



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:43 PM UTC

PDB ID : 1BD4 / pdb_00001bd4
Title : UPRT-URACIL COMPLEX
Authors : Schumacher, M.A.; Carter, D.; Scott, D.; Roos, D.; Ullman, B.; Brennan, R.G.
Deposited on : 1998-05-12
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

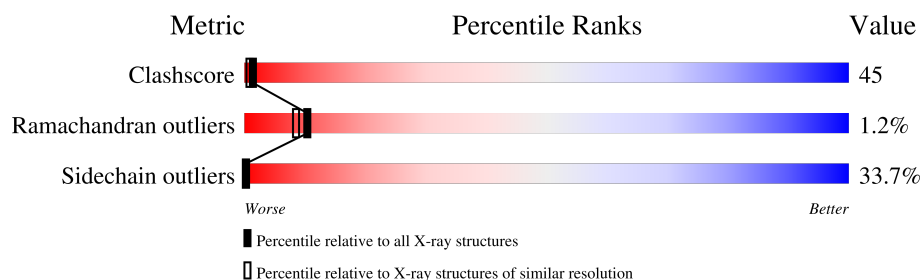
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	243	
1	B	243	
1	C	243	
1	D	243	

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	PO4	D	799	-	-	X	-
2	PO4	D	899	-	-	X	-
3	URA	C	999	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7464 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.

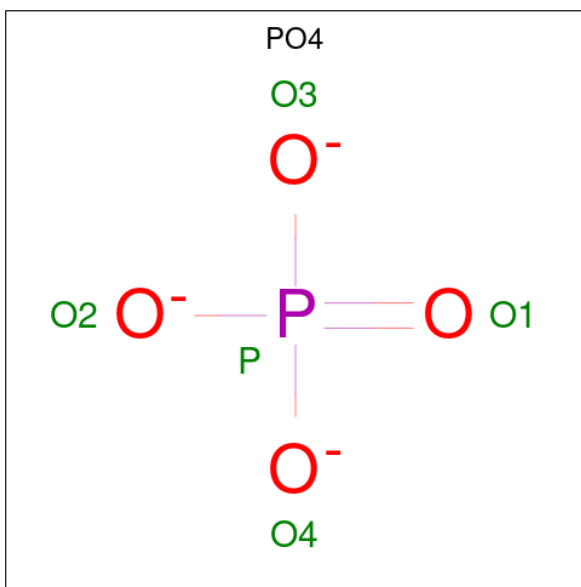
- Molecule 1 is a protein called URACIL PHOSPHORIBOSYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	224	Total	C	N	O	S	0	0	0
			1788	1146	305	324	13			
1	C	224	Total	C	N	O	S	0	0	0
			1788	1146	305	324	13			
1	B	224	Total	C	N	O	S	0	0	0
			1788	1146	305	324	13			
1	A	224	Total	C	N	O	S	0	0	0
			1788	1146	305	324	13			

There are 12 discrepancies between the modelled and reference sequences:

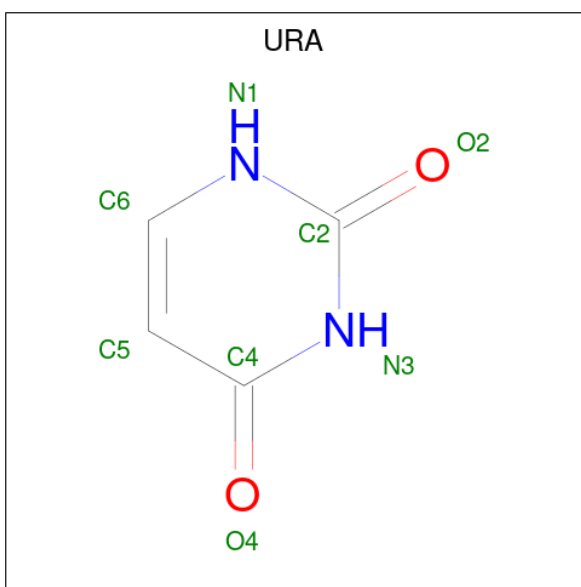
Chain	Residue	Modelled	Actual	Comment	Reference
D	84	GLN	GLU	conflict	UNP Q26998
D	128	VAL	CYS	conflict	UNP Q26998
D	157	GLU	ASP	conflict	UNP Q26998
C	84	GLN	GLU	conflict	UNP Q26998
C	128	VAL	CYS	conflict	UNP Q26998
C	157	GLU	ASP	conflict	UNP Q26998
B	84	GLN	GLU	conflict	UNP Q26998
B	128	VAL	CYS	conflict	UNP Q26998
B	157	GLU	ASP	conflict	UNP Q26998
A	84	GLN	GLU	conflict	UNP Q26998
A	128	VAL	CYS	conflict	UNP Q26998
A	157	GLU	ASP	conflict	UNP Q26998

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is URACIL (CCD ID: URA) (formula: C₄H₄N₂O₂).



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

- Molecule 4 is water.

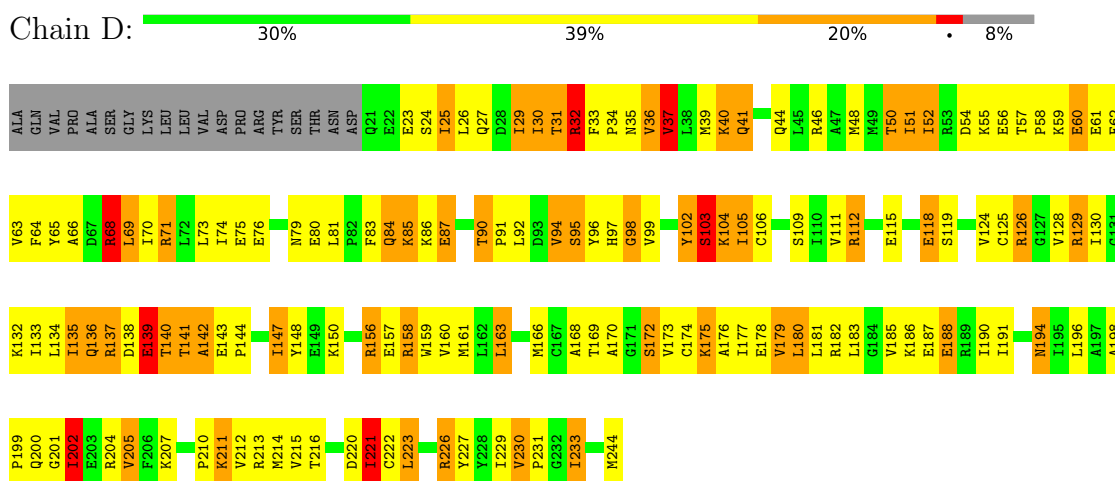
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	53	Total	O	0	0
			53	53		
4	C	74	Total	O	0	0
			74	74		
4	B	66	Total	O	0	0
			66	66		
4	A	47	Total	O	0	0
			47	47		

