Full wwPDB X-ray Structure Validation Report (i)

Aug 29, 2023 – 12:29 AM EDT

PDB ID	:	3PNS
Title	:	Crystal Structure of Uridine Phosphorylase Complexed with Uracil from Vibrio cholerae O1 biovar El Tor
Authors	:	Maltseva, N.; Kim, Y.; Hasseman, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2010-11-19
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

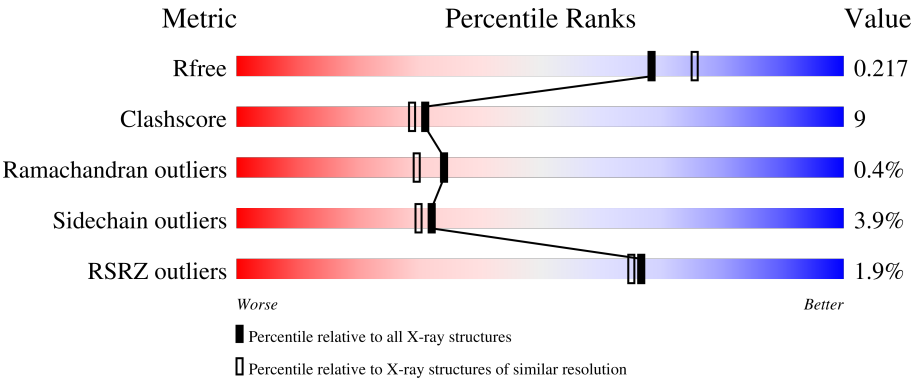
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	261	2% 77% 17% • •
1	B	261	% 77% 15% • 7%
1	C	261	% 70% 22% • 5%
1	D	261	% 78% 14% • 6%
1	E	261	2% 75% 18% • 6%

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Mol	Chain	Length	Quality of chain
1	F	261	3% 79% 15%
1	G	261	2% 84% 10%
1	H	261	4% 75% 19% 5%
1	I	261	% 78% 16%
1	J	261	2% 78% 13% 8%
1	K	261	% 82% 12%
1	L	261	79% 13% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	275	-	-	X	-
3	URA	B	271	-	X	-	-
3	URA	C	276	-	X	-	-
3	URA	D	270	-	X	-	-
3	URA	E	271	-	X	-	-
3	URA	F	274	-	X	-	-
3	URA	G	273	-	X	-	-
3	URA	H	270	-	X	-	-
3	URA	I	259	-	X	-	-
3	URA	J	271	-	X	-	-
3	URA	L	271	-	X	-	-
6	FMT	E	273	-	-	X	-
6	FMT	H	272	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25215 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	Se	0	9	0
			1951	1216	346	375	4	10			
1	B	244	Total	C	N	O	S	Se	0	10	0
			1902	1183	334	371	3	11			
1	C	248	Total	C	N	O	S	Se	0	8	0
			1925	1199	341	372	3	10			
1	D	245	Total	C	N	O	S	Se	0	8	0
			1896	1183	337	363	3	10			
1	E	245	Total	C	N	O	S	Se	0	4	0
			1864	1165	327	359	3	10			
1	F	250	Total	C	N	O	S	Se	1	7	0
			1923	1202	337	370	4	10			
1	G	250	Total	C	N	O	S	Se	0	6	0
			1916	1197	334	371	3	11			
1	H	249	Total	C	N	O	S	Se	1	15	0
			1985	1235	353	383	4	10			
1	I	250	Total	C	N	O	S	Se	0	9	0
			1937	1211	334	378	4	10			
1	J	241	Total	C	N	O	S	Se	1	4	0
			1826	1142	316	354	4	10			
1	K	251	Total	C	N	O	S	Se	0	9	0
			1941	1211	335	381	4	10			
1	L	245	Total	C	N	O	S	Se	0	6	0
			1879	1173	329	364	3	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KT71
A	-1	ASN	-	expression tag	UNP Q9KT71
A	0	ALA	-	expression tag	UNP Q9KT71
B	-2	SER	-	expression tag	UNP Q9KT71
B	-1	ASN	-	expression tag	UNP Q9KT71

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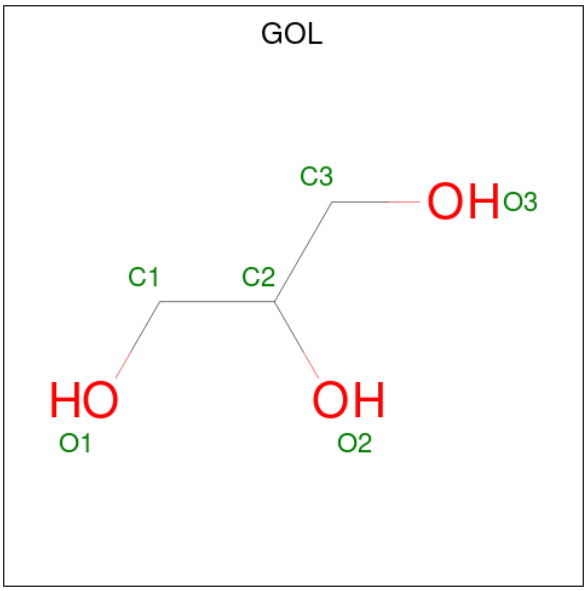
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	ALA	-	expression tag	UNP Q9KT71
C	-2	SER	-	expression tag	UNP Q9KT71
C	-1	ASN	-	expression tag	UNP Q9KT71
C	0	ALA	-	expression tag	UNP Q9KT71
D	-2	SER	-	expression tag	UNP Q9KT71
D	-1	ASN	-	expression tag	UNP Q9KT71
D	0	ALA	-	expression tag	UNP Q9KT71
E	-2	SER	-	expression tag	UNP Q9KT71
E	-1	ASN	-	expression tag	UNP Q9KT71
E	0	ALA	-	expression tag	UNP Q9KT71
F	-2	SER	-	expression tag	UNP Q9KT71
F	-1	ASN	-	expression tag	UNP Q9KT71
F	0	ALA	-	expression tag	UNP Q9KT71
G	-2	SER	-	expression tag	UNP Q9KT71
G	-1	ASN	-	expression tag	UNP Q9KT71
G	0	ALA	-	expression tag	UNP Q9KT71
H	-2	SER	-	expression tag	UNP Q9KT71
H	-1	ASN	-	expression tag	UNP Q9KT71
H	0	ALA	-	expression tag	UNP Q9KT71
I	-2	SER	-	expression tag	UNP Q9KT71
I	-1	ASN	-	expression tag	UNP Q9KT71
I	0	ALA	-	expression tag	UNP Q9KT71
J	-2	SER	-	expression tag	UNP Q9KT71
J	-1	ASN	-	expression tag	UNP Q9KT71
J	0	ALA	-	expression tag	UNP Q9KT71
K	-2	SER	-	expression tag	UNP Q9KT71
K	-1	ASN	-	expression tag	UNP Q9KT71
K	0	ALA	-	expression tag	UNP Q9KT71
L	-2	SER	-	expression tag	UNP Q9KT71
L	-1	ASN	-	expression tag	UNP Q9KT71
L	0	ALA	-	expression tag	UNP Q9KT71

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		

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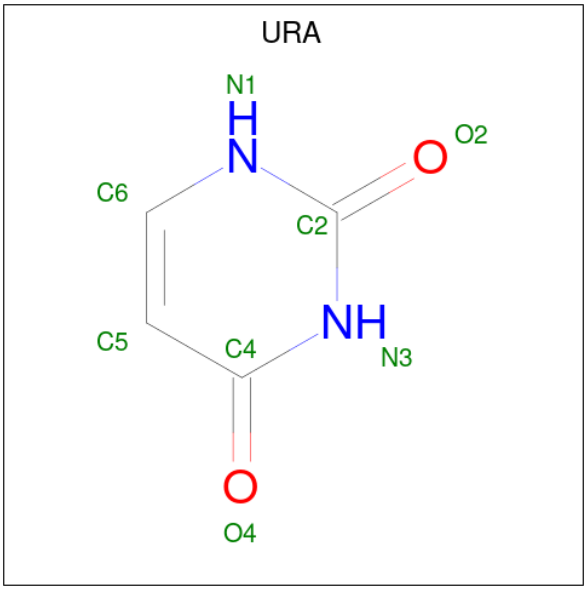
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total C O 6 3 3	0	0
2	G	1	Total C O 6 3 3	0	0
2	H	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	I	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0
2	J	1	Total C O 6 3 3	0	0
2	K	1	Total C O 6 3 3	0	0
2	K	1	Total C O 6 3 3	0	0
2	L	1	Total C O 6 3 3	0	0

- Molecule 3 is URACIL (three-letter code: URA) (formula: $C_4H_4N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 8 4 2 2	0	0

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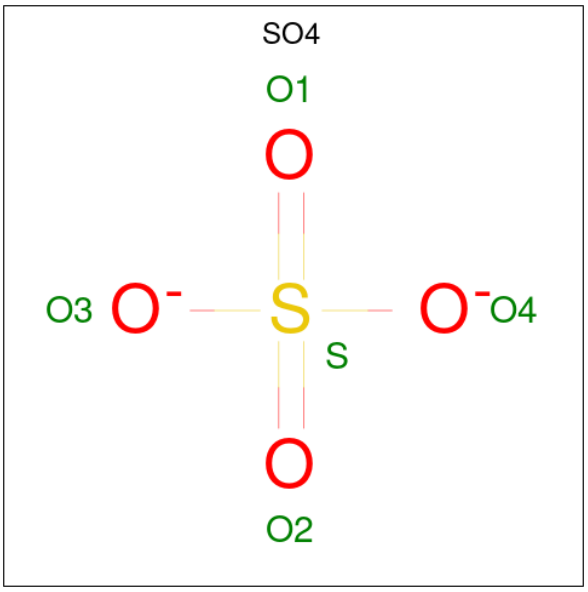
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			8	4	2	2		
3	D	1	Total	C	N	O	0	0
			8	4	2	2		
3	E	1	Total	C	N	O	0	0
			8	4	2	2		
3	F	1	Total	C	N	O	0	0
			8	4	2	2		
3	G	1	Total	C	N	O	0	0
			8	4	2	2		
3	H	1	Total	C	N	O	0	0
			8	4	2	2		
3	I	1	Total	C	N	O	0	0
			8	4	2	2		
3	J	1	Total	C	N	O	0	0
			8	4	2	2		
3	K	1	Total	C	N	O	0	0
			8	4	2	2		
3	L	1	Total	C	N	O	0	0
			8	4	2	2		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

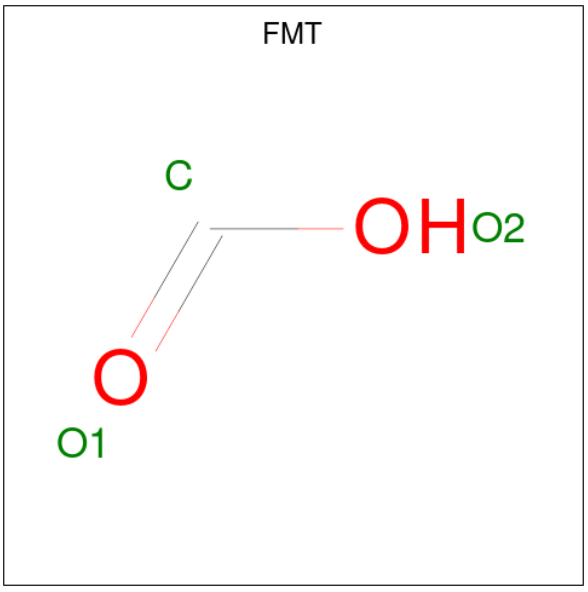
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		
4	I	2	Total	Cl	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total O S 5 4 1	0	0
5	G	1	Total O S 5 4 1	0	0
5	I	1	Total O S 5 4 1	0	0

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH_2O_2).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total C O 3 1 2	0	0

