Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:51 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

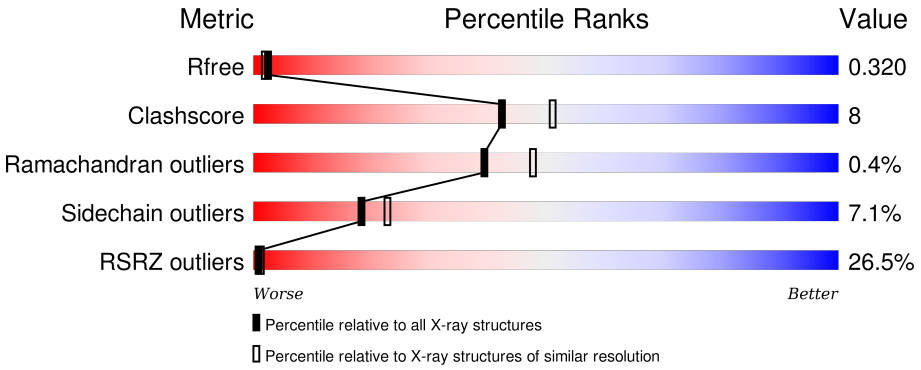
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (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. 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 <=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	11% 76% 14% • 7%
1	B	482	16% 74% 16% •• 7%
1	C	482	15% 77% 14% • 7%
1	D	482	56% 77% 13% • 7%

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.

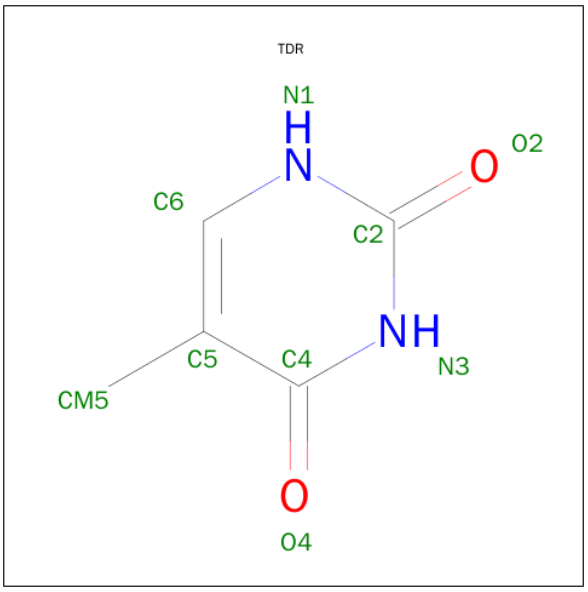
- Molecule 1 is a protein called THYMIDINE PHOSPHORYLASE.

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: $C_5H_6N_2O_2$).



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

- Molecule 3 is water.

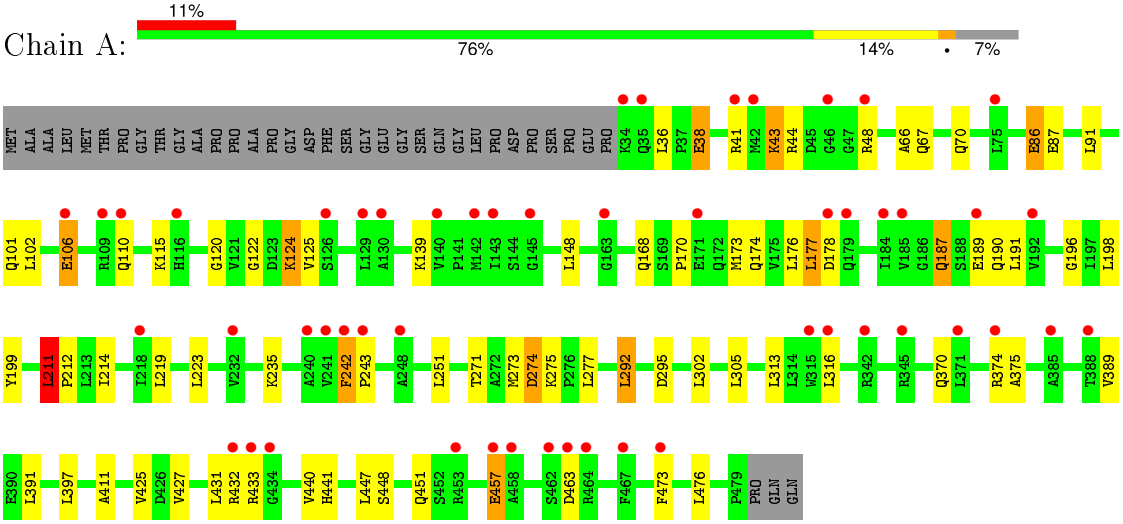
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	119	Total O 119 119	0	0
3	B	95	Total O 95 95	0	0
3	C	169	Total O 169 169	0	0
3	D	67	Total O 67 67	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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.