3 Residue-property plots

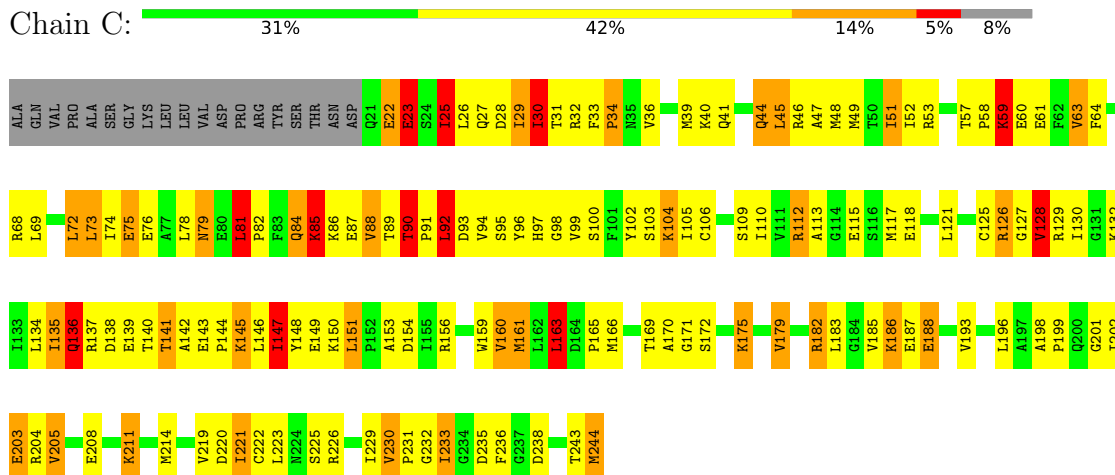
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE

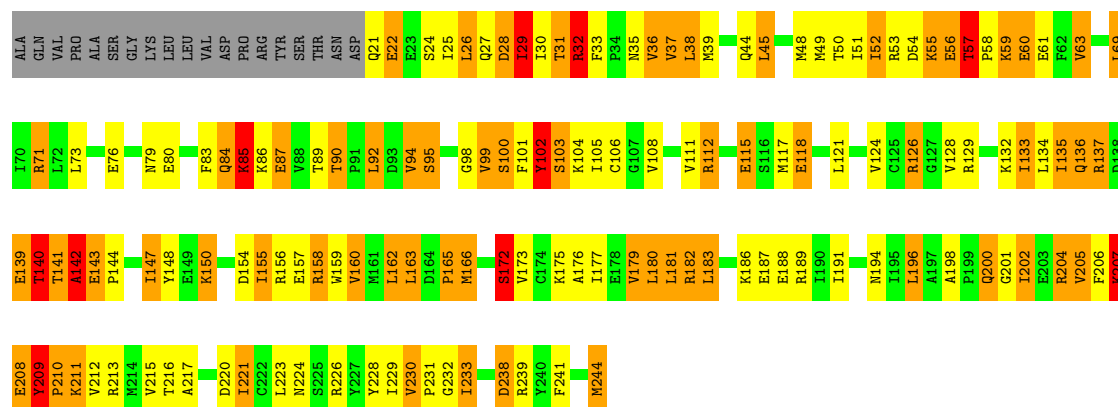


• Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE



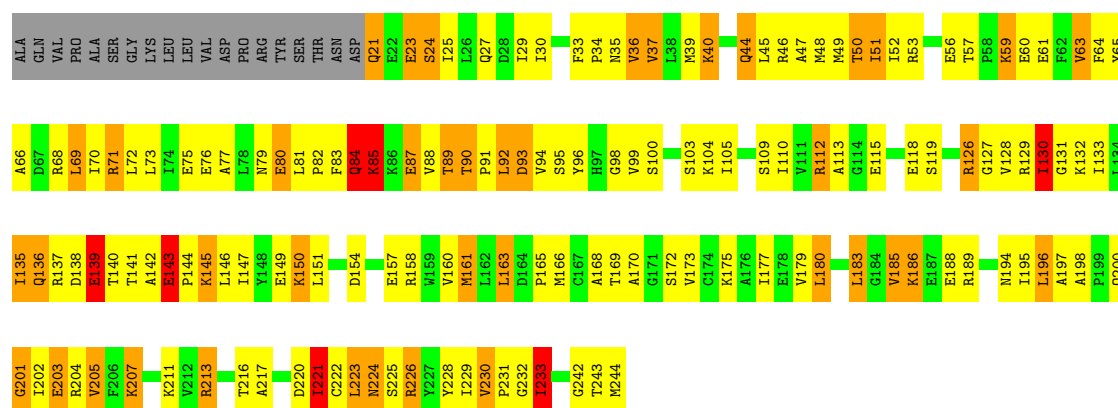
• Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE





• Molecule 1: URACIL PHOSPHORIBOSYLTRANSFERASE

Chain A: 30% 42% 17% 8%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.39 Å 141.77 Å 71.46 Å 90.00° 114.82° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	87.0 (10.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.194 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7464	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: URA, PO4

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	0.82	0/1817	1.46	21/2450 (0.9%)
1	B	0.82	0/1817	1.57	34/2450 (1.4%)
1	C	0.83	0/1817	1.45	25/2450 (1.0%)
1	D	0.84	1/1817 (0.1%)	1.48	25/2450 (1.0%)
All	All	0.83	1/7268 (0.0%)	1.49	105/9800 (1.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	229	ILE	CA-CB	-5.20	1.48	1.54

