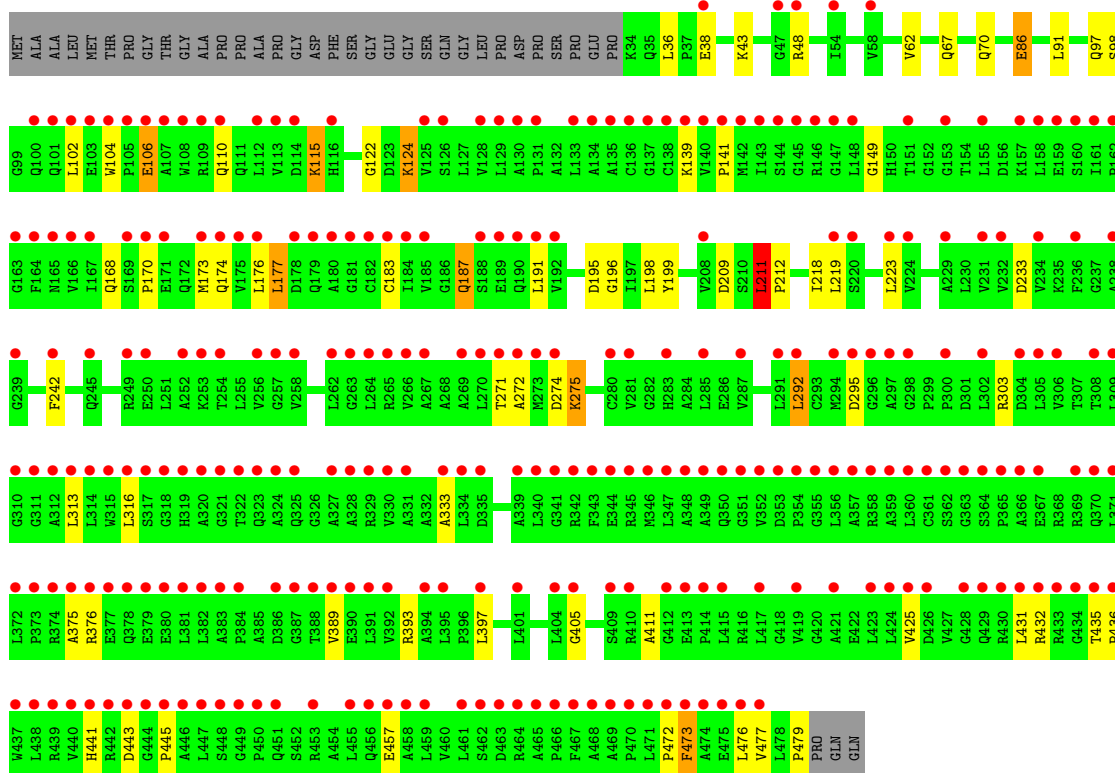
- Molecule 3 is water.

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		



● Molecule 1: THYMIDINE PHOSPHORYLASE

Chain D:



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 29.96 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.3 (102.06-2.31) 99.4 (29.96-2.31)	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 0.290 , 0.321	Depositor DCC
R_{free} test set	3368 reflections (5.34%)	DCC
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 , 8.2	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 66459 reflections (0.002%)	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.

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	0.48	0/3305	0.66	1/4483 (0.0%)
1	B	0.46	0/3305	0.65	1/4483 (0.0%)
1	C	0.46	0/3305	0.64	1/4483 (0.0%)
1	D	0.35	0/3305	0.59	1/4483 (0.0%)
All	All	0.44	0/13220	0.63	4/17932 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	LEU	CA-CB-CG	6.53	130.32	115.30
1	A	211	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	211	LEU	CA-CB-CG	5.25	127.36	115.30
1	D	211	LEU	CA-CB-CG	5.05	126.91	115.30