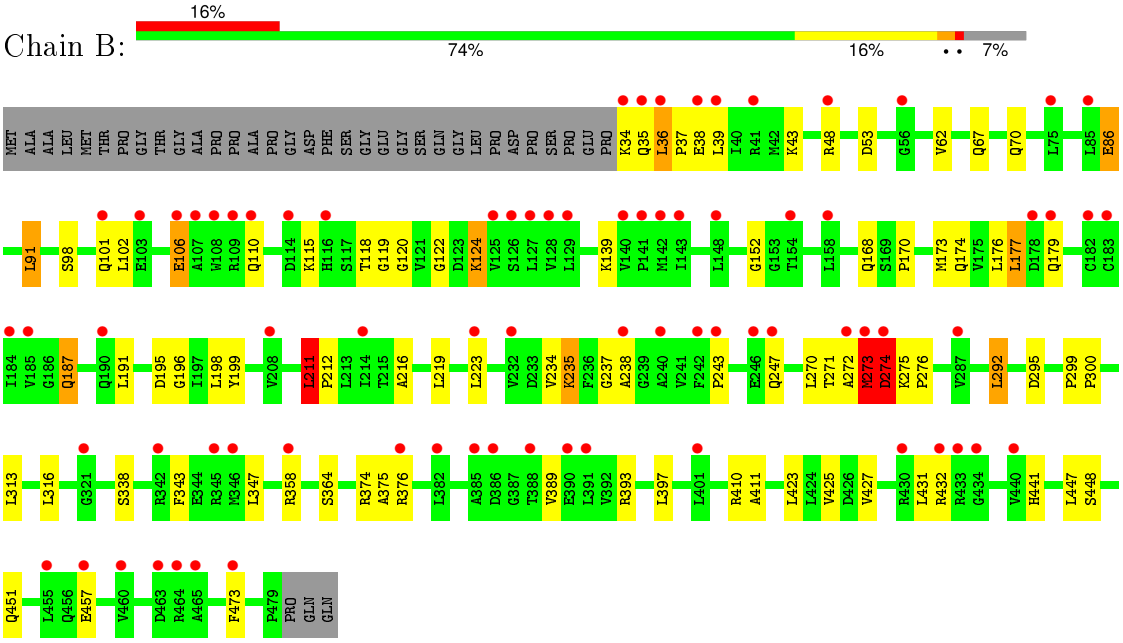
- Molecule 1: THYMIDINE PHOSPHORYLASE

Chain A:



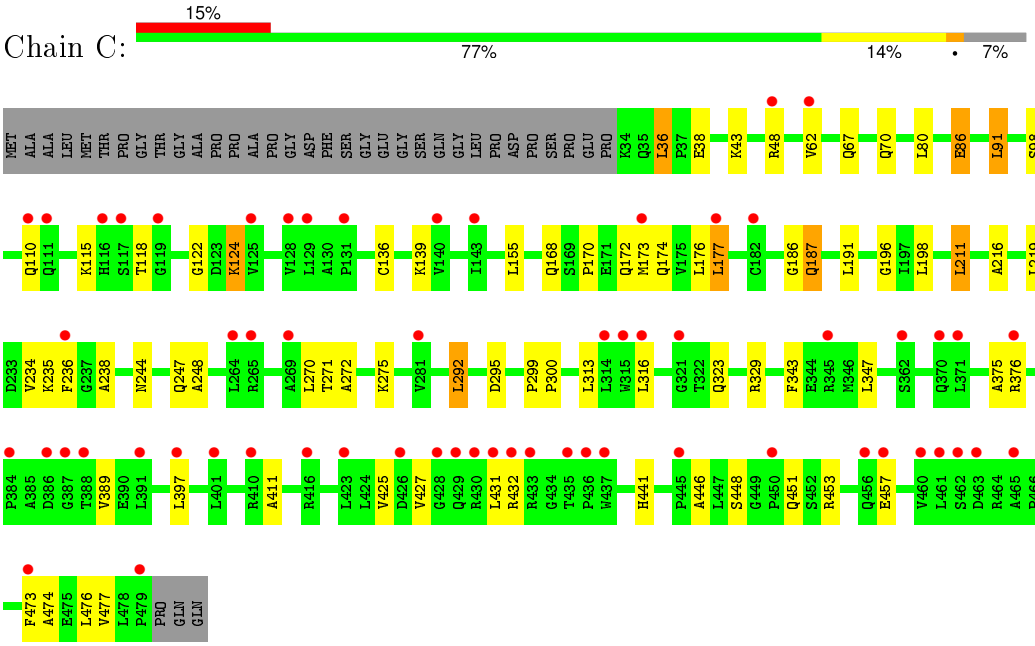
- Molecule 1: THYMIDINE PHOSPHORYLASE

Chain B:



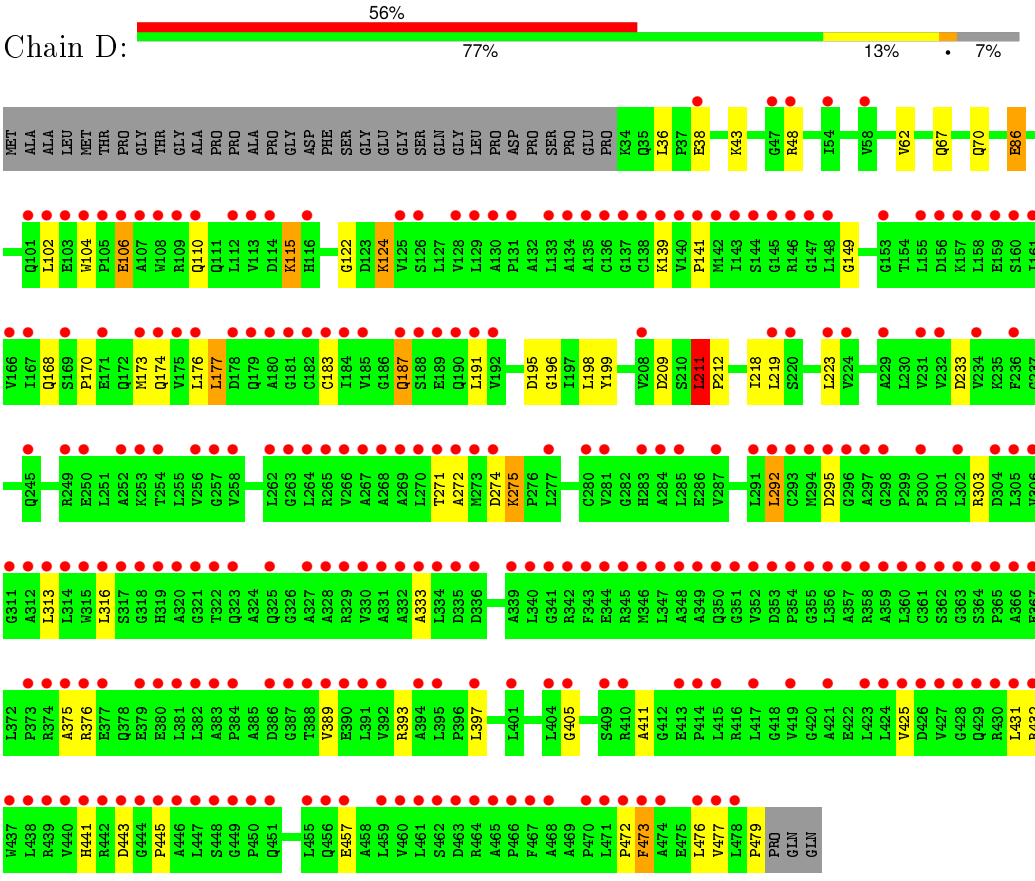
- Molecule 1: THYMIDINE PHOSPHORYLASE

Chain C:



• Molecule 1: THYMIDINE PHOSPHORYLASE

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.34%)	DCC
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.538	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 32.8	EDS
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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(^{o})	Ideal(^{o})
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 (i)

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: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

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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:D:187:GLN:HG3	1:D:196:GLY:HA3	1.90	0.50
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

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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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 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%)	52	64
1	B	444/482 (92%)	434 (98%)	8 (2%)	2 (0%)	34	40
1	C	444/482 (92%)	433 (98%)	10 (2%)	1 (0%)	52	64
1	D	444/482 (92%)	434 (98%)	7 (2%)	3 (1%)	26	31
All	All	1776/1928 (92%)	1736 (98%)	33 (2%)	7 (0%)	39	48

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%)	19 24
1	B	333/359 (93%)	308 (92%)	25 (8%)	17 20
1	C	333/359 (93%)	311 (93%)	22 (7%)	21 26
1	D	333/359 (93%)	309 (93%)	24 (7%)	18 22
All	All	1332/1436 (93%)	1238 (93%)	94 (7%)	18 23

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

There are no RNA molecules 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	-	5,9,9	2.24	1 (20%)	7,12,12	5.90	5 (71%)
2	TDR	B	1480	-	5,9,9	2.01	1 (20%)	7,12,12	6.13	5 (71%)
2	TDR	C	1480	-	5,9,9	1.82	1 (20%)	7,12,12	5.87	5 (71%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1480	TDR	O4-C4	3.85	1.33	1.24
2	B	1480	TDR	O4-C4	4.05	1.34	1.24
2	A	1480	TDR	O4-C4	4.71	1.36	1.24

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1480	TDR	N1-C2-N3	-12.70	120.23	128.33
2	C	1480	TDR	N1-C2-N3	-12.01	120.67	128.33
2	A	1480	TDR	N1-C2-N3	-11.12	121.24	128.33
2	A	1480	TDR	C5-C6-N1	-6.86	119.11	125.23
2	B	1480	TDR	C5-C6-N1	-6.53	119.40	125.23
2	C	1480	TDR	C5-C6-N1	-6.46	119.47	125.23
2	A	1480	TDR	C5-C4-N3	-5.01	119.56	125.14
2	B	1480	TDR	C5-C4-N3	-3.70	121.02	125.14
2	C	1480	TDR	C5-C4-N3	-3.62	121.11	125.14
2	A	1480	TDR	C6-N1-C2	3.55	121.17	115.47
2	C	1480	TDR	C6-N1-C2	3.69	121.40	115.47
2	B	1480	TDR	C6-N1-C2	3.79	121.56	115.47
2	C	1480	TDR	C4-N3-C2	5.28	119.81	115.25
2	B	1480	TDR	C4-N3-C2	5.50	120.00	115.25
2	A	1480	TDR	C4-N3-C2	5.89	120.33	115.25

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	B	1480	TDR	1	0
2	C	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^{th} 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%)	0.96	52 (11%) 6 10	3, 9, 28, 46	2 (0%)
1	B	446/482 (92%)	1.22	77 (17%) 2 3	4, 10, 28, 46	2 (0%)
1	C	446/482 (92%)	1.17	72 (16%) 3 4	4, 9, 27, 46	2 (0%)
1	D	446/482 (92%)	2.67	271 (60%) 0 0	4, 10, 30, 51	2 (0%)
All	All	1784/1928 (92%)	1.50	472 (26%) 1 1	3, 10, 28, 51	8 (0%)