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	ILE	N-CA-C	12.17	124.49	110.62
1	B	221	ILE	N-CA-C	10.51	120.30	110.74
1	B	22	GLU	N-CA-C	-9.45	99.88	111.40
1	D	102	TYR	N-CA-C	-9.20	93.41	108.41
1	A	243	THR	N-CA-C	-9.19	102.18	112.57
1	B	160	VAL	N-CA-C	8.14	119.64	107.75
1	C	30	ILE	N-CA-C	-7.86	102.60	110.62
1	D	147	ILE	CB-CA-C	-7.81	101.77	112.24
1	B	32	ARG	N-CA-C	7.80	119.86	111.36
1	C	103	SER	N-CA-C	7.75	120.89	110.35
1	D	163	LEU	N-CA-C	7.71	121.09	108.52
1	C	85	LYS	N-CA-C	-7.67	98.08	110.20
1	B	57	THR	CB-CA-C	7.61	120.45	109.26
1	C	236	PHE	N-CA-C	7.57	119.17	111.07
1	B	85	LYS	N-CA-C	-7.33	97.45	109.40
1	C	113	ALA	N-CA-C	7.26	119.20	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	GLU	N-CA-C	7.21	120.03	110.36
1	A	105	ILE	N-CA-C	7.07	117.44	108.82
1	B	108	VAL	N-CA-C	-7.05	98.62	108.27
1	D	139	GLU	N-CA-C	7.04	119.99	111.82
1	D	32	ARG	N-CA-C	7.04	118.95	111.28
1	B	29	ILE	N-CA-C	-6.99	103.96	110.53
1	C	59	LYS	N-CA-C	6.95	119.44	111.11
1	B	101	PHE	N-CA-C	-6.92	100.27	110.52
1	B	163	LEU	N-CA-C	6.79	119.97	108.90
1	B	198	ALA	N-CA-C	-6.76	99.93	110.14
1	B	159	TRP	N-CA-C	-6.75	98.62	109.96
1	D	160	VAL	N-CA-C	6.63	117.42	107.75
1	D	159	TRP	N-CA-C	-6.62	98.84	109.96
1	C	147	ILE	CB-CA-C	-6.53	103.36	111.92
1	D	158	ARG	N-CA-C	6.53	119.80	109.81
1	A	198	ALA	N-CA-C	-6.51	100.31	110.14
1	A	158	ARG	N-CA-C	6.45	119.62	110.14
1	A	51	ILE	CB-CA-C	-6.33	103.73	112.02
1	D	96	TYR	N-CA-C	-6.25	99.62	109.50
1	B	57	THR	N-CA-C	6.24	117.67	109.93
1	B	99	VAL	CB-CA-C	-6.23	103.31	110.41
1	D	198	ALA	N-CA-C	-6.22	99.44	109.40
1	C	128	VAL	CB-CA-C	-6.20	101.96	111.08
1	C	198	ALA	N-CA-C	-6.20	101.53	110.40
1	B	142	ALA	CA-C-N	-6.14	113.07	121.61
1	B	142	ALA	C-N-CA	-6.14	113.07	121.61
1	C	153	ALA	N-CA-C	6.14	118.94	111.82
1	D	98	GLY	N-CA-C	-6.13	102.68	111.20
1	A	85	LYS	N-CA-C	-5.94	98.15	110.80
1	B	57	THR	N-CA-CB	5.93	118.50	110.14
1	C	160	VAL	N-CA-C	5.88	116.77	108.36
1	A	205	VAL	CB-CA-C	-5.84	104.41	111.88
1	B	29	ILE	CB-CA-C	-5.83	104.38	112.02
1	C	172	SER	N-CA-C	5.82	117.42	111.14
1	A	140	THR	CB-CA-C	-5.82	101.64	110.83
1	B	210	PRO	N-CA-C	5.82	121.13	113.86
1	B	172	SER	N-CA-C	5.75	117.62	111.36
1	A	112	ARG	CB-CA-C	-5.74	99.20	110.10
1	B	158	ARG	N-CA-C	5.73	118.56	110.14
1	B	209	TYR	CA-C-N	5.73	125.34	119.56
1	B	209	TYR	C-N-CA	5.73	125.34	119.56
1	D	59	LYS	N-CA-C	5.72	117.51	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	ILE	CB-CA-C	-5.71	104.66	111.97
1	D	68	ARG	N-CA-C	-5.71	104.96	111.07
1	B	223	LEU	N-CA-C	-5.69	101.00	110.17
1	C	104	LYS	N-CA-C	-5.65	100.78	109.76
1	C	136	GLN	N-CA-C	5.64	118.67	109.24
1	D	54	ASP	CA-C-N	5.64	128.11	120.38
1	D	54	ASP	C-N-CA	5.64	128.11	120.38
1	C	163	LEU	N-CA-C	5.63	117.69	108.52
1	C	243	THR	CB-CA-C	-5.62	103.33	111.14
1	A	201	GLY	N-CA-C	-5.60	106.00	112.50
1	C	225	SER	N-CA-C	-5.56	104.63	111.75
1	B	217	ALA	N-CA-C	-5.55	106.40	114.12
1	C	90	THR	N-CA-CB	-5.53	102.69	110.04
1	B	211	LYS	N-CA-CB	-5.51	101.50	110.42
1	C	34	PRO	N-CA-C	5.49	120.78	114.03
1	C	23	GLU	N-CA-C	5.48	118.76	111.75
1	A	139	GLU	N-CA-C	5.48	119.58	113.01
1	B	35	ASN	N-CA-C	5.48	119.95	113.16
1	D	41	GLN	N-CA-C	5.46	119.17	110.70
1	B	238	ASP	N-CA-C	5.45	119.65	112.89
1	B	63	VAL	N-CA-C	5.40	116.13	110.62
1	C	75	GLU	N-CA-C	-5.39	105.41	111.28
1	A	233	ILE	CB-CA-C	-5.39	105.56	110.63
1	A	44	GLN	N-CA-C	-5.35	105.10	111.03
1	D	35	ASN	CA-C-N	-5.33	116.21	122.93
1	D	35	ASN	C-N-CA	-5.33	116.21	122.93
1	C	51	ILE	CB-CA-C	-5.32	105.05	112.02
1	A	232	GLY	N-CA-C	5.31	125.75	113.18
1	A	131	GLY	N-CA-C	-5.30	104.59	113.02
1	B	239	ARG	N-CA-C	-5.28	105.43	111.14
1	B	207	LYS	N-CA-C	-5.24	105.46	111.07
1	A	160	VAL	N-CA-C	5.21	115.60	107.99
1	D	211	LYS	N-CA-C	5.20	119.49	113.20
1	C	92	LEU	CA-CB-CG	-5.16	98.26	116.30
1	B	165	PRO	N-CA-C	5.14	120.67	113.53
1	D	140	THR	CB-CA-C	-5.13	103.00	110.95
1	D	29	ILE	CB-CA-C	-5.13	105.41	111.97
1	D	95	SER	N-CA-C	5.08	118.23	110.20
1	A	130	ILE	CB-CA-C	-5.08	104.39	110.99
1	D	194	ASN	N-CA-C	5.07	116.78	109.07
1	A	163	LEU	N-CA-C	5.05	116.75	108.52
1	C	102	TYR	N-CA-C	5.03	121.11	114.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	SER	N-CA-C	5.03	117.72	110.28
1	A	57	THR	CA-C-N	5.03	125.42	119.99
1	A	57	THR	C-N-CA	5.03	125.42	119.99
1	C	81	LEU	N-CA-C	5.01	117.07	110.36
1	D	37	VAL	N-CA-CB	5.00	117.00	110.99

There are no chirality outliers.

There are no planarity outliers.

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	1788	0	1857	196	0
1	B	1788	0	1857	161	0
1	C	1788	0	1857	180	0
1	D	1788	0	1857	180	0
2	A	10	0	0	1	0
2	B	10	0	0	2	0
2	C	10	0	0	1	0
2	D	10	0	0	5	0
3	A	8	0	3	0	0
3	B	8	0	3	2	0
3	C	8	0	3	6	0
3	D	8	0	3	3	0
4	A	47	0	0	10	0
4	B	66	0	0	6	0
4	C	74	0	0	3	0
4	D	53	0	0	4	0
All	All	7464	0	7440	659	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 45.

