



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:42 am BST

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11



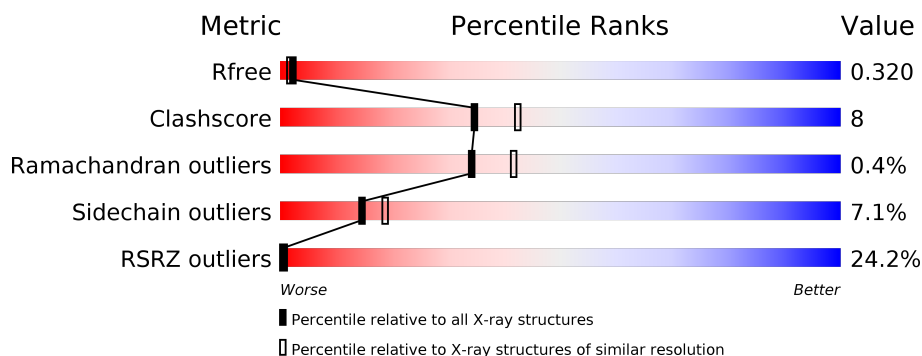
# 1 Overall quality at a glance

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))
$R_{free}$	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (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  $\geq 3$ , 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	<div> <div>9%</div> <div> <div>76%</div> <div>14%</div> <div>7%</div> </div> </div>
1	B	482	<div> <div>13%</div> <div> <div>74%</div> <div>16%</div> <div>7%</div> </div> </div>
1	C	482	<div> <div>13%</div> <div> <div>77%</div> <div>14%</div> <div>7%</div> </div> </div>
1	D	482	<div> <div>55%</div> <div> <div>77%</div> <div>13%</div> <div>7%</div> </div> </div>



## 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.

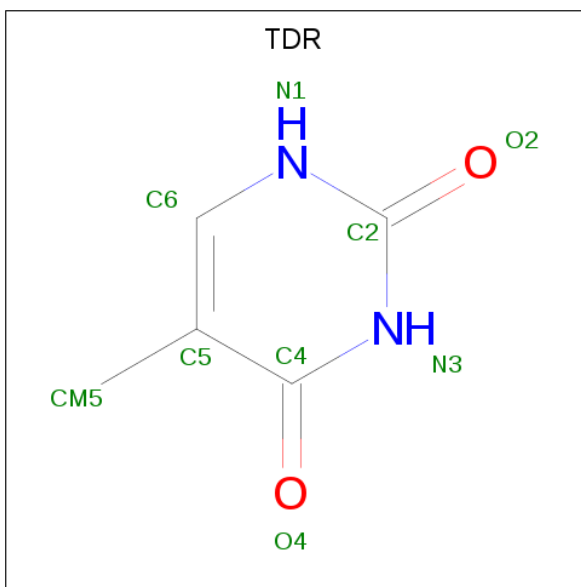
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	B	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	C	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			
1	D	446	Total	C	N	O	S	0	0	0
			3259	2038	597	608	16			

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 (three-letter code: TDR) (formula: C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>).





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.

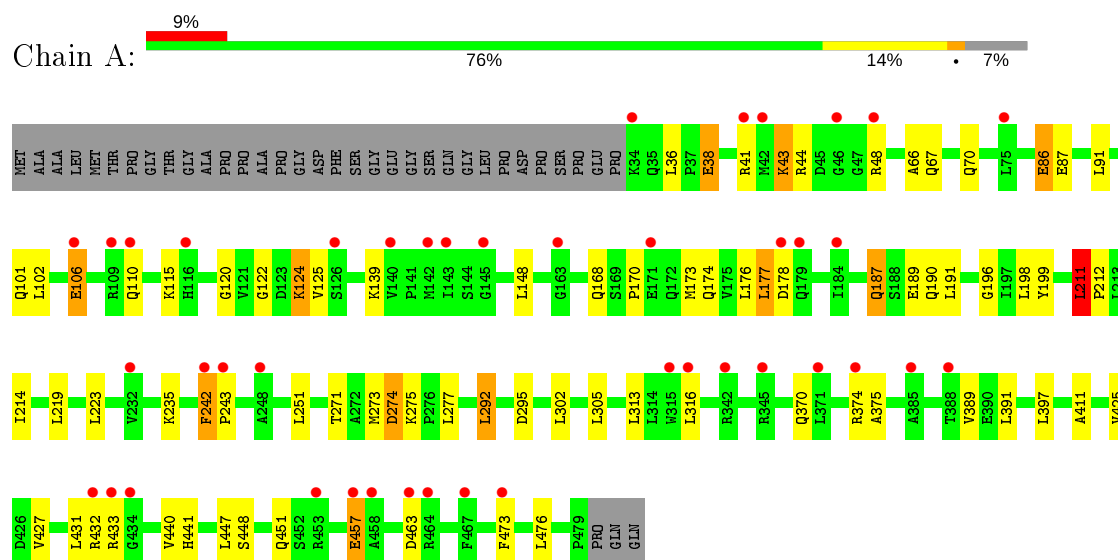
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		
3	B	95	Total	O	0	0
			95	95		
3	C	169	Total	O	0	0
			169	169		
3	D	67	Total	O	0	0
			67	67		