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3259	0	3361	69	1
1	B	3259	0	3361	60	2
1	C	3259	0	3361	53	0
1	D	3259	0	3361	53	1
2	A	9	0	6	1	0
2	B	9	0	6	1	0
2	C	9	0	6	1	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	220	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (220) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:376:ARG:NH2	3:B:2069:HOH:O	2.26	0.68
1:C:48:ARG:HH21	1:C:86:GLU:HB3	1.61	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:C:106:GLU:CD	1:C:106:GLU:H	2.03	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:115:LYS:NZ	3:D:2013:HOH:O	2.21	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:476:LEU:C	1:D:376:ARG:HH11	1.96	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:C:67:GLN:H	1:C:70:GLN:HE21	1.52	0.56
1:B:106:GLU:CD	1:B:106:GLU:H	2.09	0.56
1:A:273:MET:HG2	3:A:2074:HOH:O	2.05	0.56
1:C:477:VAL:HA	1:D:376:ARG:NH1	2.21	0.56
1:A:457:GLU:HA	1:B:179:GLN:HE22	1.70	0.56
1:B:67:GLN:H	1:B:70:GLN:HE21	1.52	0.56
1:A:106:GLU:CD	1:A:106:GLU:H	2.09	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:D:106:GLU:H	1:D:106:GLU:CD	2.10	0.55
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:C:170:PRO:HA	1:C:173:MET:HE3	1.88	0.55
1:B:139:LYS:HB3	1:B:177:LEU:HD13	1.88	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: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:D:376:ARG:HG3	1:D:443:ASP:OD1	2.09	0.53
1:B:120:GLY:HA3	1:B:235:LYS:HD2	1.90	0.53
1:B:275:LYS:HD2	1:B:427:VAL:HG21	1.90	0.52
1:C:476:LEU:C	1:D:376:ARG:NH1	2.59	0.51
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:D:187:GLN:HG3	1:D:196:GLY:HA3	1.90	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:LEU:HD21	1:A:173:MET:CE	2.41	0.50
1:A:432:ARG:HD2	1:A:432:ARG:N	2.25	0.50
1:D:405:GLY:HA2	3:D:2025:HOH:O	2.12	0.50
1:B:432:ARG:HD2	1:B:432:ARG:N	2.26	0.50
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:C:136:CYS:SG	1:C:329:ARG:HG3	2.52	0.49
1:A:101:GLN:HB2	3:A:2027:HOH:O	2.12	0.49
1:B:118:THR:O	2:B:1480:TDR:H5M1	2.12	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:173:MET:CE	1:D:191:LEU:HD11	2.42	0.49
1:C:106:GLU:N	1:C:106:GLU:CD	2.66	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:170:PRO:HA	1:B:173:MET:HE3	1.95	0.48
1:B:36:LEU:HD22	1:B:70:GLN:HB3	1.94	0.48
1:A:433:ARG:HH12	1:B:358:ARG:HG2	1.76	0.48
1:A:120:GLY:CA	1:A:235:LYS:HD2	2.42	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:A:214:ILE:HG12	2:A:1480:TDR:H5M2	1.96	0.47
1:B:173:MET:CE	1:B:191:LEU:HD11	2.44	0.47
1:D:170:PRO:HA	1:D:173:MET:HE3	1.97	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:C:271:THR:HB	1:C:473:PHE:O	2.15	0.47
1:B:234:VAL:O	1:B:270:LEU:HA	2.14	0.47
1:B:410:ARG:HD2	3:B:2081:HOH:O	2.15	0.46