All (659) 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:C:141:THR:HG22	1:C:143:GLU:H	1.09	1.10
1:B:133:ILE:HD11	1:B:135:ILE:HD12	1.34	1.08
1:D:68:ARG:HG3	1:D:68:ARG:HH11	1.26	1.01
1:B:49:MET:HE3	1:B:69:LEU:HD21	1.42	0.98
1:D:48:MET:HE3	1:D:68:ARG:HB3	1.45	0.95
1:D:136:GLN:HB3	1:D:147:ILE:HD11	1.47	0.94
1:A:186:LYS:HB2	1:A:189:ARG:HG3	1.48	0.94
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.32	0.94
1:B:117:MET:HE3	1:B:165:PRO:HD3	1.50	0.92
1:A:90:THR:HG22	1:A:92:LEU:H	1.36	0.90
1:A:224:ASN:ND2	1:A:228:TYR:H	1.69	0.90
1:C:135:ILE:HD13	1:C:135:ILE:H	1.39	0.87
1:D:87:GLU:HB2	1:D:97:HIS:CD2	2.11	0.86
1:B:137:ARG:HD3	1:B:144:PRO:HD3	1.58	0.85
1:A:21:GLN:HE21	1:A:21:GLN:HA	1.42	0.85
1:C:26:LEU:H	1:C:26:LEU:HD22	1.41	0.84
1:B:188:GLU:HB3	1:B:211:LYS:HD3	1.59	0.83
1:D:231:PRO:O	1:A:90:THR:HG21	1.78	0.82
1:D:84:GLN:HE21	1:D:84:GLN:HA	1.42	0.82
1:B:117:MET:HE3	1:B:165:PRO:CD	2.10	0.81
1:D:223:LEU:HD23	1:D:227:TYR:HA	1.62	0.81
1:C:244:MET:HE3	1:C:244:MET:C	2.05	0.81
1:D:223:LEU:CD2	1:D:227:TYR:HA	2.11	0.81
1:C:64:PHE:CZ	1:B:126:ARG:HD2	2.16	0.81
1:C:44:GLN:H	1:B:79:ASN:HD21	1.29	0.80
1:B:90:THR:CG2	1:B:92:LEU:H	1.93	0.80
1:C:141:THR:HG22	1:C:143:GLU:N	1.92	0.80
1:D:90:THR:HG23	1:D:92:LEU:H	1.47	0.80
1:A:201:GLY:O	1:A:205:VAL:HG23	1.83	0.79
1:C:199:PRO:O	1:C:203:GLU:HG2	1.83	0.79
1:D:137:ARG:HG3	1:D:142:ALA:O	1.83	0.78
1:C:127:GLY:O	1:A:59:LYS:HE3	1.83	0.78
1:C:134:LEU:HD11	1:C:136:GLN:NE2	1.98	0.78
1:C:90:THR:HG23	1:C:92:LEU:H	1.48	0.78
1:C:201:GLY:O	1:C:205:VAL:HG12	1.84	0.78
1:D:90:THR:CG2	1:D:92:LEU:H	1.97	0.78
1:B:90:THR:HG22	1:B:92:LEU:H	1.49	0.77
1:A:90:THR:CG2	1:A:92:LEU:H	1.96	0.77
1:A:173:VAL:O	1:A:177:ILE:HD12	1.85	0.77
1:D:148:TYR:OH	1:D:150:LYS:HG3	1.84	0.77
1:A:213:ARG:HH11	1:A:213:ARG:HB2	1.49	0.77
1:C:141:THR:CG2	1:C:143:GLU:H	1.95	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:LYS:HZ2	1:C:145:LYS:HA	1.49	0.77
1:C:81:LEU:HB3	1:C:82:PRO:HD2	1.67	0.76
1:C:149:GLU:OE1	1:C:151:LEU:HD22	1.85	0.76
1:D:39:MET:HE1	1:D:73:LEU:HA	1.68	0.76
1:B:187:GLU:HB3	1:B:211:LYS:HD2	1.68	0.76
1:A:186:LYS:N	1:A:186:LYS:HD2	1.99	0.75
1:D:64:PHE:CZ	1:A:126:ARG:HD2	2.21	0.75
1:D:173:VAL:O	1:D:177:ILE:HG13	1.87	0.75
1:C:88:VAL:HG23	1:C:96:TYR:HB3	1.67	0.75
1:D:226:ARG:HH11	1:D:226:ARG:HG3	1.51	0.75
1:A:90:THR:HG22	1:A:92:LEU:N	2.01	0.75
1:A:173:VAL:HG22	1:A:177:ILE:CD1	2.17	0.75
1:A:46:ARG:HD3	4:A:1021:HOH:O	1.86	0.75
1:D:201:GLY:O	1:D:205:VAL:HG12	1.86	0.74
1:C:90:THR:CG2	1:C:92:LEU:H	2.00	0.74
1:C:49:MET:O	1:C:53:ARG:HG3	1.87	0.74
1:A:84:GLN:HA	1:A:84:GLN:NE2	2.03	0.74
1:B:112:ARG:HH22	1:B:238:ASP:HB3	1.51	0.74
1:D:85:LYS:HE3	1:D:97:HIS:HB3	1.70	0.74
1:A:21:GLN:HA	1:A:21:GLN:NE2	2.01	0.73
1:D:166:MET:HE1	1:D:233:ILE:HG22	1.70	0.73
1:D:80:GLU:HB2	1:D:191:ILE:HD13	1.69	0.73
1:B:162:LEU:HD11	1:B:173:VAL:HG23	1.72	0.72
1:C:231:PRO:O	1:B:90:THR:HG21	1.90	0.72
1:C:94:VAL:HG21	1:B:231:PRO:HA	1.72	0.71
1:C:117:MET:HE1	1:C:165:PRO:N	2.04	0.71
1:B:49:MET:HE3	1:B:69:LEU:CD2	2.16	0.71
1:D:79:ASN:HD21	1:A:44:GLN:H	1.35	0.71
1:C:90:THR:HG21	1:B:231:PRO:O	1.90	0.71
1:C:121:LEU:HG	1:C:128:VAL:HG21	1.71	0.71
1:C:223:LEU:HD23	1:C:229:ILE:HA	1.71	0.71
1:D:48:MET:HE3	1:D:68:ARG:CB	2.21	0.71
1:D:115:GLU:O	1:D:118:GLU:HG3	1.91	0.71
1:C:26:LEU:HA	1:C:29:ILE:HD11	1.71	0.70
1:A:154:ASP:HB2	4:A:1040:HOH:O	1.91	0.70
1:D:233:ILE:HD13	1:D:233:ILE:O	1.91	0.70
1:C:145:LYS:HA	1:C:145:LYS:NZ	2.07	0.70
1:B:115:GLU:O	1:B:118:GLU:HG3	1.90	0.70
1:D:134:LEU:HG	1:D:147:ILE:HB	1.74	0.70
1:B:182:ARG:HG3	1:B:182:ARG:HH11	1.56	0.70
1:D:133:ILE:HG22	1:D:135:ILE:HD12	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:THR:CG2	1:A:143:GLU:HG3	2.21	0.70