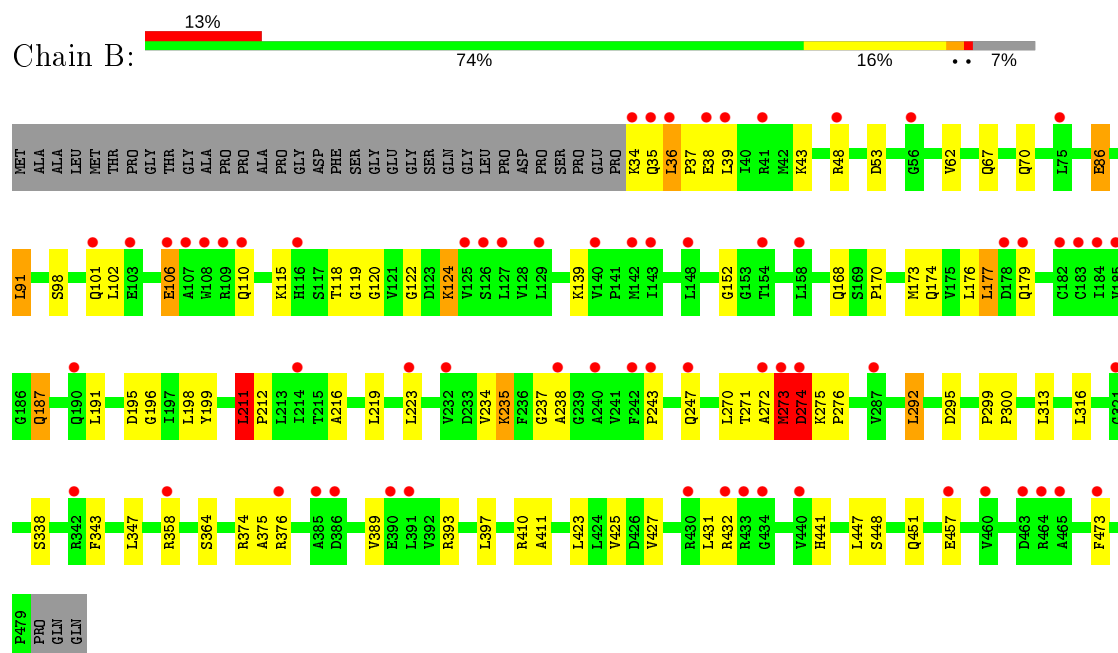
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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