1:A:38:GLU:HG2	3:A:2004: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:275:LYS:HD2	1:C:427:VAL:HG21	1.98	0.46
1:C:234:VAL:O	1:C:270:LEU:HA	2.16	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:D:272:ALA:H	1:D:473:PHE:CB	2.29	0.45
1:C:292:LEU:O	1:C:295:ASP:HB2	2.16	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:D:102:LEU:HD21	1:D:173:MET:CE	2.46	0.45
1:C:389:VAL:HG23	1:C:431:LEU:HD22	1.98	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:D:106:GLU:N	1:D:106:GLU:CD	2.71	0.45
1:A:425:VAL:HG11	1:A:431:LEU:HD13	1.99	0.45
1:B:376:ARG:NH2	3:B:2071:HOH:O	2.50	0.44
1:B:375:ALA:HB3	1:B:441:HIS:HB3	2.00	0.44
1:C:375:ALA:HB3	1:C:441:HIS:HB3	1.99	0.44
1:B:211:LEU:HB3	1:B:212:PRO:CD	2.47	0.44
1:B:122:GLY:O	1:B:124:LYS:HE2	2.18	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: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
1:A:375:ALA:HB3	1:A:441:HIS:HB3	2.00	0.44
1:B:35:GLN:HB3	1:B:37:PRO:HD2	2.00	0.43
1:C:118:THR:O	2:C:1480:TDR:H5M1	2.19	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:A:106:GLU:CD	1:A:106:GLU:N	2.71	0.43
1:D:102:LEU:HD21	1:D:173:MET:HE3	2.00	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:B:120:GLY:CA	1:B:235:LYS:HD2	2.48	0.43
1:A:148:LEU:HD13	1:A:199:TYR:CE1	2.54	0.43
1:D:211:LEU:HB3	1:D:212:PRO:CD	2.49	0.43
1:D:209:ASP:HB2	1:D:242:PHE:CE2	2.53	0.43
1:B:106:GLU:N	1:B:106:GLU:CD	2.72	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:343:PHE:O	1:B:347:LEU:HG	2.19	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:62:VAL:HG21	1:B:98:SER:HB2	2.02	0.42
1:C:248:ALA:HB1	1:C:270:LEU:HD21	2.00	0.42
1:B:139:LYS:HB3	1:B:177:LEU:CD1	2.50	0.42
1:A:41:ARG:HD2	3:A:2004:HOH:O	2.20	0.42
1:C:343:PHE:O	1:C:347:LEU:HG	2.19	0.42
1:B:448:SER:OG	1:B:451:GLN:HG2	2.20	0.41
1:B:237:GLY:H	1:B:243:PRO:HA	1.84	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:D:173:MET:HE1	1:D:191:LEU:HD11	2.02	0.41
1:C:292:LEU:HD13	3:C:2104:HOH:O	2.21	0.41
1:A:102:LEU:HD21	1:A:173:MET:HE3	2.03	0.41
1:B:299:PRO:HA	1:B:300:PRO:HD3	1.96	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:274:ASP:O	1:A:391:LEU:CD1	2.66	0.41
1:C:329:ARG:HD3	3:C:2116:HOH:O	2.20	0.41
1:C:244:ASN:ND2	1:C:247:GLN:H	2.18	0.41
1:A:102:LEU:HD21	1:A:173:MET:HE1	2.01	0.41
1:B:102:LEU:HD21	1:B:173:MET:HE3	2.03	0.41
1:D:139:LYS:HB3	1:D:177:LEU:CD1	2.50	0.41
1:A:292:LEU:O	1:A:295:ASP:HB2	2.21	0.41
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: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:C:172:GLN:O	1:C:176:LEU:HG	2.21	0.40
1:A:36:LEU:HD11	1:A:66:ALA:HB2	2.02	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: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	Distance(Å)	Clash(Å)
1:A:178:ASP:OD2	1:B:393:ARG:NH2[1_556]	2.11	0.09