1:D:98:GLY:HA3	1:A:50:THR:HG21	1.74	0.69
1:C:188:GLU:HG2	4:C:1014:HOH:O	1.93	0.69
1:D:230:VAL:HG23	1:D:231:PRO:HA	1.74	0.69
1:D:48:MET:CE	1:D:68:ARG:HB3	2.23	0.69
1:D:68:ARG:HG3	1:D:68:ARG:NH1	2.03	0.69
1:C:231:PRO:HB3	1:B:94:VAL:CG2	2.23	0.69
1:A:173:VAL:HG22	1:A:177:ILE:HD11	1.75	0.69
1:C:148:TYR:OH	1:A:112:ARG:HG3	1.93	0.69
1:B:27:GLN:O	1:B:31:THR:HG22	1.92	0.69
1:B:202:ILE:O	1:B:205:VAL:HG13	1.92	0.69
1:C:84:GLN:HA	1:C:84:GLN:HE21	1.58	0.69
1:B:201:GLY:O	1:B:205:VAL:HG12	1.93	0.68
1:D:68:ARG:NE	1:A:75:GLU:OE2	2.26	0.68
1:D:144:PRO:HB2	1:D:175:LYS:HG3	1.76	0.68
1:C:53:ARG:NH2	1:C:220:ASP:OD2	2.26	0.68
1:A:133:ILE:CG2	1:A:135:ILE:HD12	2.24	0.68
1:D:97:HIS:O	1:A:46:ARG:NH2	2.26	0.68
1:D:138:ASP:O	1:D:142:ALA:HA	1.93	0.68
1:D:166:MET:HE3	3:D:999:URA:C4	2.29	0.68
1:A:115:GLU:HG2	1:A:118:GLU:OE2	1.93	0.68
1:A:157:GLU:HB2	4:A:1040:HOH:O	1.92	0.68
1:C:230:VAL:HA	1:C:231:PRO:C	2.18	0.68
1:D:90:THR:HG21	1:A:231:PRO:O	1.92	0.68
1:A:221:ILE:HG13	1:A:222:CYS:N	2.09	0.68
1:D:126:ARG:HD2	1:A:64:PHE:CZ	2.28	0.68
1:B:154:ASP:OD2	1:B:158:ARG:NH1	2.28	0.67
1:C:144:PRO:C	1:C:145:LYS:HD2	2.19	0.67
1:A:80:GLU:HG3	1:A:213:ARG:HG2	1.76	0.67
1:D:169:THR:HG23	2:D:799:PO4:O3	1.95	0.67
1:C:39:MET:HG2	1:C:76:GLU:OE1	1.94	0.67
1:B:112:ARG:O	1:B:115:GLU:HG3	1.93	0.67
1:D:202:ILE:O	1:D:205:VAL:HG13	1.95	0.67
1:B:60:GLU:H	1:B:60:GLU:CD	2.03	0.67
1:D:33:PHE:HB2	1:D:36:VAL:CG1	2.24	0.67
1:A:82:PRO:HG2	1:A:103:SER:OG	1.95	0.67
1:A:204:ARG:HA	1:A:207:LYS:HG2	1.76	0.67
1:A:204:ARG:O	1:A:207:LYS:HG3	1.94	0.67
1:B:26:LEU:O	1:B:30:ILE:HD12	1.95	0.66
1:A:224:ASN:HD22	1:A:228:TYR:H	1.43	0.66
1:B:133:ILE:HD11	1:B:135:ILE:CD1	2.19	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ARG:NH1	2:D:899:PO4:O2	2.29	0.66
1:B:155:ILE:HA	1:B:158:ARG:HG3	1.77	0.66
1:D:50:THR:HG21	1:A:98:GLY:HA3	1.76	0.66
1:C:188:GLU:HG2	1:C:211:LYS:HZ1	1.61	0.66
1:C:115:GLU:O	1:C:118:GLU:HG3	1.96	0.65
1:D:177:ILE:HG22	1:D:181:LEU:HD12	1.78	0.65
1:D:179:VAL:HB	1:D:182:ARG:NH2	2.10	0.65
1:B:22:GLU:HG2	1:B:26:LEU:HD22	1.77	0.65
1:B:48:MET:O	1:B:52:ILE:HG22	1.97	0.65
1:A:204:ARG:HA	1:A:207:LYS:HE3	1.77	0.65
1:C:26:LEU:HA	1:C:29:ILE:CD1	2.27	0.65
1:D:134:LEU:HD23	1:D:148:TYR:HB3	1.79	0.65
1:D:32:ARG:NH1	1:D:32:ARG:HG2	2.11	0.65
1:B:154:ASP:HB3	1:B:158:ARG:NH1	2.12	0.65
1:D:137:ARG:HD2	1:D:144:PRO:HG3	1.78	0.65
1:B:176:ALA:O	1:B:180:LEU:HD22	1.96	0.65
1:D:61:GLU:OE2	1:A:126:ARG:NH2	2.30	0.64
1:D:66:ALA:O	1:D:70:ILE:HG13	1.98	0.64
1:B:80:GLU:HB2	1:B:191:ILE:HD13	1.79	0.64
1:A:88:VAL:O	1:A:96:TYR:N	2.30	0.64
1:A:49:MET:O	1:A:53:ARG:HG3	1.98	0.64
1:D:221:ILE:HG22	1:D:222:CYS:N	2.12	0.64
1:C:244:MET:CE	1:C:244:MET:H	2.10	0.64
1:B:143:GLU:O	1:B:143:GLU:HG2	1.98	0.64
1:D:230:VAL:HA	1:D:231:PRO:C	2.23	0.63
1:B:103:SER:O	1:B:105:ILE:HG23	1.98	0.63
1:D:60:GLU:CD	1:D:60:GLU:H	2.05	0.63
1:C:221:ILE:HG22	1:C:222:CYS:SG	2.39	0.63
1:D:91:PRO:HG2	1:A:233:ILE:O	1.98	0.63
1:C:90:THR:O	1:B:55:LYS:NZ	2.31	0.63
1:C:134:LEU:HD12	1:C:135:ILE:N	2.12	0.63
1:C:165:PRO:C	1:C:166:MET:HG2	2.20	0.63
1:D:37:VAL:HG22	1:D:215:VAL:HG13	1.79	0.63
1:D:79:ASN:ND2	1:A:44:GLN:HB2	2.14	0.63
1:C:134:LEU:HG	1:C:147:ILE:HB	1.80	0.63
1:C:244:MET:H	1:C:244:MET:HE2	1.64	0.63
1:B:92:LEU:N	1:B:92:LEU:HD23	2.14	0.63
1:B:230:VAL:HA	1:B:231:PRO:C	2.22	0.63
1:D:147:ILE:HD13	1:D:147:ILE:N	2.12	0.63
1:C:84:GLN:O	1:C:99:VAL:HA	1.99	0.63
1:A:48:MET:HE2	1:A:69:LEU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:ASP:OD1	1:C:140:THR:N	2.28	0.63
1:A:52:ILE:CD1	1:A:233:ILE:HD11	2.28	0.62
1:B:33:PHE:HB2	1:B:36:VAL:CG1	2.28	0.62
1:D:94:VAL:CG2	1:A:231:PRO:HB3	2.28	0.62
1:A:141:THR:HG22	1:A:143:GLU:HG3	1.82	0.62
1:D:61:GLU:CD	1:A:126:ARG:HH22	2.06	0.62