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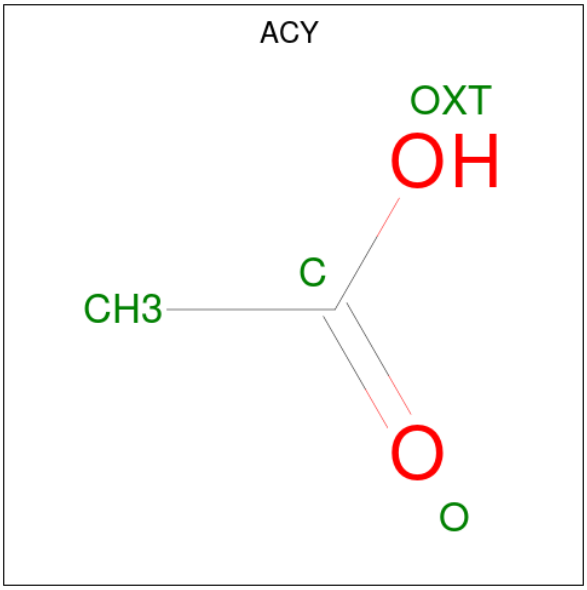
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total C O 3 1 2	0	0

- Molecule 7 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	161	Total O 161 161	0	0
8	B	190	Total O 190 190	0	0
8	C	132	Total O 132 132	0	0
8	D	197	Total O 197 197	0	0
8	E	151	Total O 151 151	0	0
8	F	161	Total O 161 161	0	0
8	G	165	Total O 165 165	0	0

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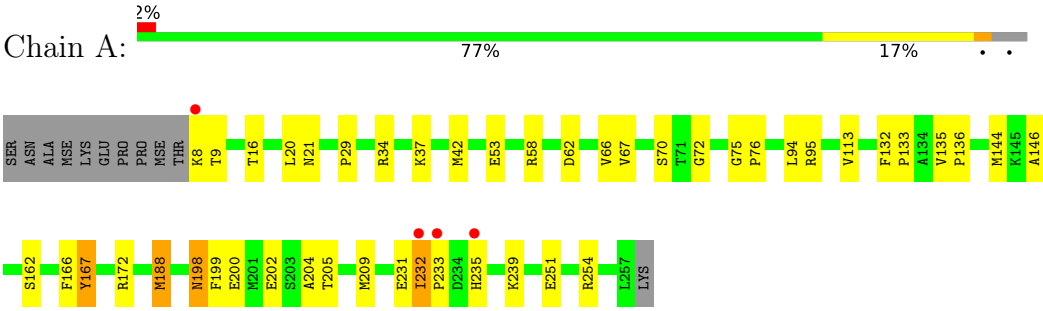
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	173	Total O 173 173	0	0
8	I	181	Total O 181 181	0	0
8	J	156	Total O 156 156	0	0
8	K	171	Total O 171 171	0	0
8	L	171	Total O 171 171	0	0

3 Residue-property plots (i)

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

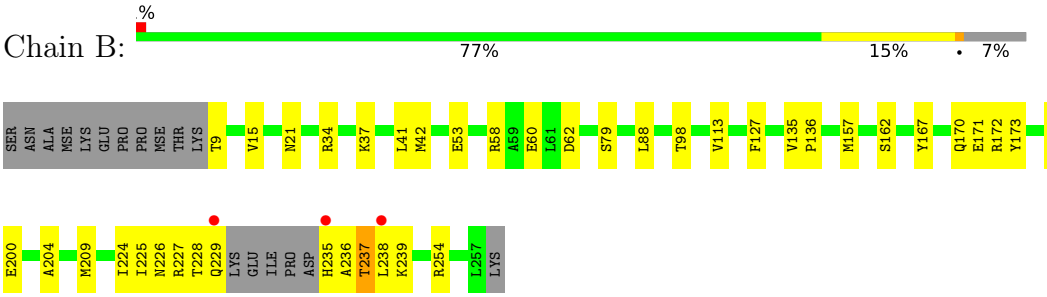
• Molecule 1: Uridine phosphorylase

Chain A:



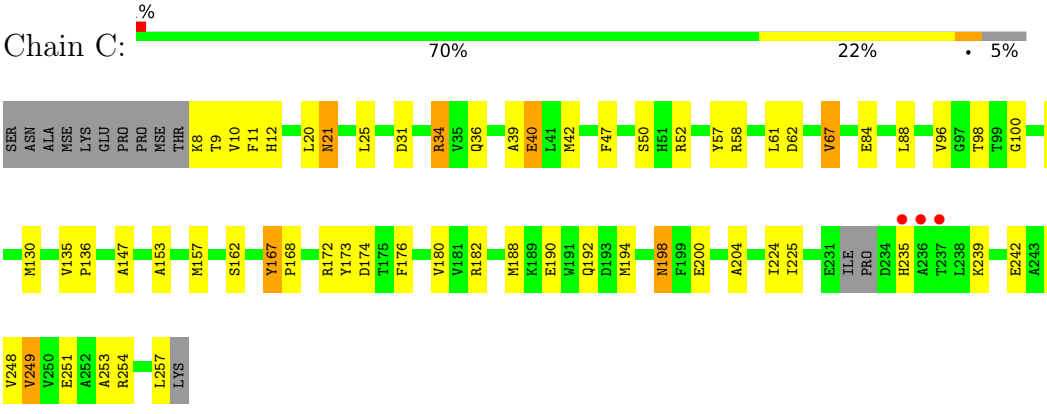
• Molecule 1: Uridine phosphorylase

Chain B:



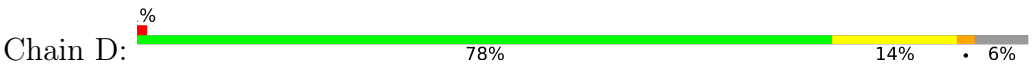
• Molecule 1: Uridine phosphorylase

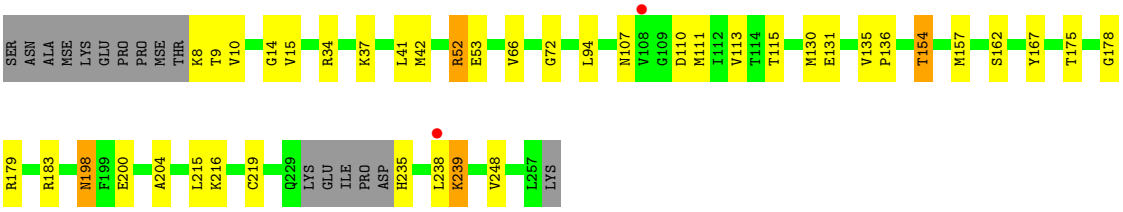
Chain C:



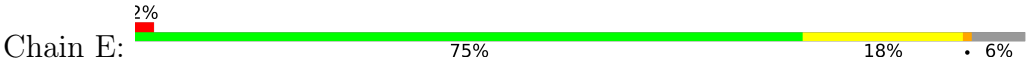
• Molecule 1: Uridine phosphorylase

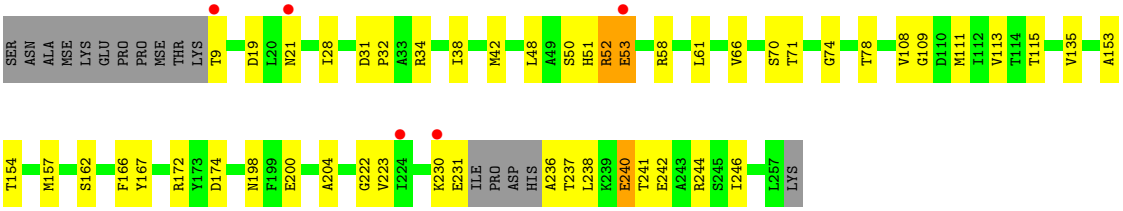
Chain D:



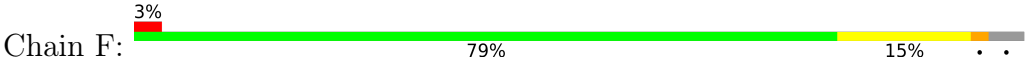


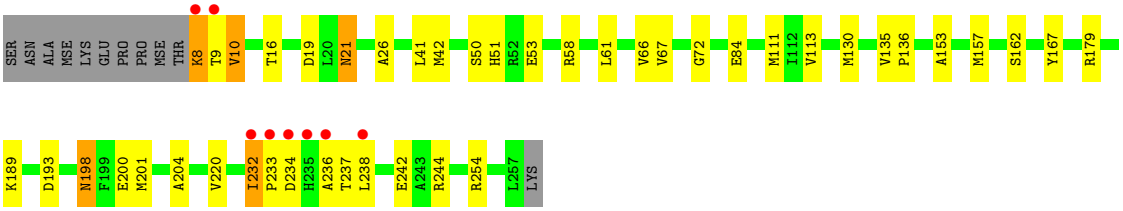
• Molecule 1: Uridine phosphorylase



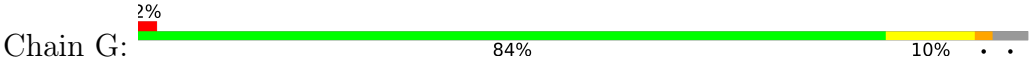


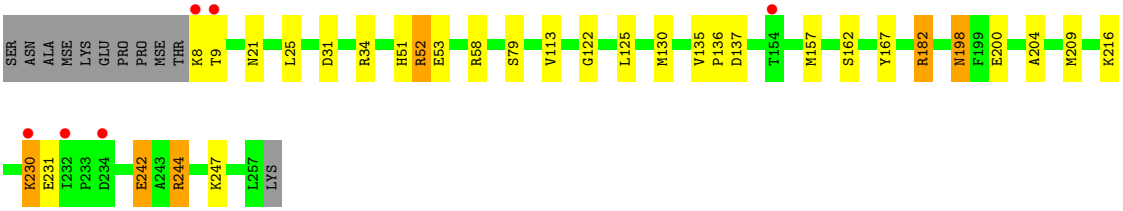
• Molecule 1: Uridine phosphorylase



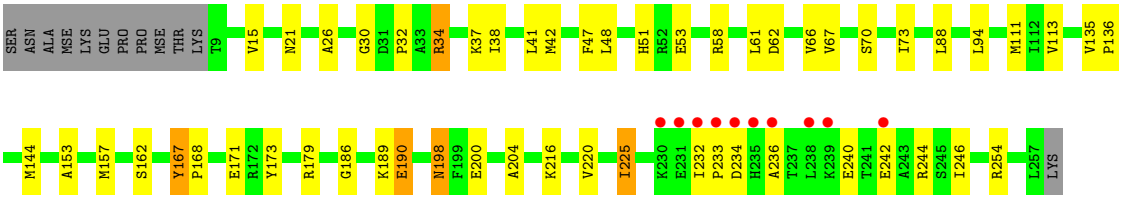


• Molecule 1: Uridine phosphorylase



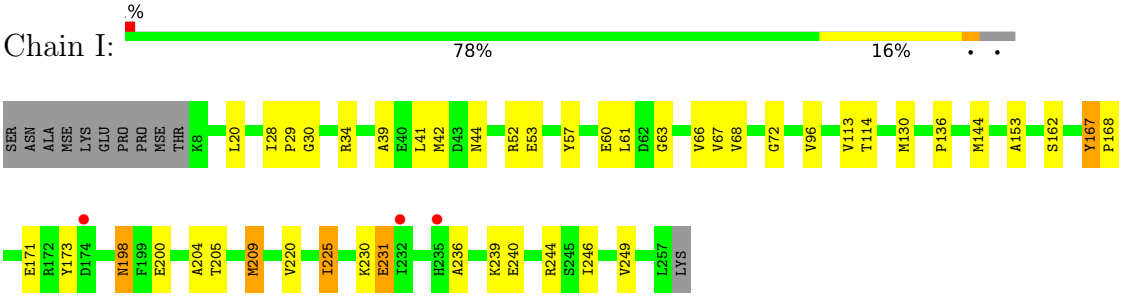


• Molecule 1: Uridine phosphorylase



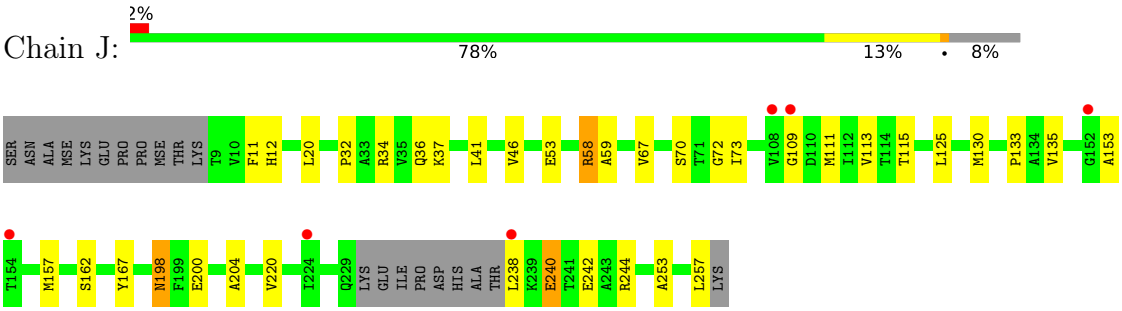
• Molecule 1: Uridine phosphorylase

Chain I:



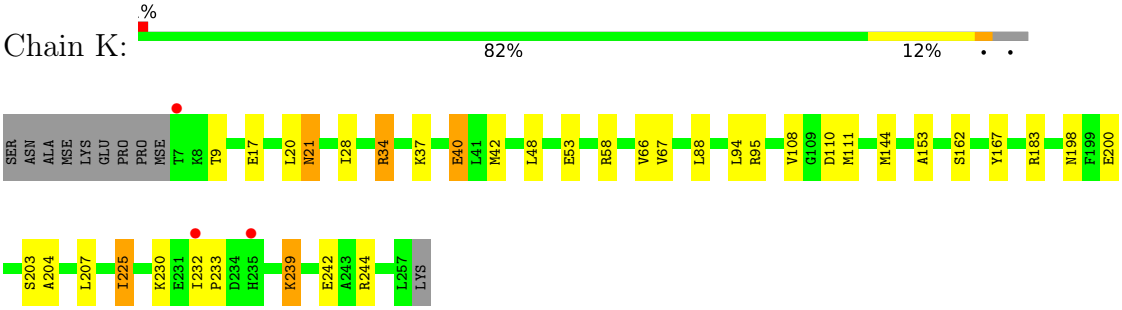
• Molecule 1: Uridine phosphorylase

Chain J:



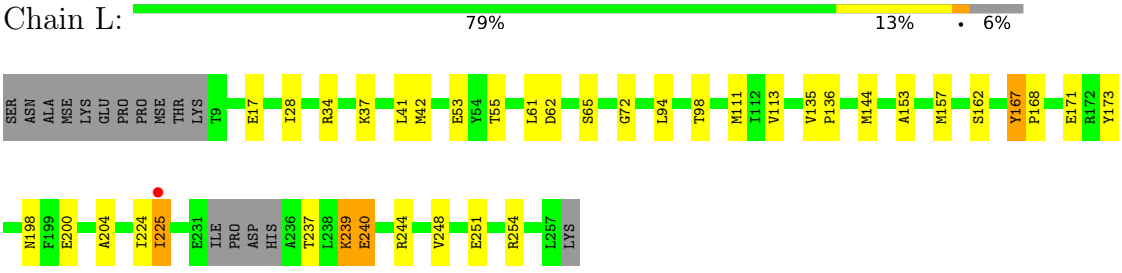
• Molecule 1: Uridine phosphorylase

Chain K:



• Molecule 1: Uridine phosphorylase

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.28Å 174.46Å 180.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 2.00 49.64 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.0 (49.64-2.00) 92.1 (49.64-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.09 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.174 , 0.226 0.168 , 0.217	Depositor DCC
R_{free} test set	10079 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	25215	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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 43.31 % 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 1.7970e-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, 0.333 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: SO4, GOL, FMT, URA, CL, ACY