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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%)	56 67
1	B	444/482 (92%)	434 (98%)	8 (2%)	2 (0%)	38 44
1	C	444/482 (92%)	433 (98%)	10 (2%)	1 (0%)	56 67
1	D	444/482 (92%)	434 (98%)	7 (2%)	3 (1%)	30 34
All	All	1776/1928 (92%)	1736 (98%)	33 (2%)	7 (0%)	43 52

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 ⓘ

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%)	310 (93%)	23 (7%)	22 27
1	B	333/359 (93%)	308 (92%)	25 (8%)	19 23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	333/359 (93%)	311 (93%)	22 (7%)	24	29
1	D	333/359 (93%)	309 (93%)	24 (7%)	21	25
All	All	1332/1436 (93%)	1238 (93%)	94 (7%)	21	25

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	115	LYS
1	A	124	LYS
1	A	174	GLN
1	A	177	LEU
1	A	187	GLN
1	A	198	LEU
1	A	211	LEU
1	A	219	LEU
1	A	223	LEU
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	457	GLU
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	115	LYS
1	B	124	LYS
1	B	174	GLN
1	B	177	LEU

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Mol	Chain	Res	Type
1	B	187	GLN
1	B	198	LEU
1	B	211	LEU
1	B	219	LEU
1	B	223	LEU
1	B	235	LYS
1	B	247	GLN
1	B	273	MET
1	B	274	ASP
1	B	292	LEU
1	B	313	LEU
1	B	316	LEU
1	B	397	LEU
1	B	457	GLU
1	C	36	LEU
1	C	38	GLU
1	C	43	LYS
1	C	86	GLU
1	C	91	LEU
1	C	106	GLU
1	C	110	GLN
1	C	115	LYS
1	C	124	LYS
1	C	174	GLN
1	C	177	LEU
1	C	187	GLN
1	C	198	LEU
1	C	211	LEU
1	C	219	LEU
1	C	223	LEU
1	C	235	LYS
1	C	292	LEU
1	C	313	LEU
1	C	316	LEU
1	C	397	LEU
1	C	457	GLU
1	D	36	LEU
1	D	38	GLU
1	D	43	LYS
1	D	86	GLU
1	D	91	LEU
1	D	106	GLU

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Mol	Chain	Res	Type
1	D	110	GLN
1	D	115	LYS
1	D	124	LYS
1	D	174	GLN
1	D	177	LEU
1	D	187	GLN
1	D	198	LEU
1	D	211	LEU
1	D	219	LEU
1	D	223	LEU
1	D	292	LEU
1	D	313	LEU
1	D	316	LEU
1	D	397	LEU
1	D	457	GLU
1	D	473	PHE
1	D	476	LEU
1	D	477	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) 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	174	GLN
1	A	190	GLN
1	A	244	ASN
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	B	325	GLN
1	C	67	GLN
1	C	70	GLN
1	C	100	GLN
1	C	101	GLN

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Mol	Chain	Res	Type
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	174	GLN
1	D	190	GLN
1	D	245	GLN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	A	1480	-	9,9,9	2.94	2 (22%)	8,12,12	1.55	2 (25%)
2	TDR	B	1480	-	9,9,9	2.89	2 (22%)	8,12,12	1.51	2 (25%)
2	TDR	C	1480	-	9,9,9	2.76	3 (33%)	8,12,12	1.51	2 (25%)

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	A	1480	-	-	0/0/0/0	0/1/1/1
2	TDR	B	1480	-	-	0/0/0/0	0/1/1/1
2	TDR	C	1480	-	-	0/0/0/0	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1480	TDR	O2-C2	5.96	1.36	1.23
2	A	1480	TDR	O4-C4	5.85	1.36	1.24
2	C	1480	TDR	O2-C2	5.49	1.35	1.23
2	A	1480	TDR	O2-C2	5.41	1.34	1.23
2	B	1480	TDR	O4-C4	5.05	1.34	1.24
2	C	1480	TDR	O4-C4	4.80	1.33	1.24
2	C	1480	TDR	C4-N3	-2.29	1.33	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1480	TDR	C5-C6-N1	-3.27	119.11	121.81
2	B	1480	TDR	C5-C6-N1	-2.91	119.40	121.81
2	C	1480	TDR	C5-C6-N1	-2.83	119.47	121.81
2	C	1480	TDR	C4-N3-C2	-2.73	119.81	125.36
2	B	1480	TDR	C4-N3-C2	-2.64	120.00	125.36
2	A	1480	TDR	C4-N3-C2	-2.48	120.33	125.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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%)	0.94	51 (11%) 6 9	3, 9, 28, 46	2 (0%)
1	B	446/482 (92%)	1.20	71 (15%) 3 5	4, 10, 28, 46	2 (0%)
1	C	446/482 (92%)	1.15	66 (14%) 3 5	4, 9, 27, 46	2 (0%)
1	D	446/482 (92%)	2.62	271 (60%) 0 0	4, 10, 30, 51	2 (0%)
All	All	1784/1928 (92%)	1.48	459 (25%) 1 2	3, 10, 28, 51	8 (0%)