1:D:85:LYS:HZ1	1:D:97:HIS:HD2	1.47	0.62
1:D:98:GLY:HA3	1:A:50:THR:CG2	2.30	0.62
1:C:59:LYS:O	1:C:63:VAL:HG13	1.99	0.62
1:A:84:GLN:HA	1:A:84:GLN:HE21	1.65	0.62
1:C:144:PRO:O	1:C:145:LYS:NZ	2.28	0.62
1:D:84:GLN:HE21	1:D:84:GLN:CA	2.12	0.62
4:D:1011:HOH:O	1:A:53:ARG:NH1	2.31	0.62
1:B:45:LEU:O	1:B:45:LEU:HD22	2.00	0.62
1:A:188:GLU:HA	1:A:211:LYS:O	1.99	0.62
1:B:136:GLN:HG2	1:B:147:ILE:HD11	1.81	0.62
1:C:39:MET:HE1	1:C:72:LEU:HB3	1.81	0.61
1:D:85:LYS:NZ	1:D:97:HIS:HD2	1.97	0.61
1:C:45:LEU:HD12	1:C:45:LEU:O	2.00	0.61
1:C:53:ARG:HH22	1:C:220:ASP:CG	2.08	0.61
1:C:186:LYS:HE3	1:C:186:LYS:HA	1.82	0.61
1:A:146:LEU:HD11	1:A:149:GLU:HB3	1.82	0.61
1:B:25:ILE:O	1:B:29:ILE:HD12	2.00	0.61
1:B:188:GLU:N	1:B:211:LYS:HD3	2.15	0.61
1:C:110:ILE:HG23	1:C:135:ILE:CD1	2.30	0.61
1:B:139:GLU:OE1	1:B:139:GLU:N	2.31	0.61
1:D:62:PHE:CE2	1:D:233:ILE:HD11	2.36	0.61
1:B:90:THR:HG22	1:B:92:LEU:N	2.14	0.61
1:D:32:ARG:HG2	1:D:32:ARG:HH11	1.66	0.61
1:D:220:ASP:OD2	1:D:231:PRO:HD2	2.01	0.61
1:B:39:MET:HG2	1:B:76:GLU:HG2	1.83	0.61
1:A:204:ARG:HA	1:A:207:LYS:CG	2.30	0.60
1:D:30:ILE:HG22	1:D:31:THR:N	2.16	0.60
1:C:137:ARG:HH22	1:C:171:GLY:HA3	1.66	0.60
1:A:45:LEU:O	1:A:45:LEU:HD12	2.02	0.60
1:D:226:ARG:HG3	1:D:226:ARG:NH1	2.15	0.60
1:C:143:GLU:HG3	1:C:144:PRO:CD	2.31	0.60
1:C:244:MET:HE1	1:A:129:ARG:HH21	1.67	0.60
1:B:154:ASP:HB3	1:B:158:ARG:HH11	1.66	0.60
1:A:23:GLU:OE1	1:A:27:GLN:HG2	2.02	0.60
1:C:188:GLU:N	1:C:211:LYS:HZ3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:HG3	1:B:71:ARG:NH1	2.07	0.59
1:C:135:ILE:HD13	1:C:135:ILE:N	2.16	0.59
1:D:126:ARG:NH2	1:A:61:GLU:OE2	2.35	0.59
1:C:205:VAL:HG11	1:C:214:MET:HE1	1.85	0.59
1:A:150:LYS:HA	1:A:150:LYS:HZ3	1.67	0.59
1:D:86:LYS:O	1:D:98:GLY:N	2.31	0.59
1:A:24:SER:O	1:A:27:GLN:HB2	2.03	0.59
1:D:126:ARG:HD2	1:A:64:PHE:CE1	2.37	0.59
1:D:62:PHE:HE2	1:D:233:ILE:HD11	1.68	0.59
1:C:129:ARG:NH1	2:C:899:PO4:O1	2.35	0.59
1:B:177:ILE:HG22	1:B:181:LEU:HD22	1.83	0.59
1:C:137:ARG:HA	1:C:143:GLU:O	2.03	0.58
1:A:226:ARG:HD2	1:A:226:ARG:O	2.03	0.58
1:D:50:THR:CG2	1:A:98:GLY:HA3	2.33	0.58
1:C:48:MET:HE1	1:C:69:LEU:CA	2.33	0.58
1:C:64:PHE:CE1	1:B:126:ARG:HD2	2.38	0.58
1:C:22:GLU:HG3	1:C:26:LEU:HD21	1.84	0.58
1:D:168:ALA:HB1	1:D:223:LEU:HD11	1.85	0.58
1:C:48:MET:HE1	1:C:69:LEU:N	2.19	0.58
1:B:177:ILE:HG22	1:B:181:LEU:CD2	2.34	0.58
1:A:221:ILE:HG23	1:A:231:PRO:HD3	1.85	0.58
1:A:194:ASN:O	1:A:216:THR:HA	2.02	0.58
1:C:202:ILE:O	1:C:205:VAL:HG13	2.04	0.58
1:A:230:VAL:HG12	1:A:231:PRO:HA	1.86	0.58
1:B:182:ARG:HH11	1:B:182:ARG:CG	2.17	0.58
1:A:145:LYS:O	1:A:147:ILE:HD12	2.03	0.58
1:D:39:MET:HE2	1:D:76:GLU:CG	2.34	0.57
1:D:103:SER:HB2	4:D:1044:HOH:O	2.03	0.57
1:B:188:GLU:CB	1:B:211:LYS:HD3	2.32	0.57
1:D:79:ASN:ND2	1:A:44:GLN:H	2.02	0.57
1:C:187:GLU:OE2	1:C:211:LYS:HB2	2.04	0.57
1:D:55:LYS:HG3	1:A:91:PRO:HA	1.84	0.57
1:A:213:ARG:HH11	1:A:213:ARG:CB	2.16	0.57
1:D:39:MET:O	1:D:41:GLN:NE2	2.33	0.57
1:D:85:LYS:HZ1	1:D:97:HIS:CD2	2.22	0.57
1:B:136:GLN:O	1:B:136:GLN:HG3	2.04	0.57
1:A:47:ALA:O	1:A:51:ILE:HG12	2.05	0.57
1:D:69:LEU:C	1:D:69:LEU:HD12	2.30	0.57
1:D:94:VAL:HG21	1:A:231:PRO:HB3	1.87	0.57
1:C:45:LEU:HD12	1:C:45:LEU:C	2.30	0.57
1:A:84:GLN:HE21	1:A:84:GLN:CA	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ALA:HB1	1:A:223:LEU:HD11	1.87	0.57
1:D:223:LEU:HD21	1:D:227:TYR:HA	1.87	0.56
1:A:221:ILE:HG13	1:A:222:CYS:H	1.68	0.56
1:C:85:LYS:NZ	1:C:97:HIS:HB3	2.20	0.56
1:B:133:ILE:O	1:B:133:ILE:HD13	2.05	0.56
1:C:134:LEU:HD11	1:C:136:GLN:HE21	1.71	0.56
1:D:85:LYS:HE2	1:D:98:GLY:O	2.04	0.56
1:B:59:LYS:NZ	4:B:1064:HOH:O	2.38	0.56
1:B:230:VAL:HG23	1:B:231:PRO:HA	1.87	0.56
1:C:115:GLU:HG2	1:C:118:GLU:OE2	2.06	0.56
1:A:52:ILE:HD12	1:A:233:ILE:HD11	1.86	0.56