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	0.52	0/1972	0.65	0/2654
1	B	0.54	0/1921	0.66	0/2585
1	C	0.49	0/1944	0.61	0/2614
1	D	0.51	0/1915	0.62	0/2578
1	E	0.48	0/1882	0.61	0/2534
1	F	0.50	0/1945	0.63	0/2621
1	G	0.52	0/1937	0.63	1/2610 (0.0%)
1	H	0.50	0/2007	0.62	0/2703
1	I	0.50	0/1958	0.62	0/2640
1	J	0.51	0/1844	0.60	0/2484
1	K	0.53	0/1962	0.63	0/2645
1	L	0.55	0/1897	0.63	0/2553
All	All	0.51	0/23184	0.63	1/31221 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	182	ARG	NE-CZ-NH1	5.37	122.99	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1951	0	1944	42	0
1	B	1902	0	1877	39	0
1	C	1925	0	1915	52	0
1	D	1896	0	1894	37	0
1	E	1864	0	1866	43	0
1	F	1923	0	1916	32	0
1	G	1916	0	1910	26	0
1	H	1985	0	1970	40	0
1	I	1937	0	1925	47	0
1	J	1826	0	1818	31	0
1	K	1941	0	1924	22	0
1	L	1879	0	1874	22	0
2	A	12	0	16	0	0
2	B	12	0	16	1	0
2	C	18	0	24	9	0
2	D	12	0	16	2	0
2	E	12	0	16	1	0
2	F	12	0	16	5	0
2	G	18	0	24	0	0
2	H	6	0	8	1	0
2	I	12	0	16	0	0
2	J	12	0	16	1	0
2	K	12	0	16	3	0
2	L	6	0	8	0	0
3	B	8	0	3	2	0
3	C	8	0	3	1	0
3	D	8	0	3	0	0
3	E	8	0	3	1	0
3	F	8	0	3	2	0
3	G	8	0	3	0	0
3	H	8	0	3	0	0
3	I	8	0	3	3	0
3	J	8	0	3	0	0
3	K	8	0	3	2	0
3	L	8	0	3	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	I	2	0	0	0	0
5	C	5	0	0	1	0
5	G	5	0	0	1	0
5	I	5	0	0	0	0
6	E	3	0	1	2	0
6	H	3	0	1	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	F	4	0	3	0	0
8	A	161	0	0	5	0
8	B	190	0	0	1	0
8	C	132	0	0	6	0
8	D	197	0	0	9	0
8	E	151	0	0	6	0
8	F	161	0	0	4	0
8	G	165	0	0	3	0
8	H	173	0	0	3	0
8	I	181	0	0	2	0
8	J	156	0	0	6	0
8	K	171	0	0	3	0
8	L	171	0	0	3	0
All	All	25215	0	23063	421	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (421) 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:34[B]:ARG:HG2	1:A:34[B]:ARG:HH11	1.08	1.16
1:E:52[A]:ARG:HG3	1:E:52[A]:ARG:HH11	1.05	1.14
1:G:244:ARG:HG2	1:G:244:ARG:HH11	1.14	1.11
1:I:144:MSE:SE	1:I:220[B]:VAL:HG23	2.05	1.07
1:D:9:THR:HG21	1:D:14:GLY:HA2	1.33	1.05
1:D:111:MSE:HE2	1:D:248:VAL:HG21	1.37	1.05
1:E:42:MSE:HE1	1:E:66:VAL:HB	1.40	1.00
1:B:235:HIS:HA	1:B:237:THR:H	1.27	1.00
1:D:219:CYS:HB3	8:D:1903:HOH:O	1.62	0.97
1:I:113:VAL:HG22	1:I:220[B]:VAL:HG22	1.45	0.95
1:B:79:SER:HA	1:B:209[A]:MSE:HE1	1.47	0.94
1:D:9:THR:HG21	1:D:14:GLY:CA	1.98	0.93
1:E:52[A]:ARG:HH11	1:E:52[A]:ARG:CG	1.81	0.92
1:B:170:GLN:HE22	3:B:271:URA:H3	1.18	0.91
1:D:111:MSE:CE	1:D:248:VAL:HG21	2.03	0.87
1:A:232:ILE:HD12	1:A:233:PRO:HD2	1.56	0.87
1:E:52[A]:ARG:HG3	1:E:52[A]:ARG:NH1	1.86	0.86
1:C:174:ASP:H	2:C:275:GOL:H31	1.40	0.86
3:K:272:URA:H5	2:K:270:GOL:HO2	1.22	0.85
1:K:34:ARG:CZ	1:K:242:GLU:HG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:PRO:HB2	1:I:34:ARG:NH1	1.92	0.84
1:J:20:LEU:HD13	1:J:67:VAL:HG21	1.59	0.84
1:C:174:ASP:HB3	2:C:275:GOL:O3	1.77	0.84
1:E:42:MSE:HE3	1:E:61:LEU:HB2	1.58	0.83
1:K:153:ALA:HB2	1:K:244:ARG:HD3	1.62	0.81
1:A:34[B]:ARG:HG2	1:A:34[B]:ARG:NH1	1.87	0.81
1:E:246:ILE:HD12	8:E:1938:HOH:O	1.79	0.81
1:H:153:ALA:HB2	1:H:244:ARG:HD3	1.61	0.80
1:I:53[B]:GLU:HG2	1:J:53:GLU:CB	2.12	0.80
1:F:10[A]:VAL:HG13	1:F:84:GLU:OE1	1.82	0.80
1:B:235:HIS:HB3	1:B:236:ALA:HA	1.62	0.79
1:A:166:PHE:O	1:A:172[B]:ARG:HD2	1.83	0.79
1:A:34[B]:ARG:HH11	1:A:34[B]:ARG:CG	1.95	0.79
1:E:71:THR:HB	1:E:78[B]:THR:HG22	1.65	0.78
1:E:153:ALA:HB2	1:E:244:ARG:HD3	1.67	0.77
1:A:251:GLU:HG2	8:A:1021:HOH:O	1.85	0.77
1:C:36[B]:GLN:HG2	1:C:57:TYR:CZ	2.21	0.76
1:G:244:ARG:HH11	1:G:244:ARG:CG	1.94	0.75
1:A:42:MSE:SE	1:A:66[B]:VAL:HG21	2.37	0.75
1:E:111:MSE:CE	1:E:222:GLY:HA2	2.17	0.74
1:K:40:GLU:HB3	8:K:1622:HOH:O	1.88	0.74
2:F:273:GOL:O2	3:F:274:URA:H5	1.71	0.73
1:I:29:PRO:HB2	1:I:34:ARG:HH11	1.50	0.73
1:D:9:THR:HG22	1:D:10:VAL:O	1.89	0.73
1:G:52[B]:ARG:HH11	1:G:52[B]:ARG:HB3	1.51	0.73
1:H:216:LYS:HE3	8:H:1969:HOH:O	1.89	0.73
1:L:224:ILE:HG13	1:L:225:ILE:HG23	1.69	0.72
1:A:20:LEU:HG	1:A:67:VAL:HG21	1.70	0.72
1:H:232:ILE:HG13	1:H:233:PRO:HD2	1.72	0.72
1:H:186:GLY:O	1:H:190[B]:GLU:HG3	1.90	0.71
2:F:273:GOL:HO2	3:F:274:URA:H5	1.38	0.71
1:F:21:ASN:HB2	1:F:58:ARG:HD2	1.73	0.71
1:H:73:ILE:HG12	2:H:271:GOL:H12	1.72	0.71
1:C:111:MSE:HE2	1:C:248:VAL:HG21	1.74	0.70
1:C:172:ARG:HB3	2:C:275:GOL:H32	1.74	0.70
1:E:111:MSE:HE2	1:E:111:MSE:HA	1.73	0.70
1:I:240[B]:GLU:HG2	1:I:244:ARG:HH22	1.57	0.70
1:A:8:LYS:O	1:A:16:THR:HA	1.91	0.69
1:B:170:GLN:NE2	1:B:172[A]:ARG:HH22	1.90	0.69
1:G:79:SER:HA	1:G:209[B]:MSE:HE1	1.73	0.69
1:B:235:HIS:HA	1:B:237:THR:N	2.04	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ASP:HB3	1:C:34[B]:ARG:HG2	1.74	0.69
1:A:53[A]:GLU:CG	1:B:53:GLU:HB3	2.23	0.69
1:B:37:LYS:HG3	8:B:267:HOH:O	1.92	0.68
1:F:42:MSE:SE	1:F:66:VAL:HG21	2.43	0.68
1:E:38:ILE:HA	8:E:1938:HOH:O	1.93	0.68
1:I:225:ILE:HD11	3:I:259:URA:O4	1.93	0.68
1:C:21:ASN:HB2	1:C:58:ARG:HD2	1.75	0.67
1:D:37:LYS:HG3	8:D:1881:HOH:O	1.94	0.67
1:K:53:GLU:HB3	1:L:53:GLU:HB3	1.76	0.67
1:B:228:THR:O	1:B:229:GLN:HB2	1.93	0.67
1:G:182:ARG:HD3	5:G:270:SO4:O3	1.94	0.67
1:A:34[B]:ARG:NH2	1:A:37:LYS:HD3	2.10	0.66
1:D:107:ASN:O	1:D:110:ASP:HB2	1.96	0.66
1:E:21:ASN:HB2	1:E:58:ARG:HD2	1.77	0.66
1:J:73:ILE:HG12	2:J:273:GOL:H31	1.78	0.66
1:H:51[B]:HIS:HE1	6:H:272:FMT:O1	1.80	0.65
1:I:205:THR:HG22	1:I:209:MSE:HE2	1.78	0.65
1:A:21:ASN:HB2	1:A:58:ARG:HD2	1.77	0.65
1:B:198:ASN:N	1:B:198:ASN:HD22	1.94	0.65
1:H:34[B]:ARG:NH1	1:H:37:LYS:HD2	2.11	0.65
1:C:153:ALA:HB2	1:C:244:ARG:HD3	1.79	0.65
1:I:162:SER:HB3	1:I:204:ALA:HB2	1.79	0.65
1:A:135:VAL:HG23	1:A:136:PRO:HD2	1.79	0.64
1:H:111:MSE:HE3	1:H:220:VAL:HG22	1.80	0.64
1:J:34:ARG:HH22	1:J:242:GLU:HB3	1.63	0.64
3:K:272:URA:H5	2:K:270:GOL:O2	1.80	0.63
1:F:179[A]:ARG:NH2	8:F:1935:HOH:O	2.21	0.63
1:I:209:MSE:SE	8:I:1985:HOH:O	2.66	0.63
1:A:251:GLU:HG3	8:A:1835:HOH:O	1.97	0.63
1:J:238:LEU:N	8:J:1405:HOH:O	2.31	0.63
1:J:125:LEU:HD21	1:J:130:MSE:HE2	1.82	0.62
1:K:162:SER:HB3	1:K:204:ALA:HB2	1.82	0.62
1:C:42:MSE:HG2	1:C:61:LEU:HD13	1.81	0.62
1:E:42:MSE:HE1	1:E:66:VAL:CB	2.25	0.62
1:C:224:ILE:C	1:C:225:ILE:HD12	2.20	0.62
1:E:52[A]:ARG:CG	1:E:52[A]:ARG:NH1	2.51	0.62
1:E:74:GLY:O	1:E:78[B]:THR:HG23	1.98	0.62
1:H:94:LEU:HG	1:H:144:MSE:HE3	1.81	0.61
1:C:130:MSE:HG3	1:I:130:MSE:HG3	1.80	0.61
1:E:111:MSE:HE1	1:E:222:GLY:HA2	1.81	0.61
1:J:133:PRO:HB2	1:J:135[B]:VAL:HG13	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34[A]:ARG:HD3	8:A:1822:HOH:O	2.00	0.60
1:H:62:ASP:OD1	1:H:254[A]:ARG:HD2	2.00	0.60
1:H:135[A]:VAL:HG23	1:H:136:PRO:HD2	1.82	0.60
1:I:53[B]:GLU:HG2	1:J:53:GLU:HB2	1.82	0.60
1:I:53[B]:GLU:HG2	1:J:53:GLU:HB3	1.80	0.60
1:J:58:ARG:HD3	8:J:766:HOH:O	2.01	0.60
1:B:34:ARG:HH21	1:B:37:LYS:HD2	1.67	0.60
1:D:42:MSE:SE	1:D:66[B]:VAL:HG21	2.51	0.60
1:F:153:ALA:HB2	1:F:244:ARG:HD3	1.83	0.60
1:J:34:ARG:NH2	1:J:242:GLU:HB3	2.16	0.60
1:C:162:SER:HB3	1:C:204:ALA:HB2	1.83	0.60
1:F:8:LYS:HB2	8:F:1941:HOH:O	2.01	0.60
1:L:135:VAL:HG23	1:L:136:PRO:HD2	1.84	0.60
1:E:111:MSE:HE2	1:E:222:GLY:HA2	1.84	0.60
1:G:125:LEU:HD21	1:G:130:MSE:HE2	1.84	0.60
1:I:144:MSE:SE	1:I:220[B]:VAL:CG2	2.94	0.60
1:A:53[A]:GLU:HG3	1:B:53:GLU:HB3	1.84	0.59
1:I:28[B]:ILE:HD13	1:I:28[B]:ILE:N	2.18	0.59
1:G:244:ARG:HG2	1:G:244:ARG:NH1	1.95	0.59
1:H:236:ALA:O	1:H:240:GLU:HG3	2.02	0.59
1:I:39:ALA:HA	1:I:42:MSE:CE	2.33	0.59
1:D:9:THR:HG21	1:D:14:GLY:C	2.23	0.59
1:I:28[B]:ILE:HD13	1:I:28[B]:ILE:H	1.68	0.59
1:C:47:PHE:HE1	1:C:50[B]:SER:HG	1.49	0.58
1:B:235:HIS:CB	1:B:236:ALA:HA	2.31	0.58
1:F:8:LYS:O	1:F:16:THR:HG22	2.04	0.57
1:E:19:ASP:HB3	1:E:48:LEU:HD13	1.86	0.57
1:J:111:MSE:HE3	1:J:220:VAL:HG22	1.86	0.57
1:L:239:LYS:HG3	1:L:240:GLU:N	2.19	0.57
1:C:20:LEU:HG	1:C:67[B]:VAL:HG21	1.86	0.57
1:G:31:ASP:HB3	1:G:34:ARG:HG2	1.86	0.57
1:F:238:LEU:O	1:F:242:GLU:HG3	2.05	0.57
1:G:113:VAL:HB	1:G:157:MSE:SE	2.55	0.56
1:C:224:ILE:O	1:C:225:ILE:HD12	2.05	0.56
1:D:53:GLU:HG3	1:D:72:GLY:HA3	1.88	0.56
1:G:51:HIS:HE1	8:G:1431:HOH:O	1.87	0.56
1:L:135:VAL:CG2	1:L:136:PRO:HD2	2.36	0.56
1:A:62:ASP:OD1	1:A:254[A]:ARG:HG3	2.06	0.56
1:L:55[B]:THR:HG23	8:L:1085:HOH:O	2.06	0.56
1:J:58:ARG:HG2	1:J:59:ALA:N	2.19	0.56
1:J:198:ASN:HD22	1:J:198:ASN:N	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:ARG:NH2	1:B:37:LYS:HD2	2.22	0.55
1:K:94:LEU:HG	1:K:144:MSE:HE3	1.88	0.55
1:J:11:PHE:HD2	1:J:12:HIS:CE1	2.23	0.55
1:G:52[A]:ARG:CG	1:G:52[A]:ARG:HH21	2.19	0.55
1:I:28[B]:ILE:HG12	1:I:28[B]:ILE:O	2.05	0.55
1:I:113:VAL:HG22	1:I:220[B]:VAL:CG2	2.26	0.55
1:I:153:ALA:HB2	1:I:244:ARG:HD2	1.87	0.55
1:D:162:SER:HB3	1:D:204:ALA:HB2	1.88	0.55
1:F:53:GLU:HG3	1:F:72:GLY:HA3	1.88	0.55
1:H:61:LEU:HG	1:H:254[A]:ARG:HG2	1.88	0.55
1:B:79:SER:CA	1:B:209[A]:MSE:HE1	2.29	0.54
1:E:28:ILE:O	1:E:28:ILE:HG13	2.07	0.54
1:H:51[B]:HIS:HD2	1:I:44:ASN:OD1	1.90	0.54
1:F:189:LYS:HE2	1:F:193:ASP:OD1	2.08	0.54
1:I:198:ASN:N	1:I:198:ASN:HD22	2.06	0.54
1:D:9:THR:HG22	1:D:10:VAL:N	2.23	0.54
1:H:232:ILE:HG13	1:H:233:PRO:CD	2.36	0.54
1:C:114:THR:O	1:C:136:PRO:HG3	2.08	0.53
1:B:172[B]:ARG:HD2	1:B:227:ARG:NH1	2.23	0.53
1:C:31:ASP:HB3	1:C:34[B]:ARG:CG	2.37	0.53
1:C:198:ASN:N	1:C:198:ASN:HD22	2.07	0.53
1:A:34[B]:ARG:NH2	1:A:37:LYS:CD	2.71	0.53
1:A:113:VAL:HB	1:A:157:MSE:SE	2.58	0.53
1:C:253:ALA:O	1:C:257:LEU:HG	2.08	0.53
1:H:179[A]:ARG:NH2	8:H:1963:HOH:O	2.41	0.53
1:B:224:ILE:HB	1:B:238:LEU:CD1	2.38	0.53
2:C:261:GOL:H11	8:C:1866:HOH:O	2.07	0.53
1:E:135[B]:VAL:CG1	1:J:135[B]:VAL:HG12	2.39	0.53
1:F:135:VAL:CG2	1:F:136:PRO:HD2	2.39	0.52
1:L:94:LEU:HG	1:L:144:MSE:HE3	1.91	0.52
1:E:52[B]:ARG:HB3	1:E:53:GLU:HG3	1.90	0.52
1:K:20:LEU:HG	1:K:67[B]:VAL:HG21	1.90	0.52
1:L:42:MSE:HG2	1:L:61:LEU:HD13	1.91	0.52
1:E:51:HIS:CE1	8:E:1594:HOH:O	2.62	0.52
1:L:62:ASP:OD2	1:L:254:ARG:NH1	2.43	0.52
1:A:146:ALA:O	1:A:150:GLU:HG3	2.08	0.52
1:B:170:GLN:NE2	3:B:271:URA:H3	1.98	0.52
2:C:275:GOL:H11	8:C:1557:HOH:O	2.09	0.52
1:E:237:THR:HA	1:E:240:GLU:HG3	1.90	0.52
1:K:183:ARG:O	2:K:271:GOL:H31	2.09	0.52
1:C:12:HIS:HE1	2:D:260:GOL:O3	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:HIS:HD2	1:C:84:GLU:OE2	1.92	0.52
1:D:131:GLU:CD	8:D:1890:HOH:O	2.47	0.52
1:E:53:GLU:HB3	1:F:53:GLU:HB3	1.91	0.52
1:K:42:MSE:SE	1:K:66[A]:VAL:HG21	2.60	0.52
1:B:235:HIS:N	1:B:235:HIS:CD2	2.78	0.52
1:H:51[B]:HIS:CE1	6:H:272:FMT:O1	2.62	0.52
1:D:130:MSE:HG3	1:F:130:MSE:HG3	1.91	0.51
1:L:162:SER:HB3	1:L:204:ALA:HB2	1.93	0.51
1:E:111:MSE:HE1	1:E:222:GLY:CA	2.40	0.51
1:D:115:THR:O	1:F:135:VAL:HG21	2.11	0.51
1:D:235:HIS:HB3	1:D:238:LEU:HG	1.92	0.51
1:E:244:ARG:HD2	8:E:756:HOH:O	2.10	0.51