All (459) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	11.8
1	D	445	PRO	8.6
1	D	465	ALA	8.3
1	C	383	ALA	8.3
1	D	352	VAL	7.6
1	C	473	PHE	7.6
1	D	171	GLU	7.5
1	D	360	LEU	7.5
1	D	430	ARG	7.3
1	D	383	ALA	7.0
1	D	382	LEU	7.0
1	B	273	MET	6.9
1	D	446	ALA	6.8
1	D	468	ALA	6.7
1	B	274	ASP	6.6
1	D	362	SER	6.6
1	D	167	ILE	6.5
1	C	435	THR	6.5
1	D	356	LEU	6.5
1	A	243	PRO	6.4
1	D	436	PRO	6.4

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Mol	Chain	Res	Type	RSRZ
1	D	371	LEU	6.2
1	D	106	GLU	6.2
1	D	358	ARG	6.2
1	D	263	GLY	6.2
1	D	388	THR	5.9
1	D	386	ASP	5.9
1	D	431	LEU	5.8
1	D	354	PRO	5.8
1	D	462	SER	5.8
1	D	309	LEU	5.8
1	D	316	LEU	5.7
1	A	109	ARG	5.7
1	D	432	ARG	5.7
1	C	465	ALA	5.6
1	C	432	ARG	5.5
1	D	364	SER	5.5
1	D	166	VAL	5.4
1	D	232	VAL	5.4
1	D	292	LEU	5.4
1	D	473	PHE	5.4
1	D	160	SER	5.4
1	D	348	ALA	5.3
1	D	361	CYS	5.3
1	D	179	GLN	5.2
1	D	253	LYS	5.2
1	D	433	ARG	5.2
1	D	384	PRO	5.2
1	D	165	ASN	5.2
1	B	238	ALA	5.2
1	D	140	VAL	5.1
1	D	387	GLY	5.1
1	D	173	MET	5.1
1	D	425	VAL	5.1
1	D	305	LEU	5.1
1	D	401	LEU	5.1
1	D	353	ASP	5.0
1	D	467	PHE	5.0
1	D	367	GLU	5.0
1	D	103	GLU	5.0
1	C	469	ALA	5.0
1	B	38	GLU	4.9
1	D	134	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	428	GLY	4.9
1	D	437	TRP	4.8
1	C	430	ARG	4.8
1	C	433	ARG	4.8
1	D	175	VAL	4.8
1	D	249	ARG	4.8
1	D	434	GLY	4.8
1	D	463	ASP	4.7
1	D	112	LEU	4.6
1	D	236	PHE	4.6
1	D	359	ALA	4.6
1	D	376	ARG	4.6
1	B	272	ALA	4.6
1	D	331	ALA	4.6
1	D	319	HIS	4.5
1	D	183	CYS	4.5
1	D	429	GLN	4.5
1	D	369	ARG	4.5
1	C	388	THR	4.4
1	D	466	PRO	4.4
1	D	161	ILE	4.4
1	D	345	ARG	4.4
1	D	450	PRO	4.3
1	D	231	VAL	4.3
1	B	109	ARG	4.3
1	D	264	LEU	4.3
1	D	476	LEU	4.3
1	D	110	GLN	4.3
1	D	129	LEU	4.3
1	C	382	LEU	4.2
1	D	366	ALA	4.2
1	B	463	ASP	4.2
1	C	386	ASP	4.2
1	C	468	ALA	4.2
1	D	410	ARG	4.2
1	D	147	GLY	4.2
1	D	365	PRO	4.2
1	D	341	GLY	4.1
1	D	294	MET	4.1
1	D	435	THR	4.1
1	D	163	GLY	4.1
1	D	109	ARG	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	135	ALA	4.0
1	D	440	VAL	4.0
1	A	315	TRP	4.0
1	C	431	LEU	4.0
1	D	271	THR	4.0
1	B	35	GLN	3.9
1	D	182	CYS	3.9
1	C	106	GLU	3.9