1:D:71:ARG:HH11	1:D:71:ARG:CG	2.19	0.56
1:D:104:LYS:HA	4:D:1039:HOH:O	2.05	0.56
1:D:39:MET:HE2	1:D:76:GLU:HG2	1.86	0.56
1:A:85:LYS:N	1:A:85:LYS:HD2	2.21	0.55
1:C:29:ILE:HD13	1:C:30:ILE:H	1.70	0.55
1:C:48:MET:HE1	1:C:69:LEU:HA	1.88	0.55
1:D:39:MET:HG3	1:D:40:LYS:HG2	1.87	0.55
1:C:231:PRO:HB3	1:B:94:VAL:HG21	1.88	0.55
1:B:90:THR:HG23	1:B:92:LEU:H	1.70	0.55
1:A:115:GLU:OE2	1:A:132:LYS:NZ	2.39	0.55
1:C:85:LYS:HD2	1:C:86:LYS:N	2.22	0.55
1:B:228:TYR:HD1	3:B:999:URA:C4	2.25	0.55
1:B:54:ASP:HB3	1:B:57:THR:CG2	2.37	0.55
1:A:48:MET:HE3	1:A:68:ARG:HB3	1.88	0.55
1:B:49:MET:HE2	1:B:52:ILE:HD13	1.87	0.55
1:D:32:ARG:HH11	1:D:32:ARG:CG	2.20	0.54
1:D:50:THR:HG21	1:A:99:VAL:H	1.71	0.54
1:A:88:VAL:CG2	1:A:96:TYR:HB3	2.37	0.54
1:A:137:ARG:HA	1:A:143:GLU:O	2.07	0.54
1:B:69:LEU:C	1:B:69:LEU:HD12	2.32	0.54
1:D:194:ASN:O	1:D:216:THR:HA	2.07	0.54
1:B:179:VAL:O	1:B:183:LEU:HD22	2.06	0.54
1:A:87:GLU:HA	1:A:96:TYR:O	2.08	0.54
1:D:91:PRO:HD3	1:A:53:ARG:O	2.08	0.54
1:C:125:CYS:O	1:C:128:VAL:HG22	2.08	0.54
1:C:231:PRO:HB3	1:B:94:VAL:HG22	1.89	0.54
1:C:98:GLY:HA3	1:B:50:THR:OG1	2.07	0.54
1:C:26:LEU:O	1:C:30:ILE:HB	2.07	0.54
1:C:110:ILE:HG23	1:C:135:ILE:HD11	1.89	0.54
1:B:44:GLN:HG2	1:B:48:MET:CE	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLN:HG2	1:B:48:MET:HE3	1.88	0.54
1:B:86:LYS:O	1:B:98:GLY:N	2.39	0.54
1:C:23:GLU:OE1	1:C:23:GLU:HA	2.08	0.53
1:B:187:GLU:HG2	1:B:211:LYS:HB3	1.89	0.53
1:A:133:ILE:HG22	1:A:135:ILE:HD12	1.89	0.53
1:A:59:LYS:O	1:A:63:VAL:HG13	2.08	0.53
1:A:224:ASN:ND2	1:A:226:ARG:H	2.06	0.53
1:C:135:ILE:H	1:C:135:ILE:CD1	2.17	0.53
1:B:105:ILE:O	1:B:106:CYS:HB3	2.08	0.53
1:A:224:ASN:HB3	1:A:230:VAL:CG2	2.38	0.53
1:D:75:GLU:OE2	1:A:68:ARG:NH2	2.26	0.53
1:C:186:LYS:HE3	1:C:186:LYS:CA	2.37	0.53
1:A:173:VAL:HG22	1:A:177:ILE:HD12	1.89	0.53
1:C:143:GLU:HG3	1:C:144:PRO:N	2.24	0.53
1:B:54:ASP:HB3	1:B:57:THR:HG23	1.89	0.53
1:A:48:MET:HE1	1:A:69:LEU:N	2.24	0.53
1:A:230:VAL:CG1	1:A:231:PRO:HA	2.39	0.53
1:D:51:ILE:HG13	1:D:52:ILE:N	2.24	0.53
1:D:79:ASN:HD21	1:A:44:GLN:HB2	1.73	0.53
1:B:188:GLU:HB3	1:B:211:LYS:CD	2.36	0.52
1:B:90:THR:HG21	1:B:92:LEU:HG	1.92	0.52
1:B:102:TYR:CD1	1:B:102:TYR:N	2.76	0.52
1:C:129:ARG:HG3	4:C:1000:HOH:O	2.09	0.52
1:B:238:ASP:O	1:B:244:MET:HG3	2.09	0.52
1:D:175:LYS:O	1:D:178:GLU:HB3	2.09	0.52
1:C:85:LYS:CE	1:C:97:HIS:HB3	2.40	0.52
1:B:33:PHE:HB3	4:B:1021:HOH:O	2.09	0.52
1:A:61:GLU:OE1	1:A:65:TYR:HE2	1.92	0.52
1:C:39:MET:O	1:C:41:GLN:NE2	2.33	0.52
1:B:85:LYS:O	1:B:85:LYS:HG3	2.09	0.52
1:B:208:GLU:HB2	1:B:209:TYR:CD1	2.45	0.52
1:C:85:LYS:HD2	1:C:86:LYS:H	1.75	0.52
1:B:45:LEU:HD22	1:B:45:LEU:C	2.35	0.52
1:C:94:VAL:HG23	1:B:231:PRO:HB3	1.91	0.51
1:A:213:ARG:HH11	1:A:213:ARG:CG	2.24	0.51
1:C:85:LYS:HE2	1:C:97:HIS:HB3	1.91	0.51
1:D:44:GLN:H	1:A:79:ASN:HD21	1.58	0.51
1:D:138:ASP:OD2	1:D:141:THR:OG1	2.29	0.51
1:B:172:SER:OG	2:B:799:PO4:O2	2.28	0.51
1:C:25:ILE:O	1:C:29:ILE:HD12	2.11	0.51
1:C:115:GLU:HA	1:C:118:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:OE1	1:A:27:GLN:HA	2.09	0.51
1:A:53:ARG:NE	4:A:1042:HOH:O	2.41	0.51
1:C:74:ILE:O	1:C:78:LEU:HG	2.11	0.51
1:A:48:MET:HE1	1:A:69:LEU:CA	2.40	0.51
4:C:1000:HOH:O	1:A:59:LYS:NZ	2.33	0.51
1:A:196:LEU:HD22	1:A:197:ALA:N	2.26	0.51
1:C:75:GLU:OE1	1:B:44:GLN:OE1	2.29	0.51
1:D:48:MET:CE	1:D:69:LEU:N	2.74	0.51
1:C:143:GLU:HG2	1:C:145:LYS:CE	2.41	0.51
1:B:24:SER:OG	1:B:25:ILE:N	2.43	0.51
1:B:57:THR:HB	1:B:58:PRO:HD2	1.92	0.50
1:B:135:ILE:CG2	1:B:144:PRO:HB3	2.40	0.50
1:D:102:TYR:N	1:D:102:TYR:CD1	2.79	0.50
1:D:230:VAL:HG23	1:D:231:PRO:CA	2.40	0.50
1:C:134:LEU:HD11	1:C:136:GLN:HE22	1.74	0.50
1:A:224:ASN:N	1:A:228:TYR:O	2.43	0.50
1:C:235:ASP:HB3	1:C:238:ASP:HB2	1.92	0.50