1:G:135[B]:VAL:HG13	1:G:136:PRO:HD2	1.93	0.51
1:G:137:ASP:OD2	1:G:216:LYS:HE3	2.11	0.51
1:I:42:MSE:HE1	1:I:68:VAL:CG2	2.41	0.51
1:E:135[A]:VAL:HG21	1:J:115:THR:O	2.10	0.51
1:F:111:MSE:HE3	1:F:220:VAL:HG22	1.92	0.51
1:G:198:ASN:N	1:G:198:ASN:HD22	2.09	0.51
1:I:230:LYS:HE3	1:L:17:GLU:OE2	2.11	0.51
8:D:1889:HOH:O	2:F:270:GOL:H11	2.09	0.50
1:B:224:ILE:HB	1:B:238:LEU:HD12	1.93	0.50
1:G:135[A]:VAL:CG2	1:G:136:PRO:HD2	2.42	0.50
1:C:174:ASP:H	2:C:275:GOL:C3	2.18	0.50
1:J:153:ALA:HB2	1:J:244:ARG:HD3	1.94	0.50
1:B:42:MSE:HB3	1:B:60[B]:GLU:O	2.12	0.50
1:E:246:ILE:HB	8:E:1938:HOH:O	2.12	0.50
1:K:17[B]:GLU:HG3	1:K:88:LEU:HD22	1.92	0.50
1:I:52:ARG:HD3	8:I:697:HOH:O	2.12	0.50
1:I:171:GLU:HG2	1:I:173:TYR:CE1	2.46	0.50
1:D:175:THR:O	1:K:230:LYS:HG3	2.11	0.50
1:E:162:SER:HB3	1:E:204:ALA:HB2	1.94	0.49
1:A:135:VAL:CG2	1:A:136:PRO:HD2	2.41	0.49
1:E:115:THR:O	1:J:135[A]:VAL:HG21	2.11	0.49
1:L:153:ALA:HB2	1:L:244:ARG:HD3	1.95	0.49
1:B:98:THR:HB	1:B:224:ILE:HG12	1.94	0.49
1:D:135[A]:VAL:HG23	1:D:136:PRO:HD2	1.93	0.49
1:F:135:VAL:HG23	1:F:136:PRO:HD2	1.94	0.49
1:G:52[B]:ARG:HH22	1:H:30:GLY:HA3	1.77	0.49
1:J:240:GLU:HG3	8:J:1405:HOH:O	2.11	0.49
1:H:162:SER:HB3	1:H:204:ALA:HB2	1.93	0.49
1:J:113:VAL:HB	1:J:157:MSE:SE	2.62	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ARG:CB	2:C:275:GOL:H32	2.40	0.49
1:G:34:ARG:NH2	1:G:242:GLU:HG2	2.28	0.48
1:B:34:ARG:HH21	1:B:37:LYS:CD	2.25	0.48
1:C:113:VAL:HB	1:C:157:MSE:SE	2.62	0.48
1:H:113:VAL:HB	1:H:157:MSE:SE	2.62	0.48
1:J:162:SER:HB3	1:J:204:ALA:HB2	1.96	0.48
1:B:162:SER:HB3	1:B:204:ALA:HB2	1.95	0.48
1:B:198:ASN:N	1:B:198:ASN:ND2	2.61	0.48
1:C:10:VAL:HG13	1:C:88:LEU:HD21	1.95	0.48
1:E:230:LYS:O	1:E:231:GLU:C	2.51	0.48
1:J:253:ALA:O	1:J:257:LEU:HG	2.13	0.48
1:G:52[A]:ARG:HH21	1:G:52[A]:ARG:HG2	1.78	0.48
1:I:30:GLY:H	1:I:34:ARG:HH12	1.61	0.48
1:B:183:ARG:O	2:B:270:GOL:H31	2.14	0.48
1:G:135[A]:VAL:HG23	1:G:136:PRO:HD2	1.95	0.48
1:I:42:MSE:HG2	1:I:61:LEU:HD13	1.95	0.48
8:D:1890:HOH:O	2:F:270:GOL:C1	2.61	0.48
1:E:109:GLY:HA2	1:E:241:THR:OG1	2.12	0.48
1:G:162:SER:HB3	1:G:204:ALA:HB2	1.95	0.48
1:B:62:ASP:OD1	1:B:254:ARG:HD3	2.14	0.48
1:F:51[A]:HIS:CD2	8:F:1634:HOH:O	2.67	0.48
1:C:52[A]:ARG:NH2	8:C:1869:HOH:O	2.38	0.48
1:L:251:GLU:HG2	8:L:1853:HOH:O	2.13	0.47
1:C:96:VAL:HB	1:C:249:VAL:HG21	1.96	0.47
1:A:188:MSE:HG2	8:A:1226:HOH:O	2.12	0.47
1:B:225:ILE:HG12	1:B:226:ASN:N	2.29	0.47
1:B:238:LEU:N	1:B:238:LEU:HD22	2.28	0.47
1:E:113:VAL:HB	1:E:157:MSE:SE	2.65	0.47
1:H:42:MSE:SE	1:H:66:VAL:HG21	2.65	0.47
1:H:48:LEU:HD11	1:H:58[B]:ARG:HB3	1.97	0.47
1:A:132:PHE:CG	1:A:133:PRO:HD2	2.49	0.47
1:D:216:LYS:HD2	8:D:1472:HOH:O	2.13	0.47
1:I:30:GLY:N	1:I:34:ARG:HH12	2.13	0.47
1:L:28:ILE:O	1:L:28:ILE:HG13	2.15	0.47
1:D:198:ASN:N	1:D:198:ASN:HD22	2.13	0.47
1:A:53[A]:GLU:HG2	8:A:1024:HOH:O	2.14	0.47
1:C:36[B]:GLN:HG3	8:C:920:HOH:O	2.14	0.46
1:H:21:ASN:HB2	1:H:58[A]:ARG:HD2	1.95	0.46
1:I:96:VAL:HB	1:I:249:VAL:HG21	1.97	0.46
1:A:9:THR:HG22	1:A:16:THR:HG22	1.97	0.46
1:A:188:MSE:CE	1:A:199:PHE:HE2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:ILE:HG12	8:K:1394:HOH:O	2.15	0.46
1:D:34:ARG:HH11	1:D:37:LYS:NZ	2.12	0.46
1:E:34:ARG:NH1	1:E:242:GLU:HG3	2.31	0.46
1:F:198:ASN:N	1:F:198:ASN:HD22	2.14	0.46
1:H:198:ASN:N	1:H:198:ASN:HD22	2.13	0.46
1:I:39:ALA:HA	1:I:42:MSE:HE3	1.96	0.46
1:I:53[A]:GLU:HB3	1:J:53:GLU:HB3	1.98	0.46
1:D:135[A]:VAL:CG2	1:D:136:PRO:HD2	2.45	0.46
1:B:21[A]:ASN:HB2	1:B:58:ARG:HD2	1.98	0.46
1:C:174:ASP:HB3	2:C:275:GOL:HO3	1.79	0.46
1:E:31:ASP:H	6:E:273:FMT:C	2.29	0.46
1:A:9:THR:HG22	1:A:16:THR:CG2	2.46	0.46
1:D:9:THR:HG23	1:D:15:VAL:O	2.15	0.46
1:H:111:MSE:HE3	1:H:220:VAL:CG2	2.46	0.46
1:A:198:ASN:N	1:A:198:ASN:HD22	2.14	0.46
1:F:201:MSE:HB2	2:F:273:GOL:H11	1.97	0.45
1:D:9:THR:HG23	1:D:15:VAL:N	2.32	0.45
1:H:135[A]:VAL:CG2	1:H:136:PRO:HD2	2.44	0.45
1:I:167:TYR:HB2	1:I:168:PRO:CD	2.47	0.45
1:C:182:ARG:HD3	5:C:259:SO4:O3	2.16	0.45
1:F:19:ASP:O	1:F:58:ARG:HD3	2.17	0.45
1:F:232:ILE:HG12	1:F:233:PRO:HD2	1.99	0.45
1:K:239:LYS:HE3	1:K:239:LYS:HA	1.98	0.45
1:I:236:ALA:O	1:I:240[A]:GLU:HG3	2.16	0.45
1:D:113:VAL:HB	1:D:157:MSE:SE	2.67	0.45
1:B:15:VAL:HG23	1:B:88:LEU:CD1	2.47	0.45
1:C:39:ALA:HA	1:C:42:MSE:HE3	1.97	0.45
1:G:25:LEU:C	1:G:25:LEU:HD23	2.37	0.45
1:A:53[B]:GLU:HG3	1:A:72:GLY:HA3	1.99	0.45
1:F:162:SER:HB3	1:F:204:ALA:HB2	1.98	0.45
1:I:20:LEU:HG	1:I:67[A]:VAL:HG11	1.98	0.45
1:B:239:LYS:HD3	1:B:239:LYS:HA	1.86	0.44
1:E:31:ASP:H	6:E:273:FMT:H	1.81	0.44
1:H:26:ALA:HA	1:H:67[B]:VAL:O	2.16	0.44
1:H:216:LYS:CE	8:H:1969:HOH:O	2.59	0.44
1:A:167:TYR:O	1:A:172[B]:ARG:HG3	2.17	0.44
1:C:167:TYR:HB2	1:C:168:PRO:CD	2.47	0.44
1:H:167:TYR:HB2	1:H:168:PRO:CD	2.47	0.44
1:C:20:LEU:HG	1:C:67[B]:VAL:CG2	2.47	0.44
1:F:10[A]:VAL:CG1	1:F:84:GLU:OE1	2.58	0.44
1:I:41:LEU:HD11	1:I:246:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HG	1:A:144:MSE:HE3	1.98	0.44
1:D:9:THR:CG2	1:D:10:VAL:N	2.81	0.44
1:J:109:GLY:HA3	8:J:1042:HOH:O	2.17	0.44
1:A:29:PRO:O	1:A:70:SER:HA	2.18	0.44
1:A:95:ARG:NH2	1:A:202:GLU:OE1	2.50	0.44
1:C:244:ARG:HD2	8:C:1868:HOH:O	2.16	0.44
1:J:37:LYS:HG3	8:J:1992:HOH:O	2.17	0.44
1:A:205:THR:O	1:A:209:MSE:HG2	2.18	0.44
1:C:135:VAL:HG23	1:C:136:PRO:HD2	2.00	0.44
1:H:189[A]:LYS:HD2	1:H:189[A]:LYS:O	2.17	0.44
1:D:9:THR:CG2	1:D:15:VAL:N	2.81	0.44
1:L:113:VAL:HB	1:L:157:MSE:SE	2.68	0.44
1:B:238:LEU:CD2	1:B:238:LEU:H	2.30	0.44
1:F:26:ALA:HA	1:F:67[B]:VAL:O	2.18	0.44
1:I:53[A]:GLU:HG3	1:I:72:GLY:HA3	2.00	0.44
1:I:225:ILE:HD11	3:I:259:URA:C4	2.53	0.44
1:A:20:LEU:HG	1:A:67:VAL:CG2	2.44	0.43
1:C:100:GLY:HA2	1:C:225:ILE:O	2.18	0.43
2:C:261:GOL:HO2	3:C:276:URA:H5	1.66	0.43
1:D:179:ARG:HD3	8:D:1898:HOH:O	2.18	0.43
1:K:21:ASN:HB2	1:K:58:ARG:HD2	2.00	0.43
1:L:254:ARG:NH2	8:L:676:HOH:O	2.51	0.43
1:C:235:HIS:CE1	1:C:239:LYS:HE3	2.53	0.43
1:I:167:TYR:CB	1:I:168:PRO:CD	2.96	0.43
1:L:111:MSE:HE2	1:L:248:VAL:HG21	1.99	0.43
1:A:232:ILE:HD12	1:A:233:PRO:CD	2.39	0.43
1:H:32:PRO:HA	1:H:70:SER:HB3	2.00	0.43
1:H:47:PHE:CD2	1:I:57:TYR:HE1	2.36	0.43
1:L:167:TYR:HB2	1:L:168:PRO:CD	2.48	0.43
1:L:171:GLU:HG2	1:L:173:TYR:CE1	2.54	0.43
1:A:231[A]:GLU:H	1:A:231[A]:GLU:CD	2.21	0.43
1:A:239:LYS:NZ	1:A:239:LYS:HB3	2.34	0.43
1:F:50:SER:O	1:F:51[A]:HIS:ND1	2.51	0.43
1:I:231:GLU:H	1:I:231:GLU:HG3	1.38	0.43
1:C:62:ASP:OD1	1:C:254:ARG:HD2	2.19	0.43
1:J:36:GLN:HB3	8:J:1992:HOH:O	2.17	0.43
1:B:135:VAL:CG2	1:B:136:PRO:HD2	2.47	0.43
1:C:188:MSE:O	1:C:192:GLN:HG3	2.18	0.43
1:E:19:ASP:O	1:E:58:ARG:HD3	2.19	0.43
1:F:113:VAL:HB	1:F:157:MSE:SE	2.68	0.43
1:G:21:ASN:HB2	1:G:58:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:GLU:HG2	1:H:173:TYR:CE1	2.53	0.43
1:H:225:ILE:HD13	1:H:225:ILE:C	2.39	0.43
1:C:36[B]:GLN:HG2	1:C:57:TYR:OH	2.19	0.43
1:D:239:LYS:HE3	8:D:1194:HOH:O	2.17	0.43
1:A:34[B]:ARG:NH1	1:A:34[B]:ARG:CG	2.61	0.43
1:B:135:VAL:HG23	1:B:136:PRO:HD2	2.01	0.43
1:E:32:PRO:HA	1:E:70:SER:HB3	2.01	0.43
1:E:166:PHE:O	1:E:172[A]:ARG:HD2	2.19	0.43
1:F:8:LYS:HB2	1:F:9:THR:H	1.61	0.43
1:H:61:LEU:CG	1:H:254[A]:ARG:HG2	2.48	0.43
1:H:153:ALA:HB2	1:H:244:ARG:CD	2.39	0.43
8:G:2004:HOH:O	6:H:272:FMT:H	2.19	0.42
1:D:94:LEU:N	1:D:94:LEU:HD12	2.34	0.42
1:E:108:VAL:HA	1:E:223:VAL:HG12	2.01	0.42
1:J:46:VAL:HB	1:J:58:ARG:HD2	2.01	0.42
1:C:147:ALA:HB1	1:C:251:GLU:HB3	2.01	0.42
1:F:50:SER:C	1:F:51[A]:HIS:ND1	2.73	0.42
1:I:225:ILE:HD11	3:I:259:URA:C5	2.54	0.42
1:A:132:PHE:CD1	1:A:133:PRO:HD2	2.54	0.42
1:H:38:ILE:HG12	1:H:246:ILE:HB	2.01	0.42
1:D:183:ARG:O	2:D:271:GOL:H31	2.20	0.42
1:I:114:THR:O	1:I:136:PRO:HG3	2.20	0.42
1:C:25:LEU:C	1:C:25:LEU:HD23	2.40	0.42
1:F:61:LEU:HD21	1:F:254:ARG:HG3	2.02	0.42
1:I:39:ALA:HA	1:I:42:MSE:HE2	2.02	0.42
1:D:154:THR:HG23	8:D:1764:HOH:O	2.20	0.42
1:G:230:LYS:HE3	1:G:230:LYS:HA	2.02	0.42
1:K:203:SER:O	1:K:207:LEU:HG	2.20	0.42
1:F:10[A]:VAL:CG2	1:F:84:GLU:HB3	2.50	0.42
1:F:234:ASP:OD2	1:F:236:ALA:HB3	2.19	0.42
1:I:240[B]:GLU:CG	1:I:244:ARG:HH22	2.28	0.42
1:J:53:GLU:HG3	1:J:72:GLY:HA3	2.02	0.42
1:K:108:VAL:HG11	1:K:233:PRO:HB3	2.00	0.42
1:K:110:ASP:O	1:K:111:MSE:HE2	2.20	0.42
1:B:113:VAL:HB	1:B:157:MSE:SE	2.70	0.42
1:D:34:ARG:HH11	1:D:37:LYS:HZ3	1.68	0.42
1:J:37:LYS:O	1:J:41:LEU:HD13	2.19	0.42
1:C:224:ILE:HG13	1:C:225:ILE:CD1	2.50	0.41
1:I:60[B]:GLU:OE2	1:I:63:GLY:HA2	2.20	0.41
1:H:15:VAL:HG23	1:H:88:LEU:CD1	2.51	0.41
3:E:271:URA:N1	2:E:272:GOL:H31	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52[A]:ARG:CG	1:G:52[A]:ARG:NH2	2.80	0.41
1:C:36[B]:GLN:O	1:C:40[B]:GLU:HG3	2.20	0.41
1:C:62:ASP:OD1	1:C:254:ARG:CD	2.68	0.41
1:C:176:PHE:CE1	1:D:215:LEU:HD21	2.56	0.41
1:K:37:LYS:NZ	8:K:1705:HOH:O	2.54	0.41
1:A:75:GLY:N	1:A:76:PRO:CD	2.83	0.41
1:D:178:GLY:HA3	1:K:230:LYS:HB3	2.02	0.41
1:L:53:GLU:HG3	1:L:72:GLY:HA3	2.02	0.41
1:B:127:PHE:CE1	1:B:209[A]:MSE:HE2	2.56	0.41
1:C:31:ASP:OD2	1:D:52[A]:ARG:HD3	2.20	0.41
1:H:32:PRO:HG3	1:H:53:GLU:O	2.20	0.41
1:B:171:GLU:HG2	1:B:173:TYR:CE1	2.56	0.41
1:C:98:THR:O	8:C:1123:HOH:O	2.22	0.41
1:K:48:LEU:HD11	1:K:58:ARG:HB2	2.02	0.41
1:C:173:TYR:CE2	1:C:180:VAL:HG23	2.56	0.40
1:G:216:LYS:CD	8:G:1959:HOH:O	2.68	0.40
1:C:11:PHE:HD2	1:C:12:HIS:CD2	2.40	0.40
1:C:246:ILE:HD13	1:C:246:ILE:HG21	1.85	0.40
1:I:42:MSE:SE	1:I:66:VAL:HG21	2.71	0.40
1:K:20:LEU:HG	1:K:67[B]:VAL:CG2	2.50	0.40
1:K:28:ILE:HG13	1:K:95:ARG:HA	2.02	0.40
1:B:238:LEU:HD22	1:B:238:LEU:H	1.85	0.40
1:C:190:GLU:HG3	1:C:194:MSE:HE3	2.03	0.40
1:E:236:ALA:N	8:E:1422:HOH:O	2.53	0.40
1:F:51[B]:HIS:HE1	8:F:1538:HOH:O	2.04	0.40
1:A:162:SER:HB3	1:A:204:ALA:HB2	2.04	0.40
1:G:52[B]:ARG:HD3	1:H:73:ILE:HD11	2.04	0.40
1:J:32:PRO:HA	1:J:70:SER:HB3	2.04	0.40
1:L:34:ARG:NH1	1:L:37:LYS:HD2	2.36	0.40
1:L:167:TYR:CB	1:L:168:PRO:CD	2.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/261 (98%)	253 (98%)	3 (1%)	1 (0%)	34	30
1	B	250/261 (96%)	245 (98%)	4 (2%)	1 (0%)	34	30
1	C	252/261 (97%)	247 (98%)	4 (2%)	1 (0%)	34	30
1	D	249/261 (95%)	244 (98%)	4 (2%)	1 (0%)	34	30
1	E	245/261 (94%)	240 (98%)	4 (2%)	1 (0%)	34	30
1	F	255/261 (98%)	247 (97%)	7 (3%)	1 (0%)	34	30
1	G	254/261 (97%)	249 (98%)	3 (1%)	2 (1%)	19	13
1	H	262/261 (100%)	256 (98%)	5 (2%)	1 (0%)	34	30
1	I	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	30
1	J	241/261 (92%)	236 (98%)	4 (2%)	1 (0%)	34	30
1	K	258/261 (99%)	253 (98%)	4 (2%)	1 (0%)	34	30
1	L	247/261 (95%)	240 (97%)	6 (2%)	1 (0%)	34	30
All	All	3027/3132 (97%)	2961 (98%)	53 (2%)	13 (0%)	34	30