All (472) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	107	ALA	10.9
1	D	445	PRO	9.5
1	D	446	ALA	8.3
1	C	383	ALA	8.2
1	D	465	ALA	8.1
1	B	273	MET	8.0
1	D	352	VAL	7.8
1	D	383	ALA	7.6
1	D	430	ARG	7.6
1	D	171	GLU	7.4
1	C	473	PHE	7.4
1	D	167	ILE	7.1
1	D	362	SER	7.0
1	D	382	LEU	7.0
1	D	360	LEU	6.7
1	C	435	THR	6.7
1	B	274	ASP	6.6
1	D	436	PRO	6.6
1	D	263	GLY	6.5
1	D	166	VAL	6.4
1	D	356	LEU	6.3

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Mol	Chain	Res	Type	RSRZ
1	A	243	PRO	6.3
1	D	384	PRO	6.3
1	D	358	ARG	6.2
1	C	432	ARG	6.1
1	D	388	THR	6.1
1	D	292	LEU	6.0
1	D	431	LEU	5.9
1	D	432	ARG	5.9
1	D	253	LYS	5.8
1	D	106	GLU	5.8
1	D	316	LEU	5.8
1	D	434	GLY	5.8
1	D	468	ALA	5.7
1	D	348	ALA	5.7
1	D	462	SER	5.7
1	D	433	ARG	5.7
1	D	354	PRO	5.6
1	D	309	LEU	5.6
1	D	371	LEU	5.6
1	C	465	ALA	5.5
1	A	109	ARG	5.5
1	D	401	LEU	5.4
1	D	361	CYS	5.4
1	D	386	ASP	5.3
1	D	140	VAL	5.3
1	D	165	ASN	5.2
1	D	160	SER	5.2
1	D	467	PHE	5.2
1	D	364	SER	5.2
1	D	428	GLY	5.2
1	D	179	GLN	5.2
1	D	103	GLU	5.2
1	D	473	PHE	5.1
1	D	476	LEU	5.1
1	D	367	GLU	5.1
1	D	305	LEU	5.0
1	D	353	ASP	5.0
1	D	134	ALA	5.0
1	D	410	ARG	5.0
1	C	469	ALA	4.9
1	D	369	ARG	4.9
1	D	175	VAL	4.9