1	B	473	PHE	3.9
1	D	404	LEU	3.9
1	D	355	GLY	3.9
1	D	357	ALA	3.9
1	D	138	CYS	3.9
1	D	414	PRO	3.9
1	D	313	LEU	3.8
1	D	104	TRP	3.8
1	D	394	ALA	3.8
1	D	395	LEU	3.8
1	D	455	LEU	3.8
1	D	287	VAL	3.8
1	D	133	LEU	3.8
1	D	291	LEU	3.8
1	D	343	PHE	3.8
1	C	436	PRO	3.7
1	D	318	GLY	3.7
1	D	180	ALA	3.7
1	B	106	GLU	3.7
1	D	374	ARG	3.7
1	D	363	GLY	3.7
1	D	330	VAL	3.7
1	D	312	ALA	3.7
1	A	432	ARG	3.7
1	D	136	CYS	3.7
1	D	224	VAL	3.7
1	D	191	LEU	3.6
1	B	433	ARG	3.6
1	D	308	THR	3.6
1	D	346	MET	3.6
1	A	434	GLY	3.6
1	D	265	ARG	3.6
1	B	154	THR	3.6
1	D	162	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	125	VAL	3.5
1	D	266	VAL	3.5
1	D	477	VAL	3.5
1	B	179	GLN	3.5
1	D	444	GLY	3.5
1	A	457	GLU	3.5
1	D	349	ALA	3.5
1	C	376	ARG	3.4
1	B	142	MET	3.4
1	D	426	ASP	3.4
1	D	333	ALA	3.4
1	D	381	LEU	3.4
1	D	328	ALA	3.4
1	D	409	SER	3.4
1	B	101	GLN	3.4
1	D	229	ALA	3.3
1	D	272	ALA	3.3
1	D	315	TRP	3.3
1	D	322	THR	3.3
1	D	389	VAL	3.3
1	D	347	LEU	3.3
1	D	157	LYS	3.3
1	D	192	VAL	3.3
1	A	316	LEU	3.3
1	D	189	GLU	3.3
1	D	102	LEU	3.2
1	B	434	GLY	3.2
1	B	432	ARG	3.2
1	D	470	PRO	3.2
1	D	176	LEU	3.2
1	D	461	LEU	3.2
1	B	385	ALA	3.2
1	C	445	PRO	3.2
1	D	373	PRO	3.2
1	C	321	GLY	3.2
1	C	467	PHE	3.2
1	D	108	TRP	3.2
1	C	461	LEU	3.1
1	C	110	GLN	3.1
1	D	159	GLU	3.1
1	D	323	GLN	3.1
1	D	344	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	164	PHE	3.1
1	C	429	GLN	3.1
1	D	185	VAL	3.1
1	D	141	PRO	3.1
1	C	380	GLU	3.1
1	D	250	GLU	3.1
1	B	178	ASP	3.1
1	D	148	LEU	3.1
1	D	262	LEU	3.1
1	A	143	ILE	3.1
1	D	270	LEU	3.0
1	C	426	ASP	3.0
1	C	462	SER	3.0
1	D	281	VAL	3.0
1	C	479	PRO	3.0
1	D	238	ALA	3.0
1	D	459	LEU	3.0
1	D	321	GLY	3.0
1	D	390	GLU	3.0
1	D	188	SER	3.0
1	A	140	VAL	3.0
1	D	392	VAL	3.0
1	D	239	GLY	3.0
1	D	314	LEU	2.9
1	D	438	LEU	2.9
1	A	116	HIS	2.9
1	C	463	ASP	2.9
1	B	41	ARG	2.9
1	B	148	LEU	2.9
1	D	139	LYS	2.9
1	D	274	ASP	2.9
1	B	110	GLN	2.9
1	B	358	ARG	2.9
1	D	256	VAL	2.9
1	A	171	GLU	2.9
1	D	457	GLU	2.9
1	D	105	PRO	2.9
1	A	42	MET	2.9
1	A	142	MET	2.9
1	B	39	LEU	2.9
1	B	391	LEU	2.9
1	A	433	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	48	ARG	2.9