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	167	TYR
1	J	167	TYR
1	L	167	TYR
1	A	167	TYR
1	B	167	TYR
1	C	167	TYR
1	E	167	TYR
1	F	167	TYR
1	G	167	TYR
1	H	167	TYR
1	K	167	TYR
1	D	167	TYR
1	G	122	GLY

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	209/198 (106%)	204 (98%)	5 (2%)	49	51
1	B	204/198 (103%)	199 (98%)	5 (2%)	47	49
1	C	206/198 (104%)	193 (94%)	13 (6%)	18	13
1	D	203/198 (102%)	195 (96%)	8 (4%)	32	30
1	E	199/198 (100%)	188 (94%)	11 (6%)	21	17
1	F	207/198 (104%)	198 (96%)	9 (4%)	29	26
1	G	206/198 (104%)	194 (94%)	12 (6%)	20	15
1	H	214/198 (108%)	204 (95%)	10 (5%)	26	22
1	I	209/198 (106%)	203 (97%)	6 (3%)	42	43
1	J	196/198 (99%)	192 (98%)	4 (2%)	55	58
1	K	210/198 (106%)	201 (96%)	9 (4%)	29	26
1	L	201/198 (102%)	192 (96%)	9 (4%)	27	24
All	All	2464/2376 (104%)	2363 (96%)	101 (4%)	32	28

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	MSE
1	A	198	ASN
1	A	200	GLU
1	A	232	ILE
1	A	235	HIS
1	B	9	THR
1	B	41	LEU
1	B	198	ASN
1	B	200	GLU
1	B	237	THR
1	C	8	LYS
1	C	9	THR
1	C	21	ASN
1	C	34[A]	ARG
1	C	34[B]	ARG
1	C	40[A]	GLU
1	C	40[B]	GLU
1	C	67[A]	VAL
1	C	67[B]	VAL

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Mol	Chain	Res	Type
1	C	198	ASN
1	C	200	GLU
1	C	242	GLU
1	C	249	VAL
1	D	8	LYS
1	D	41	LEU
1	D	52[A]	ARG
1	D	52[B]	ARG
1	D	154	THR
1	D	198	ASN
1	D	200	GLU
1	D	239	LYS
1	E	9	THR
1	E	50	SER
1	E	52[A]	ARG
1	E	52[B]	ARG
1	E	53	GLU
1	E	154	THR
1	E	174	ASP
1	E	198	ASN
1	E	200	GLU
1	E	238	LEU
1	E	240	GLU
1	F	8	LYS
1	F	10[A]	VAL
1	F	10[B]	VAL
1	F	21	ASN
1	F	41	LEU
1	F	198	ASN
1	F	200	GLU
1	F	232	ILE
1	F	237	THR
1	G	8	LYS
1	G	9	THR
1	G	52[A]	ARG
1	G	52[B]	ARG
1	G	53	GLU
1	G	198	ASN
1	G	200	GLU
1	G	230	LYS
1	G	231	GLU
1	G	242	GLU

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Mol	Chain	Res	Type
1	G	244	ARG
1	G	247	LYS
1	H	34[A]	ARG
1	H	34[B]	ARG
1	H	41	LEU
1	H	190[A]	GLU
1	H	190[B]	GLU
1	H	198	ASN
1	H	200	GLU
1	H	225	ILE
1	H	234	ASP
1	H	242	GLU
1	I	198	ASN
1	I	200	GLU
1	I	209	MSE
1	I	225	ILE
1	I	231	GLU
1	I	239	LYS
1	J	58	ARG
1	J	198	ASN
1	J	200	GLU
1	J	240	GLU
1	K	9	THR
1	K	21	ASN
1	K	34	ARG
1	K	40	GLU
1	K	198	ASN
1	K	200	GLU
1	K	225	ILE
1	K	232	ILE
1	K	239	LYS
1	L	41	LEU
1	L	65	SER
1	L	98	THR
1	L	198	ASN
1	L	200	GLU
1	L	225	ILE
1	L	237	THR
1	L	239	LYS
1	L	240	GLU

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

Mol	Chain	Res	Type
1	A	198	ASN
1	B	36	GLN
1	B	170	GLN
1	B	198	ASN
1	B	235	HIS
1	C	12	HIS
1	C	198	ASN
1	D	198	ASN
1	E	198	ASN
1	F	198	ASN
1	G	198	ASN
1	H	198	ASN
1	I	198	ASN
1	J	198	ASN
1	K	198	ASN
1	L	198	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 45 ligands modelled in this entry, 4 are monoatomic - leaving 41 for Mogul analysis.