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Mol	Chain	Res	Type	RSRZ
1	D	236	PHE	4.9
1	D	249	ARG	4.8
1	B	38	GLU	4.8
1	D	232	VAL	4.8
1	D	173	MET	4.8
1	D	109	ARG	4.8
1	D	463	ASP	4.7
1	B	473	PHE	4.7
1	D	110	GLN	4.7
1	C	430	ARG	4.7
1	D	345	ARG	4.7
1	D	387	GLY	4.7
1	B	272	ALA	4.7
1	D	435	THR	4.6
1	D	425	VAL	4.6
1	B	238	ALA	4.6
1	D	437	TRP	4.6
1	D	147	GLY	4.5
1	C	433	ARG	4.5
1	D	376	ARG	4.5
1	D	112	LEU	4.4
1	D	294	MET	4.4
1	D	341	GLY	4.4
1	B	106	GLU	4.4
1	C	382	LEU	4.3
1	D	135	ALA	4.3
1	D	349	ALA	4.3
1	D	359	ALA	4.3
1	D	331	ALA	4.3
1	D	414	PRO	4.3
1	D	129	LEU	4.3
1	B	109	ARG	4.3
1	D	318	GLY	4.3
1	B	463	ASP	4.2
1	D	271	THR	4.2
1	D	365	PRO	4.2
1	D	231	VAL	4.2
1	D	308	THR	4.2
1	D	404	LEU	4.2
1	D	450	PRO	4.2
1	D	477	VAL	4.2
1	D	429	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	265	ARG	4.1
1	D	312	ALA	4.1
1	C	388	THR	4.1
1	D	466	PRO	4.1
1	D	363	GLY	4.1
1	D	138	CYS	4.1
1	D	182	CYS	4.1
1	A	434	GLY	4.1
1	D	319	HIS	4.0
1	A	315	TRP	4.0
1	D	104	TRP	4.0
1	D	180	ALA	3.9
1	D	136	CYS	3.9
1	D	224	VAL	3.9
1	B	179	GLN	3.9
1	D	355	GLY	3.9
1	C	468	ALA	3.9
1	D	343	PHE	3.9
1	D	313	LEU	3.8
1	C	436	PRO	3.8
1	D	322	THR	3.7
1	B	433	ARG	3.7
1	C	110	GLN	3.7
1	D	192	VAL	3.7
1	D	366	ALA	3.7
1	D	346	MET	3.7
1	D	264	LEU	3.7
1	D	440	VAL	3.7
1	D	357	ALA	3.7
1	D	125	VAL	3.7
1	C	445	PRO	3.6
1	D	330	VAL	3.6
1	D	374	ARG	3.6
1	D	161	ILE	3.6
1	B	35	GLN	3.6
1	D	183	CYS	3.6
1	D	291	LEU	3.6
1	C	386	ASP	3.6
1	D	266	VAL	3.6
1	D	347	LEU	3.6
1	D	409	SER	3.5
1	D	333	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	238	ALA	3.5
1	D	185	VAL	3.5
1	D	287	VAL	3.5
1	B	142	MET	3.5
1	C	376	ARG	3.5
1	B	154	THR	3.5
1	D	323	GLN	3.5
1	A	432	ARG	3.4
1	D	250	GLU	3.4
1	D	137	GLY	3.4
1	B	101	GLN	3.4
1	A	433	ARG	3.4
1	C	461	LEU	3.4
1	D	395	LEU	3.4
1	D	455	LEU	3.4
1	B	385	ALA	3.4
1	C	426	ASP	3.4
1	D	102	LEU	3.4
1	D	270	LEU	3.4
1	D	457	GLU	3.3
1	D	256	VAL	3.3
1	D	133	LEU	3.3
1	C	467	PHE	3.3
1	D	163	GLY	3.3
1	D	269	ALA	3.3
1	C	462	SER	3.3
1	D	285	LEU	3.3
1	D	272	ALA	3.3
1	D	315	TRP	3.3
1	D	426	ASP	3.3
1	D	373	PRO	3.2
1	D	344	GLU	3.2
1	C	431	LEU	3.2
1	D	176	LEU	3.2
1	D	191	LEU	3.2
1	D	229	ALA	3.2
1	C	106	GLU	3.2
1	B	432	ARG	3.2
1	A	457	GLU	3.2
1	D	461	LEU	3.2
1	D	105	PRO	3.2
1	B	434	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	148	LEU	3.2
1	D	295	ASP	3.2
1	D	392	VAL	3.2
1	D	157	LYS	3.2
1	B	107	ALA	3.2
1	D	389	VAL	3.2
1	D	456	GLN	3.1
1	D	188	SER	3.1
1	D	328	ALA	3.1
1	D	394	ALA	3.1
1	B	457	GLU	3.1
1	D	139	LYS	3.1
1	A	143	ILE	3.1
1	D	189	GLU	3.1
1	D	257	GLY	3.1
1	A	316	LEU	3.1