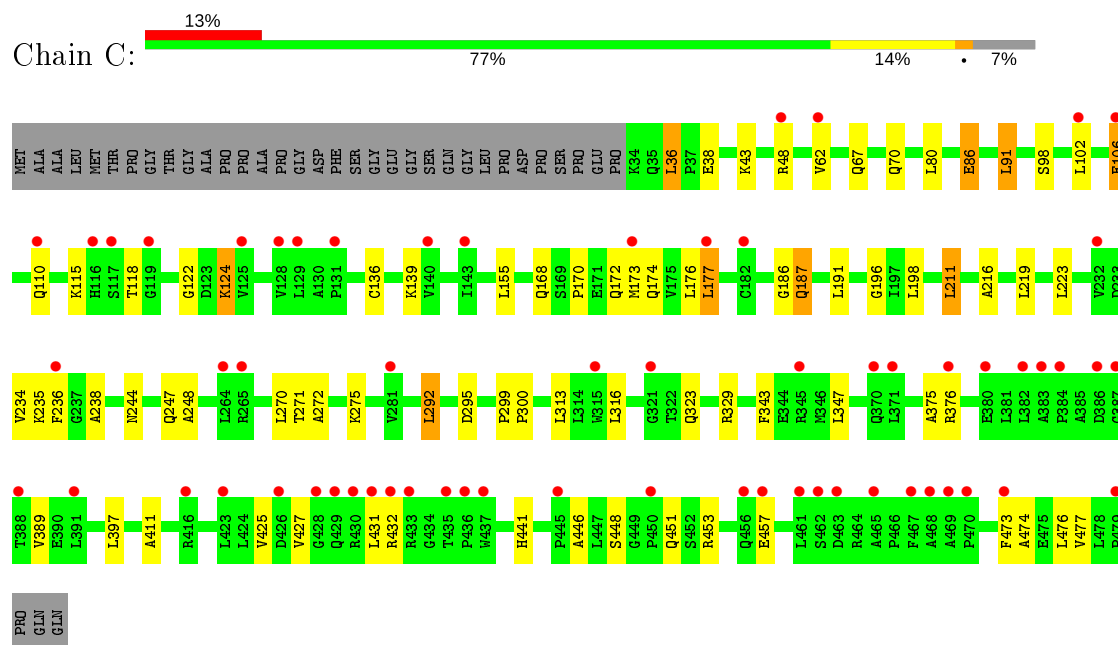


#### • Molecule 1: THYMIDINE PHOSPHORYLASE

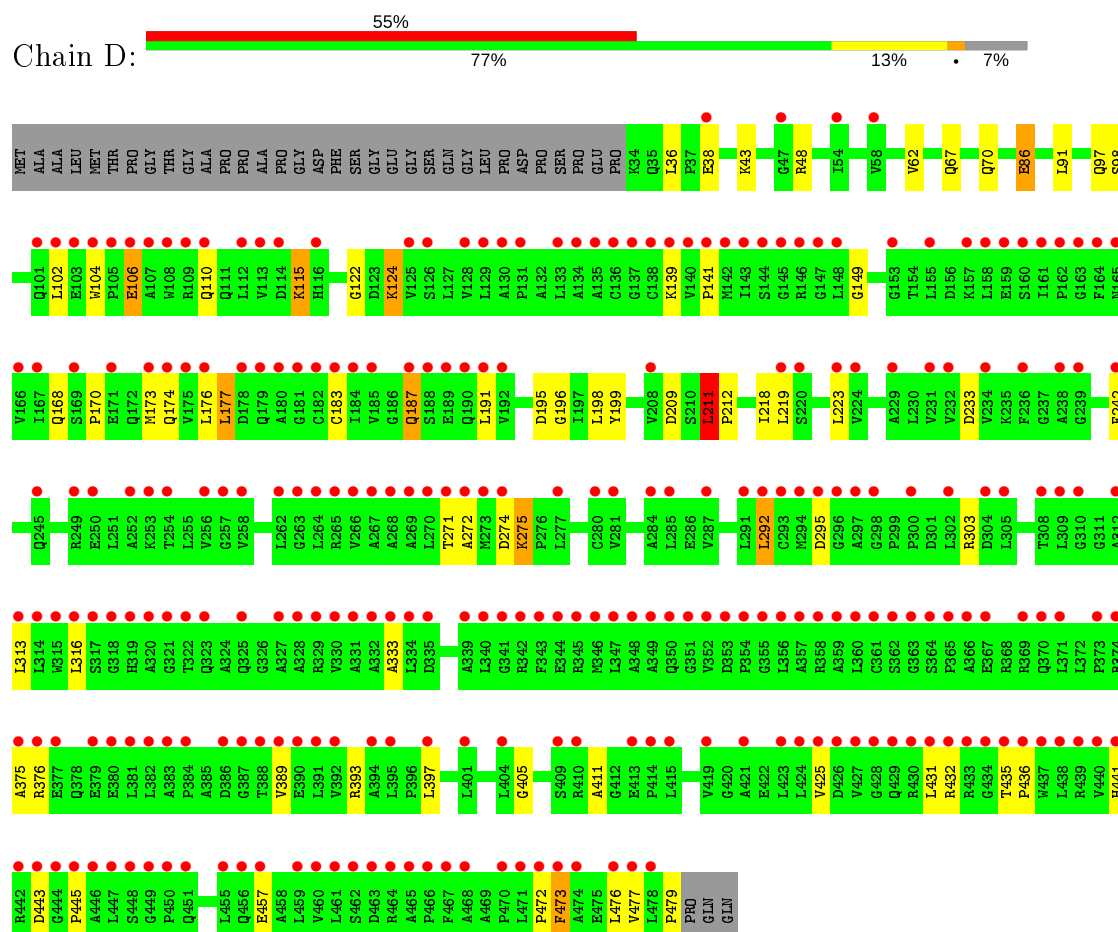




● Molecule 1: THYMIDINE PHOSPHORYLASE



● Molecule 1: THYMIDINE PHOSPHORYLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	32.0	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 32.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	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 <sup>2</sup> )	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.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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	0.48	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( $^{\circ}$ )	Ideal( $^{\circ}$ )
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 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	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

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 (220) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:PRO:HD3	3:D:2039:HOH:O	1.99	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: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:236:PHE:CZ	1:C:272:ALA:HB2	2.39	0.57
1:C:476:LEU:C	1:D:376:ARG:HH11	1.96	0.57
1:C:173:MET:CE	1:C:191:LEU:HD11	2.35	0.57
1:B:106:GLU:CD	1:B:106:GLU:H	2.09	0.56
1:C:67:GLN:H	1:C:70:GLN:HE21	1.52	0.56
1:A:273:MET:HG2	3:A:2074:HOH:O	2.05	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:B:273:MET:HB3	1:B:275:LYS:O	2.13	0.49
1:C:106:GLU:N	1:C:106:GLU:CD	2.66	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: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: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: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:N	1:D:432:ARG:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:102:LEU:HD21	1:C:173:MET:CE	2.46	0.45
1:C:36:LEU:HD22	1:C:70:GLN:HB3	1.97	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:D:106:GLU:N	1:D:106:GLU:CD	2.71	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