1	D	370	GLN	2.9
1	D	451	GLN	2.9
1	D	158	LEU	2.8
1	D	310	GLY	2.8
1	D	456	GLN	2.8
1	B	457	GLU	2.8
1	A	385	ALA	2.8
1	D	441	HIS	2.8
1	C	470	PRO	2.8
1	D	443	ASP	2.8
1	D	474	ALA	2.8
1	B	183	CYS	2.8
1	D	101	GLN	2.8
1	B	460	VAL	2.8
1	D	334	LEU	2.8
1	D	184	ILE	2.8
1	B	247	GLN	2.7
1	D	471	LEU	2.7
1	D	421	ALA	2.7
1	C	387	GLY	2.7
1	D	449	GLY	2.7
1	C	384	PRO	2.7
1	D	285	LEU	2.7
1	D	302	LEU	2.7
1	C	450	PRO	2.7
1	D	128	VAL	2.7
1	A	46	GLY	2.7
1	D	137	GLY	2.7
1	D	351	GLY	2.7
1	C	345	ARG	2.7
1	D	464	ARG	2.6
1	D	130	ALA	2.6
1	C	371	LEU	2.6
1	D	116	HIS	2.6
1	B	36	LEU	2.6
1	B	376	ARG	2.6
1	D	342	ARG	2.6
1	D	254	THR	2.6
1	B	223	LEU	2.6
1	D	113	VAL	2.6
1	D	174	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	473	PHE	2.6
1	B	116	HIS	2.6
1	B	430	ARG	2.6
1	C	265	ARG	2.6
1	B	34	LYS	2.6
1	A	126	SER	2.6
1	C	117	SER	2.6
1	C	423	LEU	2.6
1	D	442	ARG	2.6
1	D	114	ASP	2.5
1	D	257	GLY	2.5
1	D	296	GLY	2.5
1	B	232	VAL	2.5
1	C	125	VAL	2.5
1	D	419	VAL	2.5
1	B	143	ILE	2.5
1	D	295	ASP	2.5
1	B	125	VAL	2.5
1	B	103	GLU	2.5
1	D	181	GLY	2.5
1	D	329	ARG	2.5
1	A	178	ASP	2.5
1	D	439	ARG	2.5
1	B	126	SER	2.5
1	D	142	MET	2.5
1	D	143	ILE	2.5
1	D	146	ARG	2.5
1	D	131	PRO	2.5
1	C	116	HIS	2.5
1	D	280	CYS	2.5
1	D	297	ALA	2.5
1	D	320	ALA	2.5
1	D	375	ALA	2.5
1	A	467	PHE	2.4
1	D	377	GLU	2.4
1	D	412	GLY	2.4
1	A	179	GLN	2.4
1	C	456	GLN	2.4
1	D	178	ASP	2.4
1	D	397	LEU	2.4
1	D	447	LEU	2.4
1	D	252	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	269	ALA	2.4
1	B	242	PHE	2.4
1	D	335	ASP	2.4
1	D	391	LEU	2.4
1	C	182	CYS	2.4
1	D	415	LEU	2.4
1	B	107	ALA	2.4
1	B	243	PRO	2.4
1	A	163	GLY	2.4
1	C	119	GLY	2.4
1	B	104	TRP	2.4
1	B	184	ILE	2.4
1	A	345	ARG	2.4
1	B	75	LEU	2.3
1	B	127	LEU	2.3
1	D	155	LEU	2.3
1	B	185	VAL	2.3
1	D	234	VAL	2.3
1	D	306	VAL	2.3
1	D	469	ALA	2.3
1	D	413	GLU	2.3
1	C	236	PHE	2.3
1	A	145	GLY	2.3
1	C	281	VAL	2.3
1	D	58	VAL	2.3
1	A	242	PHE	2.3
1	B	108	TRP	2.3
1	C	315	TRP	2.3
1	C	177	LEU	2.3
1	C	128	VAL	2.3
1	C	131	PRO	2.3
1	D	472	PRO	2.3
1	B	214	ILE	2.3
1	C	171	GLU	2.3
1	B	440	VAL	2.3
1	D	339	ALA	2.3
1	A	41	ARG	2.3
1	D	153	GLY	2.3