1	D	381	LEU	3.1
1	D	415	LEU	3.1
1	B	41	ARG	3.1
1	D	390	GLU	3.1
1	B	110	GLN	3.1
1	B	178	ASP	3.1
1	A	42	MET	3.0
1	C	479	PRO	3.0
1	B	148	LEU	3.0
1	B	183	CYS	3.0
1	C	321	GLY	3.0
1	D	116	HIS	3.0
1	D	128	VAL	3.0
1	D	178	ASP	3.0
1	A	171	GLU	3.0
1	D	162	PRO	3.0
1	D	460	VAL	3.0
1	B	242	PHE	3.0
1	C	48	ARG	2.9
1	D	280	CYS	2.9
1	D	370	GLN	2.9
1	D	158	LEU	2.9
1	D	438	LEU	2.9
1	D	310	GLY	2.9
1	A	116	HIS	2.9
1	C	380	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	441	HIS	2.9
1	D	281	VAL	2.9
1	A	242	PHE	2.9
1	B	125	VAL	2.8
1	D	470	PRO	2.8
1	D	262	LEU	2.8
1	D	314	LEU	2.8
1	D	159	GLU	2.8
1	D	339	ALA	2.8
1	D	296	GLY	2.8
1	D	113	VAL	2.8
1	D	164	PHE	2.8
1	B	391	LEU	2.8
1	D	459	LEU	2.8
1	A	385	ALA	2.8
1	A	140	VAL	2.8
1	B	376	ARG	2.8
1	A	473	PHE	2.8
1	B	39	LEU	2.8
1	B	126	SER	2.8
1	D	302	LEU	2.8
1	C	450	PRO	2.8
1	D	141	PRO	2.8
1	D	379	GLU	2.8
1	D	443	ASP	2.8
1	D	335	ASP	2.8
1	B	240	ALA	2.8
1	B	358	ARG	2.8
1	C	345	ARG	2.8
1	C	384	PRO	2.8
1	D	317	SER	2.8
1	A	142	MET	2.8
1	D	320	ALA	2.8
1	D	474	ALA	2.8
1	D	444	GLY	2.7
1	D	334	LEU	2.7
1	D	342	ARG	2.7
1	C	387	GLY	2.7
1	D	449	GLY	2.7
1	B	48	ARG	2.7
1	D	108	TRP	2.7
1	D	321	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	460	VAL	2.7
1	C	177	LEU	2.7
1	C	429	GLN	2.7
1	B	103	GLU	2.7
1	D	254	THR	2.7
1	B	34	LYS	2.7
1	D	274	ASP	2.7
1	D	101	GLN	2.6
1	D	267	ALA	2.6
1	D	181	GLY	2.6
1	D	451	GLN	2.6
1	D	142	MET	2.6
1	C	119	GLY	2.6
1	C	463	ASP	2.6
1	C	62	VAL	2.6
1	C	371	LEU	2.6
1	B	143	ILE	2.6
1	D	329	ARG	2.6
1	D	464	ARG	2.6
1	B	430	ARG	2.6
1	D	146	ARG	2.6
1	D	421	ALA	2.6
1	A	126	SER	2.6
1	D	442	ARG	2.6
1	D	424	LEU	2.6
1	D	377	GLU	2.5
1	D	220	SER	2.5
1	D	252	ALA	2.5
1	B	184	ILE	2.5
1	D	114	ASP	2.5
1	A	179	GLN	2.5
1	A	178	ASP	2.5
1	A	463	ASP	2.5
1	B	232	VAL	2.5
1	D	130	ALA	2.5
1	A	464	ARG	2.5
1	B	75	LEU	2.5
1	C	102	LEU	2.5
1	C	265	ARG	2.5
1	A	163	GLY	2.5
1	D	184	ILE	2.5
1	A	110	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	391	LEU	2.5
1	C	182	CYS	2.5
1	C	470	PRO	2.5
1	D	439	ARG	2.5
1	B	56	GLY	2.4
1	C	117	SER	2.4
1	C	391	LEU	2.4
1	C	128	VAL	2.4
1	C	428	GLY	2.4
1	D	153	GLY	2.4
1	C	423	LEU	2.4
1	D	447	LEU	2.4
1	C	143	ILE	2.4
1	D	143	ILE	2.4
1	D	258	VAL	2.4
1	D	297	ALA	2.4
1	D	155	LEU	2.4
1	A	106	GLU	2.4
1	D	380	GLU	2.4
1	C	125	VAL	2.4
1	A	345	ARG	2.4
1	C	456	GLN	2.4
1	D	242	PHE	2.4
1	C	116	HIS	2.4
1	B	129	LEU	2.4
1	B	223	LEU	2.4
1	D	397	LEU	2.4
1	D	234	VAL	2.4
1	D	304	ASP	2.4
1	B	116	HIS	2.4
1	B	182	CYS	2.4
1	B	342	ARG	2.4
1	B	127	LEU	2.4
1	D	219	LEU	2.4
1	D	273	MET	2.4
1	D	58	VAL	2.4
1	B	243	PRO	2.4