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: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:D:102:LEU:HD21	1:D:173:MET:HE3	2.00	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:195:ASP:O	1:B:199:TYR:HB2	2.19	0.42
1:B:62:VAL:HG21	1:B:98:SER:HB2	2.02	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: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:D:173:MET:HE1	1:D:191:LEU:HD11	2.02	0.41
1:A:102:LEU:HD21	1:A:173:MET:HE3	2.03	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: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: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
1:B:102:LEU:HD21	1:B:173:MET:HE3	2.03	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: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: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 sym-



metry 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 [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	444/482 (92%)	435 (98%)	8 (2%)	1 (0%)	47 58
1	B	444/482 (92%)	434 (98%)	8 (2%)	2 (0%)	29 35
1	C	444/482 (92%)	433 (98%)	10 (2%)	1 (0%)	47 58
1	D	444/482 (92%)	434 (98%)	7 (2%)	3 (1%)	22 26
All	All	1776/1928 (92%)	1736 (98%)	33 (2%)	7 (0%)	34 41

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%)	310 (93%)	23 (7%)	15	20
1	B	333/359 (93%)	308 (92%)	25 (8%)	13	16
1	C	333/359 (93%)	311 (93%)	22 (7%)	16	22
1	D	333/359 (93%)	309 (93%)	24 (7%)	14	18
All	All	1332/1436 (93%)	1238 (93%)	94 (7%)	14	19

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

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Mol	Chain	Res	Type
1	B	124	LYS
1	B	174	GLN
1	B	177	LEU
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

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Mol	Chain	Res	Type
1	D	86	GLU
1	D	91	LEU
1	D	106	GLU
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