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	$\#\|Z\|>2$
3	URA	E	271	-	8,8,8	1.78	3 (37%)	9,10,10	3.08	6 (66%)
6	FMT	H	272	-	2,2,2	0.76	0	1,1,1	0.32	0
5	SO4	C	259	-	4,4,4	0.17	0	6,6,6	0.08	0
2	GOL	J	273	-	5,5,5	0.33	0	5,5,5	0.38	0
6	FMT	E	273	-	2,2,2	0.72	0	1,1,1	0.28	0
2	GOL	J	270	-	5,5,5	0.41	0	5,5,5	0.18	0
2	GOL	D	260	-	5,5,5	0.33	0	5,5,5	0.38	0
2	GOL	B	270	-	5,5,5	0.45	0	5,5,5	0.22	0
2	GOL	G	272	-	5,5,5	0.31	0	5,5,5	0.37	0
2	GOL	I	272	-	5,5,5	0.28	0	5,5,5	0.15	0
3	URA	G	273	-	8,8,8	1.56	2 (25%)	9,10,10	3.23	6 (66%)
5	SO4	I	271	-	4,4,4	0.33	0	6,6,6	0.17	0
3	URA	J	271	-	8,8,8	1.71	3 (37%)	9,10,10	2.81	5 (55%)
3	URA	K	272	-	8,8,8	1.74	2 (25%)	9,10,10	2.76	5 (55%)
2	GOL	E	259	-	5,5,5	0.49	0	5,5,5	0.77	0
3	URA	D	270	-	8,8,8	1.63	2 (25%)	9,10,10	3.05	6 (66%)
2	GOL	L	270	-	5,5,5	0.39	0	5,5,5	0.41	0
2	GOL	A	260	-	5,5,5	0.36	0	5,5,5	0.36	0
3	URA	H	270	-	8,8,8	1.76	3 (37%)	9,10,10	2.82	5 (55%)
3	URA	I	259	-	8,8,8	1.75	2 (25%)	9,10,10	2.79	6 (66%)
2	GOL	D	271	-	5,5,5	0.47	0	5,5,5	0.87	0
3	URA	L	271	-	8,8,8	1.53	2 (25%)	9,10,10	2.87	6 (66%)
2	GOL	I	270	-	5,5,5	0.36	0	5,5,5	0.24	0
2	GOL	A	270	-	5,5,5	0.44	0	5,5,5	0.31	0
2	GOL	E	272	-	5,5,5	0.42	0	5,5,5	0.64	0
7	ACY	F	275	-	3,3,3	0.77	0	3,3,3	1.04	0
3	URA	F	274	-	8,8,8	1.53	2 (25%)	9,10,10	3.14	6 (66%)
5	SO4	G	270	-	4,4,4	0.43	0	6,6,6	0.46	0
2	GOL	F	270	-	5,5,5	0.40	0	5,5,5	0.58	0
2	GOL	K	270	-	5,5,5	0.41	0	5,5,5	0.27	0
2	GOL	C	275	-	5,5,5	0.33	0	5,5,5	0.39	0
3	URA	C	276	-	8,8,8	1.68	3 (37%)	9,10,10	3.02	6 (66%)
2	GOL	B	261	-	5,5,5	0.34	0	5,5,5	0.35	0
2	GOL	C	261	-	5,5,5	0.30	0	5,5,5	0.26	0
2	GOL	C	271	-	5,5,5	0.45	0	5,5,5	0.37	0
2	GOL	F	273	-	5,5,5	0.38	0	5,5,5	0.26	0
3	URA	B	271	-	8,8,8	2.64	5 (62%)	9,10,10	2.92	5 (55%)
2	GOL	K	271	-	5,5,5	0.46	0	5,5,5	0.58	0
2	GOL	G	271	-	5,5,5	0.32	0	5,5,5	0.55	0
2	GOL	H	271	-	5,5,5	0.36	0	5,5,5	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GOL	G	274	-	5,5,5	0.43	0	5,5,5	0.77	0

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
3	URA	E	271	-	-	-	0/1/1/1
2	GOL	J	273	-	-	2/4/4/4	-
2	GOL	J	270	-	-	4/4/4/4	-
2	GOL	D	260	-	-	4/4/4/4	-
2	GOL	B	270	-	-	2/4/4/4	-
2	GOL	G	272	-	-	0/4/4/4	-
2	GOL	I	272	-	-	2/4/4/4	-
3	URA	G	273	-	-	-	0/1/1/1
3	URA	J	271	-	-	-	0/1/1/1
3	URA	K	272	-	-	-	0/1/1/1
2	GOL	E	259	-	-	0/4/4/4	-
3	URA	D	270	-	-	-	0/1/1/1
2	GOL	L	270	-	-	2/4/4/4	-
2	GOL	A	260	-	-	4/4/4/4	-
3	URA	H	270	-	-	-	0/1/1/1
3	URA	I	259	-	-	-	0/1/1/1
2	GOL	D	271	-	-	4/4/4/4	-
3	URA	L	271	-	-	-	0/1/1/1
2	GOL	I	270	-	-	0/4/4/4	-
2	GOL	A	270	-	-	0/4/4/4	-
2	GOL	E	272	-	-	4/4/4/4	-
3	URA	F	274	-	-	-	0/1/1/1
2	GOL	F	270	-	-	0/4/4/4	-
2	GOL	K	270	-	-	2/4/4/4	-
2	GOL	C	275	-	-	2/4/4/4	-
3	URA	C	276	-	-	-	0/1/1/1
2	GOL	B	261	-	-	4/4/4/4	-
2	GOL	C	261	-	-	2/4/4/4	-
2	GOL	C	271	-	-	0/4/4/4	-
2	GOL	F	273	-	-	4/4/4/4	-
3	URA	B	271	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	K	271	-	-	2/4/4/4	-
2	GOL	G	271	-	-	2/4/4/4	-
2	GOL	H	271	-	-	2/4/4/4	-
2	GOL	G	274	-	-	0/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	271	URA	C4-N3	-4.50	1.30	1.38
3	B	271	URA	C2-N3	-3.33	1.31	1.37
3	B	271	URA	C6-N1	-3.07	1.31	1.36
3	I	259	URA	C6-C5	2.99	1.40	1.34
3	H	270	URA	C6-C5	2.84	1.40	1.34
3	I	259	URA	C4-N3	-2.71	1.33	1.38
3	K	272	URA	C6-C5	2.69	1.40	1.34
3	E	271	URA	C4-N3	-2.63	1.33	1.38
3	K	272	URA	C4-N3	-2.59	1.33	1.38
3	J	271	URA	C6-C5	2.55	1.40	1.34
3	B	271	URA	C5-C4	-2.48	1.38	1.43
3	G	273	URA	C6-C5	2.48	1.39	1.34
3	H	270	URA	C4-N3	-2.48	1.34	1.38
3	F	274	URA	C6-C5	2.46	1.39	1.34
3	L	271	URA	C6-C5	2.39	1.39	1.34
3	B	271	URA	C2-N1	-2.38	1.33	1.36
3	C	276	URA	C6-C5	2.34	1.39	1.34
3	E	271	URA	C6-C5	2.33	1.39	1.34
3	D	270	URA	C4-N3	-2.31	1.34	1.38
3	D	270	URA	C6-C5	2.30	1.39	1.34
3	C	276	URA	C4-N3	-2.27	1.34	1.38
3	J	271	URA	C4-N3	-2.27	1.34	1.38
3	C	276	URA	C5-C4	-2.23	1.38	1.43
3	F	274	URA	C4-N3	-2.19	1.34	1.38
3	H	270	URA	C2-N3	-2.17	1.33	1.37
3	L	271	URA	C4-N3	-2.16	1.34	1.38
3	J	271	URA	C2-N3	-2.14	1.33	1.37
3	E	271	URA	C2-N3	-2.13	1.33	1.37
3	G	273	URA	C5-C4	-2.01	1.39	1.43

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	274	URA	N1-C2-N3	5.44	121.29	115.13
3	G	273	URA	C4-N3-C2	-5.28	120.46	125.70
3	E	271	URA	N1-C2-N3	5.14	120.95	115.13
3	G	273	URA	N1-C2-N3	5.12	120.93	115.13
3	B	271	URA	C4-N3-C2	-5.11	120.64	125.70
3	D	270	URA	C4-N3-C2	-4.93	120.81	125.70
3	E	271	URA	C4-N3-C2	-4.87	120.87	125.70
3	H	270	URA	N1-C2-N3	4.79	120.56	115.13
3	J	271	URA	N1-C2-N3	4.79	120.55	115.13
3	L	271	URA	C4-N3-C2	-4.74	121.00	125.70
3	L	271	URA	N1-C2-N3	4.71	120.47	115.13
3	I	259	URA	N1-C2-N3	4.70	120.45	115.13
3	D	270	URA	N1-C2-N3	4.64	120.39	115.13
3	F	274	URA	C4-N3-C2	-4.63	121.10	125.70
3	C	276	URA	C4-N3-C2	-4.62	121.11	125.70
3	C	276	URA	N1-C2-N3	4.62	120.37	115.13
3	K	272	URA	C6-N1-C2	-4.39	119.71	122.40
3	K	272	URA	N1-C2-N3	4.31	120.01	115.13
3	J	271	URA	C6-N1-C2	-4.30	119.76	122.40
3	B	271	URA	N1-C2-N3	4.17	119.85	115.13
3	H	270	URA	C4-N3-C2	-4.13	121.60	125.70
3	I	259	URA	C4-N3-C2	-4.00	121.73	125.70
3	B	271	URA	C5-C4-N3	4.00	120.82	114.84
3	F	274	URA	C6-N1-C2	-3.81	120.06	122.40
3	J	271	URA	C4-N3-C2	-3.43	122.30	125.70
3	K	272	URA	C4-N3-C2	-3.41	122.32	125.70
3	E	271	URA	C5-C4-N3	3.25	119.70	114.84
3	D	270	URA	C5-C4-N3	3.22	119.66	114.84
3	G	273	URA	O2-C2-N1	-3.22	119.25	122.79
3	K	272	URA	C5-C4-N3	3.18	119.60	114.84
3	H	270	URA	C5-C4-N3	3.17	119.59	114.84
3	I	259	URA	C5-C4-N3	3.15	119.56	114.84
3	C	276	URA	O4-C4-C5	-3.11	119.69	125.16
3	C	276	URA	O2-C2-N1	-3.10	119.37	122.79
3	D	270	URA	O4-C4-C5	-3.09	119.73	125.16
3	C	276	URA	C5-C4-N3	3.04	119.39	114.84
3	G	273	URA	O4-C4-C5	-3.02	119.85	125.16
3	D	270	URA	O2-C2-N1	-2.97	119.52	122.79
3	L	271	URA	C5-C4-N3	2.92	119.21	114.84
3	G	273	URA	C5-C4-N3	2.91	119.20	114.84
3	H	270	URA	C6-N1-C2	-2.90	120.62	122.40
3	I	259	URA	C6-N1-C2	-2.88	120.64	122.40
3	E	271	URA	O2-C2-N1	-2.77	119.75	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	274	URA	O2-C2-N1	-2.74	119.77	122.79
3	F	274	URA	C5-C4-N3	2.71	118.89	114.84
3	H	270	URA	O2-C2-N3	-2.67	116.78	121.82
3	B	271	URA	O4-C4-C5	-2.63	120.53	125.16
3	E	271	URA	O4-C4-C5	-2.59	120.61	125.16
3	J	271	URA	C5-C4-N3	2.59	118.71	114.84
3	G	273	URA	C6-N1-C2	-2.53	120.85	122.40
3	C	276	URA	C6-N1-C2	-2.50	120.87	122.40
3	L	271	URA	O4-C4-C5	-2.48	120.80	125.16
3	L	271	URA	O2-C2-N1	-2.45	120.09	122.79
3	E	271	URA	C6-N1-C2	-2.36	120.95	122.40
3	D	270	URA	C6-N1-C2	-2.28	121.00	122.40
3	I	259	URA	O4-C4-C5	-2.27	121.17	125.16
3	L	271	URA	C6-N1-C2	-2.19	121.05	122.40
3	I	259	URA	O2-C2-N1	-2.15	120.43	122.79
3	B	271	URA	C5-C6-N1	-2.14	118.54	121.31
3	J	271	URA	O4-C4-C5	-2.13	121.42	125.16
3	F	274	URA	O4-C4-C5	-2.08	121.50	125.16
3	K	272	URA	O4-C4-C5	-2.07	121.52	125.16