1	D	419	VAL	2.3
1	D	208	VAL	2.3
1	B	465	ALA	2.3
1	D	47	GLY	2.3
1	D	239	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	75	LEU	2.3
1	B	440	VAL	2.3
1	B	190	GLN	2.3
1	D	187	GLN	2.3
1	D	223	LEU	2.3
1	D	471	LEU	2.3
1	A	248	ALA	2.3
1	D	126	SER	2.3
1	B	108	TRP	2.3
1	C	129	LEU	2.3
1	D	131	PRO	2.3
1	D	375	ALA	2.3
1	D	144	SER	2.3
1	D	169	SER	2.3
1	D	351	GLY	2.2
1	C	232	VAL	2.2
1	D	293	CYS	2.2
1	D	332	ALA	2.2
1	C	236	PHE	2.2
1	D	413	GLU	2.2
1	A	41	ARG	2.2
1	C	416	ARG	2.2
1	B	36	LEU	2.2
1	D	478	LEU	2.2
1	A	145	GLY	2.2
1	D	145	GLY	2.2
1	D	427	VAL	2.2
1	A	453	ARG	2.2
1	A	34	LYS	2.2
1	A	371	LEU	2.2
1	A	46	GLY	2.2
1	B	321	GLY	2.2
1	A	48	ARG	2.2
1	D	54	ILE	2.2
1	A	232	VAL	2.2
1	B	247	GLN	2.2
1	B	158	LEU	2.2
1	C	173	MET	2.2
1	D	190	GLN	2.2
1	D	268	ALA	2.2
1	D	284	ALA	2.2
1	A	184	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	472	PRO	2.2
1	B	185	VAL	2.2
1	C	140	VAL	2.2
1	C	437	TRP	2.2
1	B	386	ASP	2.2
1	A	374	ARG	2.2
1	A	467	PHE	2.2
1	C	131	PRO	2.2
1	D	245	GLN	2.2
1	C	457	GLU	2.2
1	B	140	VAL	2.1
1	B	287	VAL	2.1
1	C	281	VAL	2.1
1	D	298	GLY	2.1
1	D	325	GLN	2.1
1	D	350	GLN	2.1
1	D	300	PRO	2.1
1	B	214	ILE	2.1
1	B	128	VAL	2.1
1	D	448	SER	2.1
1	C	264	LEU	2.1
1	D	277	LEU	2.1
1	D	423	LEU	2.1
1	A	388	THR	2.1
1	A	240	ALA	2.1
1	A	458	ALA	2.1
1	C	370	GLN	2.1
1	D	174	GLN	2.1
1	D	327	ALA	2.1
1	A	185	VAL	2.1
1	A	192	VAL	2.1
1	B	390	GLU	2.1
1	C	315	TRP	2.1
1	D	38	GLU	2.1
1	B	382	LEU	2.1
1	C	401	LEU	2.1
1	D	340	LEU	2.1
1	A	218	ILE	2.1
1	A	189	GLU	2.1
1	B	464	ARG	2.1
1	D	306	VAL	2.1
1	C	381	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	397	LEU	2.1
1	A	342	ARG	2.1
1	C	362	SER	2.1
1	C	460	VAL	2.1
1	A	129	LEU	2.1
1	B	388	THR	2.1
1	B	401	LEU	2.1
1	A	35	GLN	2.1
1	B	114	ASP	2.1
1	A	462	SER	2.1
1	B	141	PRO	2.1
1	A	241	VAL	2.1
1	D	48	ARG	2.0
1	B	455	LEU	2.0
1	C	314	LEU	2.0
1	C	316	LEU	2.0
1	C	269	ALA	2.0
1	D	336	ASP	2.0
1	B	345	ARG	2.0
1	B	208	VAL	2.0
1	D	405	GLY	2.0
1	D	156	ASP	2.0
1	A	130	ALA	2.0
1	B	85	LEU	2.0
1	B	346	MET	2.0
1	B	246	GLU	2.0
1	D	283	HIS	2.0
1	C	410	ARG	2.0
1	D	311	GLY	2.0
1	C	111	GLN	2.0
1	D	417	LEU	2.0

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

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

6.3 Carbohydrates (i)

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, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	TDR	C	1480	9/9	0.94	0.22	0.19	2,2,2,2	0
2	TDR	A	1480	9/9	0.94	0.21	-0.39	2,2,2,2	0
2	TDR	B	1480	9/9	0.94	0.23	-0.45	2,3,3,4	0

6.5 Other polymers

There are no such residues in this entry.