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Mol	Chain	Res	Type
1	C	70	GLN
1	C	100	GLN
1	C	101	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	174	GLN
1	D	190	GLN
1	D	245	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 carbohydrates 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	A	1480	-	8,9,9	1.97	1 (12%)	6,12,12	5.29	4 (66%)
2	TDR	C	1480	-	8,9,9	1.70	1 (12%)	6,12,12	5.34	4 (66%)
2	TDR	B	1480	-	8,9,9	1.78	1 (12%)	6,12,12	5.57	4 (66%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1480	TDR	O4-C4	4.54	1.36	1.24
2	B	1480	TDR	O4-C4	3.92	1.34	1.24
2	C	1480	TDR	O4-C4	3.73	1.33	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1480	TDR	N1-C2-N3	-10.31	120.23	128.43
2	C	1480	TDR	N1-C2-N3	-9.76	120.67	128.43
2	A	1480	TDR	N1-C2-N3	-9.04	121.24	128.43
2	A	1480	TDR	C4-N3-C2	6.15	120.33	115.14
2	A	1480	TDR	C5-C6-N1	-5.94	119.11	125.16
2	B	1480	TDR	C4-N3-C2	5.76	120.00	115.14
2	B	1480	TDR	C5-C6-N1	-5.65	119.40	125.16
2	C	1480	TDR	C5-C6-N1	-5.59	119.47	125.16
2	C	1480	TDR	C4-N3-C2	5.53	119.81	115.14
2	B	1480	TDR	C6-N1-C2	3.76	121.56	115.36
2	C	1480	TDR	C6-N1-C2	3.66	121.40	115.36
2	A	1480	TDR	C6-N1-C2	3.52	121.17	115.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.



3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1480	TDR	1	0
2	C	1480	TDR	1	0
2	B	1480	TDR	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	446/482 (92%)	0.88	42 (9%) <b>8</b> <b>11</b>	3, 9, 28, 46	2 (0%)
1	B	446/482 (92%)	1.14	65 (14%) <b>2</b> <b>3</b>	4, 10, 28, 46	2 (0%)
1	C	446/482 (92%)	1.08	62 (13%) <b>2</b> <b>4</b>	4, 9, 27, 46	2 (0%)
1	D	446/482 (92%)	2.55	263 (58%) <b>0</b> <b>0</b>	4, 10, 30, 51	2 (0%)
All	All	1784/1928 (92%)	1.41	432 (24%) <b>0</b> <b>1</b>	3, 10, 28, 51	8 (0%)

All (432) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	10.5
1	D	445	PRO	9.2
1	D	446	ALA	8.0
1	C	383	ALA	8.0
1	D	465	ALA	7.8
1	B	273	MET	7.8
1	D	352	VAL	7.5
1	D	430	ARG	7.3
1	D	383	ALA	7.3
1	D	171	GLU	7.2
1	C	473	PHE	7.1
1	D	167	ILE	6.9
1	D	362	SER	6.8
1	D	382	LEU	6.7
1	D	360	LEU	6.5
1	C	435	THR	6.4
1	B	274	ASP	6.4
1	D	436	PRO	6.4
1	D	263	GLY	6.2
1	D	166	VAL	6.2
1	D	356	LEU	6.1

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Mol	Chain	Res	Type	RSRZ
1	D	358	ARG	6.1
1	D	384	PRO	6.1
1	A	243	PRO	6.0
1	C	432	ARG	6.0
1	D	388	THR	5.9
1	D	292	LEU	5.8
1	D	432	ARG	5.8
1	D	253	LYS	5.7
1	D	431	LEU	5.7
1	D	106	GLU	5.7
1	D	316	LEU	5.6
1	D	434	GLY	5.6
1	D	433	ARG	5.5
1	D	462	SER	5.5
1	D	348	ALA	5.5
1	D	468	ALA	5.5
1	A	109	ARG	5.4
1	D	354	PRO	5.4
1	D	309	LEU	5.4
1	D	371	LEU	5.3
1	C	465	ALA	5.3
1	D	401	LEU	5.2
1	D	386	ASP	5.2
1	D	361	CYS	5.1
1	D	140	VAL	5.1
1	D	467	PHE	5.1
1	D	179	GLN	5.1
1	D	103	GLU	5.0
1	D	160	SER	5.0
1	D	165	ASN	5.0
1	D	364	SER	5.0
1	D	476	LEU	5.0
1	D	367	GLU	4.9
1	D	428	GLY	4.9
1	D	473	PHE	4.9
1	D	305	LEU	4.9
1	D	353	ASP	4.9
1	D	410	ARG	4.8
1	D	134	ALA	4.8
1	D	369	ARG	4.8
1	C	469	ALA	4.8
1	D	249	ARG	4.7