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	261	GOL	O1-C1-C2-C3
2	B	270	GOL	O1-C1-C2-C3
2	C	261	GOL	O1-C1-C2-C3
2	C	275	GOL	O1-C1-C2-C3
2	D	260	GOL	O1-C1-C2-C3
2	D	260	GOL	C1-C2-C3-O3
2	D	271	GOL	O1-C1-C2-C3
2	H	271	GOL	O1-C1-C2-C3
2	I	272	GOL	O1-C1-C2-C3
2	J	273	GOL	C1-C2-C3-O3
2	K	271	GOL	O1-C1-C2-C3
2	K	270	GOL	O1-C1-C2-C3
2	L	270	GOL	O1-C1-C2-C3
2	B	270	GOL	O1-C1-C2-O2
2	D	260	GOL	O2-C2-C3-O3
2	D	271	GOL	O1-C1-C2-O2
2	H	271	GOL	O1-C1-C2-O2
2	I	272	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	K	270	GOL	O1-C1-C2-O2
2	A	260	GOL	O1-C1-C2-C3
2	A	260	GOL	C1-C2-C3-O3
2	B	261	GOL	C1-C2-C3-O3
2	E	272	GOL	O1-C1-C2-C3
2	E	272	GOL	C1-C2-C3-O3
2	J	270	GOL	C1-C2-C3-O3
2	C	261	GOL	O1-C1-C2-O2
2	C	275	GOL	O1-C1-C2-O2
2	K	271	GOL	O1-C1-C2-O2
2	L	270	GOL	O1-C1-C2-O2
2	A	260	GOL	O1-C1-C2-O2
2	B	261	GOL	O1-C1-C2-O2
2	D	271	GOL	O2-C2-C3-O3
2	E	272	GOL	O1-C1-C2-O2
2	J	270	GOL	O2-C2-C3-O3
2	J	273	GOL	O2-C2-C3-O3
2	A	260	GOL	O2-C2-C3-O3
2	D	260	GOL	O1-C1-C2-O2
2	F	273	GOL	O1-C1-C2-O2
2	F	273	GOL	O2-C2-C3-O3
2	G	271	GOL	O1-C1-C2-O2
2	F	273	GOL	O1-C1-C2-C3
2	J	270	GOL	O1-C1-C2-C3
2	D	271	GOL	C1-C2-C3-O3
2	B	261	GOL	O2-C2-C3-O3
2	E	272	GOL	O2-C2-C3-O3
2	F	273	GOL	C1-C2-C3-O3
2	G	271	GOL	O1-C1-C2-C3
2	J	270	GOL	O1-C1-C2-O2

There are no ring outliers.

22 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	271	URA	1	0
6	H	272	FMT	3	0
5	C	259	SO4	1	0
2	J	273	GOL	1	0
6	E	273	FMT	2	0
2	D	260	GOL	1	0
2	B	270	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	272	URA	2	0
3	I	259	URA	3	0
2	D	271	GOL	1	0
2	E	272	GOL	1	0
3	F	274	URA	2	0
5	G	270	SO4	1	0
2	F	270	GOL	2	0
2	K	270	GOL	2	0
2	C	275	GOL	7	0
3	C	276	URA	1	0
2	C	261	GOL	2	0
2	F	273	GOL	3	0
3	B	271	URA	2	0
2	K	271	GOL	1	0
2	H	271	GOL	1	0

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, 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	240/261 (91%)	-0.23	4 (1%)	70	68	11, 20, 38, 87	5 (2%)
1	B	234/261 (89%)	-0.32	3 (1%)	77	76	9, 20, 39, 88	1 (0%)
1	C	238/261 (91%)	-0.12	3 (1%)	77	76	12, 27, 56, 102	4 (1%)
1	D	235/261 (90%)	-0.39	2 (0%)	84	83	11, 20, 43, 89	1 (0%)
1	E	235/261 (90%)	-0.04	5 (2%)	63	62	11, 26, 55, 101	5 (2%)
1	F	240/261 (91%)	-0.18	8 (3%)	46	45	10, 22, 60, 110	3 (1%)
1	G	240/261 (91%)	-0.09	6 (2%)	57	56	11, 22, 51, 83	5 (2%)
1	H	239/261 (91%)	-0.08	10 (4%)	36	35	11, 21, 45, 82	1 (0%)
1	I	240/261 (91%)	-0.36	3 (1%)	77	76	11, 22, 45, 71	3 (1%)
1	J	231/261 (88%)	-0.17	6 (2%)	56	54	12, 25, 51, 72	3 (1%)
1	K	241/261 (92%)	-0.40	3 (1%)	79	78	10, 20, 42, 71	4 (1%)
1	L	235/261 (90%)	-0.31	1 (0%)	92	92	10, 20, 42, 75	4 (1%)
All	All	2848/3132 (90%)	-0.23	54 (1%)	66	65	9, 22, 49, 110	39 (1%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	LYS	5.8
1	G	9	THR	5.6
1	C	236	ALA	5.6
1	F	232	ILE	4.8
1	H	232	ILE	4.4
1	E	230	LYS	4.3
1	A	232	ILE	4.2
1	J	224	ILE	4.1
1	A	235	HIS	4.0
1	F	8	LYS	3.9
1	C	235	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	235	HIS	3.5
1	G	230	LYS	3.5
1	H	234	ASP	3.3
1	F	233	PRO	3.3
1	F	234	ASP	3.2
1	H	231	GLU	3.1
1	F	9	THR	3.0
1	F	238	LEU	3.0
1	J	238	LEU	3.0
1	D	108	VAL	3.0
1	K	235	HIS	3.0
1	H	238	LEU	2.9
1	J	108	VAL	2.9
1	F	236	ALA	2.9
1	C	237	THR	2.9
1	A	233	PRO	2.8
1	H	235	HIS	2.8
1	G	8	LYS	2.8
1	H	236	ALA	2.8
1	I	235	HIS	2.7
1	H	239	LYS	2.7
1	H	230	LYS	2.6
1	G	232	ILE	2.6
1	F	235	HIS	2.5
1	L	225	ILE	2.4
1	E	53	GLU	2.4
1	J	109	GLY	2.4
1	G	234	ASP	2.3
1	E	9	THR	2.3
1	E	224	ILE	2.3
1	I	232	ILE	2.3
1	J	154	THR	2.3
1	E	21	ASN	2.3
1	J	152	GLY	2.3
1	G	154	THR	2.2
1	H	242	GLU	2.2
1	B	229	GLN	2.1
1	I	174	ASP	2.1
1	B	238	LEU	2.1
1	D	238	LEU	2.1
1	H	233	PRO	2.0
1	K	232	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	K	7	THR	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 monosaccharides 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^{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	B-factors(Å^2)	Q<0.9
3	URA	B	271	8/8	0.83	0.21	31,52,55,59	0
3	URA	C	276	8/8	0.84	0.27	15,22,30,31	8
7	ACY	F	275	4/4	0.86	0.21	31,34,37,38	0
2	GOL	J	270	6/6	0.87	0.16	33,35,37,38	0
2	GOL	I	272	6/6	0.87	0.18	28,30,35,35	0
2	GOL	F	270	6/6	0.88	0.18	38,46,49,54	0
3	URA	D	270	8/8	0.89	0.17	28,45,49,52	0
2	GOL	F	273	6/6	0.89	0.15	32,39,41,42	0
2	GOL	G	271	6/6	0.90	0.20	39,45,47,53	0
2	GOL	C	261	6/6	0.91	0.17	40,42,44,50	0
2	GOL	G	272	6/6	0.91	0.15	34,39,42,44	0
2	GOL	B	261	6/6	0.92	0.14	36,42,45,51	0
3	URA	J	271	8/8	0.92	0.11	28,33,39,39	0
4	CL	I	273	1/1	0.92	0.14	72,72,72,72	0
2	GOL	C	275	6/6	0.92	0.14	39,48,54,54	0
2	GOL	A	270	6/6	0.93	0.15	30,31,32,37	0
3	URA	L	271	8/8	0.93	0.10	19,33,34,36	0
4	CL	C	274	1/1	0.93	0.10	59,59,59,59	0
2	GOL	I	270	6/6	0.93	0.14	20,24,29,29	0
4	CL	I	274	1/1	0.93	0.07	54,54,54,54	0
2	GOL	K	270	6/6	0.93	0.11	28,30,35,35	0
3	URA	G	273	8/8	0.94	0.10	19,26,29,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GOL	D	260	6/6	0.94	0.12	34,36,41,44	0
2	GOL	L	270	6/6	0.94	0.10	40,42,42,44	0
2	GOL	A	260	6/6	0.94	0.14	35,38,44,48	0
2	GOL	J	273	6/6	0.94	0.13	45,46,48,49	0
2	GOL	K	271	6/6	0.94	0.20	22,27,30,30	0
6	FMT	H	272	3/3	0.94	0.19	59,59,59,60	0
3	URA	F	274	8/8	0.94	0.12	18,26,31,34	0
2	GOL	E	259	6/6	0.95	0.15	18,20,23,25	0
6	FMT	E	273	3/3	0.95	0.15	45,45,46,48	0
2	GOL	C	271	6/6	0.95	0.14	26,29,30,32	0
2	GOL	E	272	6/6	0.95	0.15	33,40,41,46	0
2	GOL	H	271	6/6	0.96	0.10	31,36,43,44	0
3	URA	H	270	8/8	0.96	0.09	16,20,23,24	0
5	SO4	C	259	5/5	0.96	0.13	37,46,49,53	0
2	GOL	B	270	6/6	0.96	0.19	20,21,23,23	0
3	URA	E	271	8/8	0.96	0.10	35,40,45,46	0
2	GOL	D	271	6/6	0.96	0.18	16,25,27,28	0
5	SO4	I	271	5/5	0.97	0.09	29,30,34,41	0
3	URA	K	272	8/8	0.97	0.08	11,15,21,23	0
2	GOL	G	274	6/6	0.97	0.14	15,16,19,20	0
5	SO4	G	270	5/5	0.97	0.10	19,19,24,32	0
3	URA	I	259	8/8	0.98	0.08	15,17,18,22	0
4	CL	E	270	1/1	0.99	0.09	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.