1	D	144	SER	2.3
1	A	141	PRO	2.3
1	B	240	ALA	2.3
1	D	219	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	428	GLY	2.3
1	D	317	SER	2.3
1	A	463	ASP	2.3
1	C	381	LEU	2.3
1	D	208	VAL	2.2
1	D	145	GLY	2.2
1	B	182	CYS	2.2
1	D	220	SER	2.2
1	D	48	ARG	2.2
1	A	397	LEU	2.2
1	A	458	ALA	2.2
1	D	340	LEU	2.2
1	A	165	ASN	2.2
1	C	457	GLU	2.2
1	D	304	ASP	2.2
1	B	48	ARG	2.2
1	D	417	LEU	2.2
1	B	128	VAL	2.2
1	C	62	VAL	2.2
1	D	273	MET	2.2
1	C	437	TRP	2.2
1	A	248	ALA	2.2
1	B	321	GLY	2.2
1	B	465	ALA	2.2
1	D	298	GLY	2.2
1	C	129	LEU	2.2
1	D	100	GLN	2.2
1	D	258	VAL	2.2
1	B	190	GLN	2.2
1	B	474	ALA	2.2
1	D	350	GLN	2.2
1	B	129	LEU	2.2
1	D	448	SER	2.2
1	A	110	GLN	2.2
1	B	56	GLY	2.2
1	D	300	PRO	2.2
1	D	380	GLU	2.2
1	D	327	ALA	2.2
1	C	173	MET	2.2
1	C	391	LEU	2.2
1	A	218	ILE	2.1
1	A	129	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	223	LEU	2.1
1	A	370	GLN	2.1
1	D	405	GLY	2.1
1	A	479	PRO	2.1
1	D	475	GLU	2.1
1	A	464	ARG	2.1
1	B	227	LEU	2.1
1	B	345	ARG	2.1
1	C	364	SER	2.1
1	D	190	GLN	2.1
1	D	372	LEU	2.1
1	D	423	LEU	2.1
1	A	231	VAL	2.1
1	D	47	GLY	2.1
1	D	311	GLY	2.1
1	B	342	ARG	2.1
1	D	267	ALA	2.1
1	D	169	SER	2.1
1	A	75	LEU	2.1
1	C	264	LEU	2.1
1	B	390	GLU	2.1
1	C	109	ARG	2.1
1	D	54	ILE	2.1
1	D	242	PHE	2.1
1	A	371	LEU	2.1
1	A	106	GLU	2.1
1	B	145	GLY	2.1
1	B	246	GLU	2.1
1	C	232	VAL	2.1
1	C	370	GLN	2.1
1	D	325	GLN	2.1
1	A	274	ASP	2.1
1	B	158	LEU	2.1
1	B	381	LEU	2.1
1	D	424	LEU	2.1
1	D	453	ARG	2.1
1	B	287	VAL	2.1
1	D	170	PRO	2.1
1	D	283	HIS	2.1
1	A	34	LYS	2.1
1	D	324	ALA	2.1
1	D	458	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	378	GLN	2.0
1	D	38	GLU	2.0
1	D	379	GLU	2.0
1	C	143	ILE	2.0
1	D	151	THR	2.0
1	A	356	LEU	2.0
1	B	382	LEU	2.0
1	A	192	VAL	2.0
1	A	35	GLN	2.0
1	D	245	GLN	2.0
1	C	181	GLY	2.0
1	A	130	ALA	2.0
1	C	211	LEU	2.0
1	A	48	ARG	2.0
1	A	342	ARG	2.0
1	A	374	ARG	2.0
1	C	249	ARG	2.0
1	D	126	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TDR	C	1480	9/9	0.21	0.05	2,2,2,2	0
2	TDR	B	1480	9/9	0.22	-0.66	2,3,3,4	0
2	TDR	A	1480	9/9	0.20	-0.83	2,2,2,2	0

6.5 Other polymers ⓘ

There are no such residues in this entry.