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Mol	Chain	Res	Type	RSRZ
1	B	38	GLU	4.7
1	D	236	PHE	4.7
1	D	173	MET	4.7
1	D	109	ARG	4.7
1	D	175	VAL	4.6
1	D	232	VAL	4.6
1	D	345	ARG	4.6
1	D	110	GLN	4.6
1	D	463	ASP	4.6
1	C	430	ARG	4.5
1	D	387	GLY	4.5
1	B	473	PHE	4.5
1	B	272	ALA	4.5
1	D	435	THR	4.4
1	B	238	ALA	4.4
1	C	433	ARG	4.4
1	D	437	TRP	4.4
1	D	425	VAL	4.4
1	D	376	ARG	4.4
1	D	147	GLY	4.3
1	D	294	MET	4.3
1	D	112	LEU	4.3
1	D	341	GLY	4.3
1	B	106	GLU	4.3
1	D	331	ALA	4.2
1	B	109	ARG	4.2
1	D	349	ALA	4.2
1	D	414	PRO	4.2
1	D	135	ALA	4.2
1	D	359	ALA	4.2
1	C	382	LEU	4.1
1	D	129	LEU	4.1
1	D	318	GLY	4.1
1	B	463	ASP	4.1
1	D	271	THR	4.1
1	D	365	PRO	4.1
1	D	450	PRO	4.0
1	D	404	LEU	4.0
1	D	429	GLN	4.0
1	D	308	THR	4.0
1	D	231	VAL	4.0
1	D	477	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	265	ARG	4.0
1	D	312	ALA	4.0
1	D	466	PRO	4.0
1	C	388	THR	4.0
1	D	363	GLY	3.9
1	D	319	HIS	3.9
1	A	434	GLY	3.9
1	D	182	CYS	3.9
1	A	315	TRP	3.9
1	D	104	TRP	3.8
1	B	179	GLN	3.8
1	D	138	CYS	3.8
1	D	180	ALA	3.8
1	C	468	ALA	3.8
1	D	136	CYS	3.7
1	D	355	GLY	3.7
1	D	224	VAL	3.7
1	D	343	PHE	3.7
1	D	313	LEU	3.7
1	C	436	PRO	3.7
1	B	433	ARG	3.6
1	D	322	THR	3.6
1	C	110	GLN	3.6
1	D	346	MET	3.6
1	D	366	ALA	3.6
1	D	192	VAL	3.6
1	D	374	ARG	3.5
1	D	125	VAL	3.5
1	D	264	LEU	3.5
1	C	445	PRO	3.5
1	D	357	ALA	3.5
1	B	35	GLN	3.5
1	D	161	ILE	3.5
1	D	330	VAL	3.5
1	D	440	VAL	3.5
1	C	386	ASP	3.5
1	D	291	LEU	3.5
1	D	266	VAL	3.4
1	D	183	CYS	3.4
1	D	347	LEU	3.4
1	D	409	SER	3.4
1	D	333	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	238	ALA	3.4
1	C	376	ARG	3.4
1	A	432	ARG	3.4
1	D	185	VAL	3.3
1	D	287	VAL	3.3
1	B	142	MET	3.3
1	D	323	GLN	3.3
1	B	101	GLN	3.3
1	D	250	GLU	3.3
1	B	154	THR	3.3
1	A	433	ARG	3.3
1	D	137	GLY	3.3
1	C	461	LEU	3.3
1	C	426	ASP	3.3
1	D	395	LEU	3.2
1	B	385	ALA	3.2
1	D	457	GLU	3.2
1	D	270	LEU	3.2
1	D	102	LEU	3.2
1	D	455	LEU	3.2
1	D	269	ALA	3.2
1	D	133	LEU	3.2
1	D	163	GLY	3.2
1	C	467	PHE	3.2
1	D	256	VAL	3.2
1	D	344	GLU	3.2
1	D	315	TRP	3.1
1	D	285	LEU	3.1
1	C	462	SER	3.1
1	D	229	ALA	3.1
1	D	272	ALA	3.1
1	D	426	ASP	3.1
1	D	176	LEU	3.1
1	A	457	GLU	3.1
1	C	106	GLU	3.1
1	D	373	PRO	3.1
1	B	432	ARG	3.1
1	D	191	LEU	3.1
1	D	157	LYS	3.1
1	C	431	LEU	3.1
1	D	456	GLN	3.1
1	D	105	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	107	ALA	3.1
1	D	188	SER	3.0
1	D	461	LEU	3.0
1	D	295	ASP	3.0
1	D	139	LYS	3.0
1	D	389	VAL	3.0
1	B	434	GLY	3.0
1	D	328	ALA	3.0
1	D	148	LEU	3.0
1	B	457	GLU	3.0
1	D	189	GLU	3.0
1	B	41	ARG	3.0
1	D	390	GLU	3.0
1	D	392	VAL	3.0
1	D	381	LEU	3.0
1	D	394	ALA	3.0
1	D	415	LEU	2.9
1	A	143	ILE	2.9
1	D	257	GLY	2.9
1	A	316	LEU	2.9
1	B	110	GLN	2.9
1	B	178	ASP	2.9
1	A	42	MET	2.9
1	C	321	GLY	2.9
1	C	479	PRO	2.9
1	D	116	HIS	2.9
1	A	171	GLU	2.9
1	B	148	LEU	2.9
1	D	128	VAL	2.9
1	D	178	ASP	2.9
1	D	162	PRO	2.9
1	C	48	ARG	2.9
1	B	183	CYS	2.8
1	D	310	GLY	2.8
1	D	370	GLN	2.8
1	B	242	PHE	2.8
1	C	380	GLU	2.8
1	D	158	LEU	2.8
1	D	438	LEU	2.8
1	D	460	VAL	2.8
1	D	280	CYS	2.8
1	A	116	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	159	GLU	2.8
1	A	242	PHE	2.7
1	D	379	GLU	2.7
1	B	376	ARG	2.7
1	D	441	HIS	2.7
1	D	470	PRO	2.7
1	D	339	ALA	2.7
1	D	164	PHE	2.7
1	D	314	LEU	2.7
1	B	126	SER	2.7
1	D	141	PRO	2.7
1	A	140	VAL	2.7
1	B	125	VAL	2.7
1	B	358	ARG	2.7
1	C	345	ARG	2.7
1	D	281	VAL	2.7
1	D	262	LEU	2.7
1	D	296	GLY	2.7
1	D	443	ASP	2.7
1	B	39	LEU	2.7
1	B	391	LEU	2.7
1	D	302	LEU	2.7
1	D	459	LEU	2.7
1	A	142	MET	2.7
1	C	384	PRO	2.7
1	D	342	ARG	2.7
1	A	385	ALA	2.7
1	D	335	ASP	2.7
1	A	473	PHE	2.7
1	D	113	VAL	2.7
1	D	334	LEU	2.7
1	C	450	PRO	2.6
1	B	240	ALA	2.6
1	D	320	ALA	2.6
1	B	48	ARG	2.6
1	D	317	SER	2.6
1	D	321	GLY	2.6
1	C	429	GLN	2.6
1	B	34	LYS	2.6
1	C	387	GLY	2.6
1	D	444	GLY	2.6
1	D	449	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	254	THR	2.6
1	B	460	VAL	2.6
1	B	103	GLU	2.6
1	D	108	TRP	2.6
1	D	474	ALA	2.6
1	C	177	LEU	2.6
1	D	101	GLN	2.6
1	D	142	MET	2.5
1	D	274	ASP	2.5
1	D	181	GLY	2.5
1	D	451	GLN	2.5
1	D	329	ARG	2.5
1	C	119	GLY	2.5
1	D	146	ARG	2.5
1	D	464	ARG	2.5
1	D	267	ALA	2.5
1	C	463	ASP	2.5
1	B	430	ARG	2.5
1	C	371	LEU	2.5
1	B	143	ILE	2.5
1	A	126	SER	2.4
1	D	220	SER	2.4
1	C	62	VAL	2.4
1	D	442	ARG	2.4
1	D	377	GLU	2.4
1	D	114	ASP	2.4
1	A	464	ARG	2.4
1	B	184	ILE	2.4
1	C	265	ARG	2.4
1	D	424	LEU	2.4
1	A	179	GLN	2.4
1	D	252	ALA	2.4
1	D	421	ALA	2.4
1	A	178	ASP	2.4
1	A	463	ASP	2.4
1	D	184	ILE	2.4
1	C	102	LEU	2.4
1	D	391	LEU	2.4
1	A	163	GLY	2.4
1	D	130	ALA	2.4
1	D	439	ARG	2.4
1	B	232	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	110	GLN	2.4
1	B	75	LEU	2.4
1	D	380	GLU	2.3
1	A	106	GLU	2.3
1	D	143	ILE	2.3
1	C	456	GLN	2.3
1	C	470	PRO	2.3
1	C	117	SER	2.3
1	C	182	CYS	2.3
1	C	391	LEU	2.3
1	C	423	LEU	2.3
1	D	297	ALA	2.3
1	B	56	GLY	2.3
1	D	242	PHE	2.3
1	A	345	ARG	2.3
1	D	304	ASP	2.3
1	B	223	LEU	2.3
1	D	447	LEU	2.3
1	C	428	GLY	2.3
1	D	153	GLY	2.3
1	C	116	HIS	2.3
1	C	128	VAL	2.3
1	D	258	VAL	2.3
1	B	342	ARG	2.3
1	C	143	ILE	2.3
1	B	129	LEU	2.3
1	D	155	LEU	2.3
1	B	116	HIS	2.3
1	C	125	VAL	2.3
1	B	127	LEU	2.2
1	D	219	LEU	2.2
1	D	273	MET	2.2
1	B	182	CYS	2.2
1	D	58	VAL	2.2
1	D	419	VAL	2.2
1	B	243	PRO	2.2
1	D	397	LEU	2.2
1	D	187	GLN	2.2
1	D	126	SER	2.2
1	D	47	GLY	2.2
1	B	190	GLN	2.2
1	D	234	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	465	ALA	2.2
1	D	471	LEU	2.2
1	D	208	VAL	2.2
1	D	239	GLY	2.2
1	A	248	ALA	2.2
1	B	108	TRP	2.2
1	A	41	ARG	2.2
1	A	75	LEU	2.2
1	A	453	ARG	2.2
1	C	416	ARG	2.2
1	D	223	LEU	2.2
1	D	131	PRO	2.2
1	B	440	VAL	2.2
1	C	129	LEU	2.2
1	D	144	SER	2.2
1	D	169	SER	2.2
1	A	34	LYS	2.1
1	D	145	GLY	2.2
1	D	413	GLU	2.1
1	B	36	LEU	2.1
1	C	236	PHE	2.1
1	D	332	ALA	2.1
1	B	247	GLN	2.1
1	A	46	GLY	2.1
1	A	48	ARG	2.1
1	A	145	GLY	2.1
1	D	351	GLY	2.1
1	C	232	VAL	2.1
1	D	375	ALA	2.1
1	D	54	ILE	2.1
1	A	371	LEU	2.1
1	B	158	LEU	2.1
1	D	478	LEU	2.1
1	C	173	MET	2.1
1	D	190	GLN	2.1
1	D	245	GLN	2.1
1	D	472	PRO	2.1
1	A	184	ILE	2.1
1	B	386	ASP	2.1
1	D	325	GLN	2.1
1	A	374	ARG	2.1
1	C	457	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	293	CYS	2.1
1	D	268	ALA	2.1
1	A	232	VAL	2.1
1	C	131	PRO	2.1
1	D	350	GLN	2.1
1	D	284	ALA	2.1
1	B	321	GLY	2.1
1	C	437	TRP	2.1
1	D	427	VAL	2.1
1	A	467	PHE	2.1
1	D	298	GLY	2.0
1	B	140	VAL	2.0
1	B	185	VAL	2.0
1	D	300	PRO	2.0
1	B	214	ILE	2.0
1	D	277	LEU	2.0
1	D	340	LEU	2.0
1	D	423	LEU	2.0
1	B	390	GLU	2.0
1	C	370	GLN	2.0
1	D	174	GLN	2.0
1	D	327	ALA	2.0
1	D	448	SER	2.0
1	B	464	ARG	2.0
1	B	287	VAL	2.0
1	C	140	VAL	2.0
1	C	281	VAL	2.0
1	C	315	TRP	2.0
1	C	264	LEU	2.0
1	D	38	GLU	2.0
1	A	342	ARG	2.0
1	A	388	THR	2.0
1	A	458	ALA	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 [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, 95<sup>th</sup> 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	0.94	0.22	2,2,2,2	0
2	TDR	B	1480	9/9	0.94	0.23	2,3,3,4	0
2	TDR	A	1480	9/9	0.95	0.21	2,2,2,2	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.