1:D:133:ILE:CG2	1:D:135:ILE:HD12	2.41	0.50
1:C:166:MET:CE	3:C:999:URA:N3	2.75	0.50
1:C:182:ARG:HG3	1:C:183:LEU:N	2.26	0.50
1:C:137:ARG:NH2	1:C:171:GLY:HA3	2.27	0.50
1:C:64:PHE:CE2	1:B:126:ARG:HD2	2.47	0.50
1:C:85:LYS:HZ3	1:C:97:HIS:HB3	1.76	0.50
1:C:233:ILE:HD13	1:C:233:ILE:O	2.12	0.50
1:B:121:LEU:HG	1:B:128:VAL:HG11	1.94	0.50
1:A:126:ARG:HD3	4:A:1019:HOH:O	2.11	0.50
1:D:75:GLU:HG2	1:A:72:LEU:HD11	1.94	0.50
4:D:1037:HOH:O	1:B:241:PHE:HE1	1.95	0.50
1:D:136:GLN:CB	1:D:147:ILE:HD11	2.30	0.50
1:C:84:GLN:HB3	1:C:100:SER:HB3	1.94	0.50
1:C:143:GLU:HG3	1:C:144:PRO:HD2	1.94	0.50
1:C:179:VAL:O	1:C:183:LEU:HG	2.10	0.50
1:C:221:ILE:HD13	1:C:221:ILE:N	2.26	0.50
1:B:208:GLU:HB2	1:B:209:TYR:CE1	2.46	0.50
1:C:112:ARG:CZ	1:A:150:LYS:HG2	2.42	0.49
1:B:32:ARG:HG2	1:B:32:ARG:HH11	1.76	0.49
1:A:89:THR:HA	1:A:95:SER:HA	1.93	0.49
1:A:115:GLU:HA	1:A:118:GLU:OE2	2.11	0.49
1:C:48:MET:HE3	1:C:68:ARG:HB3	1.94	0.49
1:A:180:LEU:O	1:A:185:VAL:HG13	2.12	0.49
1:D:220:ASP:CG	1:D:231:PRO:HD2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:148:TYR:CZ	1:D:150:LYS:HG3	2.47	0.49
1:B:115:GLU:HA	1:B:118:GLU:CG	2.42	0.49
1:B:137:ARG:HA	1:B:144:PRO:HA	1.94	0.49
1:C:110:ILE:HG23	1:C:135:ILE:HD12	1.94	0.49
1:C:235:ASP:HA	3:C:999:URA:O2	2.12	0.49
1:B:206:PHE:O	1:B:210:PRO:HD3	2.13	0.49
1:A:224:ASN:HB3	1:A:230:VAL:HG21	1.94	0.49
1:D:27:GLN:O	1:D:30:ILE:HB	2.13	0.49
1:C:48:MET:HE2	1:C:69:LEU:HB2	1.94	0.49
1:B:204:ARG:HD3	1:B:208:GLU:OE2	2.13	0.49
1:C:84:GLN:HB2	1:C:100:SER:O	2.13	0.49
1:B:117:MET:HE3	1:B:165:PRO:N	2.28	0.49
1:B:142:ALA:O	1:B:144:PRO:HD3	2.12	0.49
1:C:22:GLU:O	1:C:26:LEU:HD22	2.11	0.49
1:B:233:ILE:HG12	1:B:233:ILE:O	2.12	0.49
1:D:231:PRO:HA	1:A:94:VAL:HG21	1.95	0.49
1:B:135:ILE:HG12	1:B:175:LYS:HG2	1.93	0.49
1:B:207:LYS:HB2	1:B:207:LYS:NZ	2.26	0.49
1:A:200:GLN:HA	1:A:203:GLU:HB2	1.94	0.49
1:D:32:ARG:NH1	1:D:32:ARG:CG	2.76	0.48
1:C:138:ASP:N	1:C:143:GLU:O	2.40	0.48
1:B:33:PHE:O	1:B:36:VAL:HG13	2.13	0.48
1:B:37:VAL:HG13	1:B:215:VAL:HG22	1.93	0.48
1:D:105:ILE:CG1	1:D:106:CYS:N	2.77	0.48
1:D:166:MET:CE	3:D:999:URA:N3	2.76	0.48
1:D:177:ILE:HG22	1:D:181:LEU:CD1	2.42	0.48
1:C:117:MET:CE	1:C:165:PRO:HG3	2.43	0.48
1:C:166:MET:HE3	3:C:999:URA:N3	2.28	0.48
1:B:133:ILE:HD13	1:B:133:ILE:C	2.39	0.48
1:A:211:LYS:HE2	4:A:1016:HOH:O	2.11	0.48
1:A:220:ASP:OD2	1:A:231:PRO:HD2	2.13	0.48
1:D:48:MET:HE2	1:D:69:LEU:CA	2.44	0.48
1:B:209:TYR:O	1:B:212:VAL:HG22	2.12	0.48
1:A:141:THR:HG22	1:A:143:GLU:H	1.78	0.48
1:A:161:MET:CA	1:A:161:MET:HE2	2.42	0.48
1:B:111:VAL:HA	1:B:112:ARG:HA	1.64	0.48
1:C:44:GLN:O	1:C:47:ALA:HB3	2.14	0.48
1:C:86:LYS:O	1:C:98:GLY:N	2.42	0.48
1:C:134:LEU:HD12	1:C:134:LEU:C	2.39	0.48
1:A:84:GLN:NE2	1:A:85:LYS:HE3	2.28	0.48
1:A:226:ARG:HB3	1:A:228:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:ARG:HH11	1:A:71:ARG:CG	2.26	0.48
1:D:85:LYS:HG2	1:D:98:GLY:O	2.14	0.47
1:C:166:MET:HE1	1:C:233:ILE:CG2	2.44	0.47
1:A:130:ILE:HG22	1:A:130:ILE:O	2.14	0.47
1:D:172:SER:OG	2:D:799:PO4:O2	2.29	0.47
1:C:166:MET:HE3	3:C:999:URA:C4	2.50	0.47
1:B:166:MET:HE2	1:B:166:MET:HA	1.95	0.47
1:A:88:VAL:HG22	1:A:96:TYR:HB3	1.96	0.47
1:A:136:GLN:N	1:A:147:ILE:HD13	2.29	0.47
1:D:27:GLN:O	1:D:31:THR:HG22	2.14	0.47
1:D:44:GLN:H	1:A:79:ASN:ND2	2.13	0.47
1:D:187:GLU:OE2	1:D:210:PRO:HD2	2.15	0.47
1:C:141:THR:O	1:C:142:ALA:HB3	2.14	0.47
1:A:230:VAL:HA	1:A:231:PRO:C	2.39	0.47
1:A:186:LYS:CB	1:A:189:ARG:HG3	2.33	0.47
1:C:175:LYS:O	1:C:179:VAL:HG13	2.13	0.47
1:B:207:LYS:HB2	1:B:207:LYS:HE3	1.69	0.47
1:D:85:LYS:NZ	1:D:97:HIS:CD2	2.82	0.47
1:D:141:THR:O	1:D:142:ALA:HB2	2.15	0.47
1:B:83:PHE:HD1	1:B:84:GLN:O	1.98	0.47
1:B:99:VAL:HG23	1:B:99:VAL:O	2.15	0.47
1:A:71:ARG:CG	1:A:71:ARG:NH1	2.77	0.47
1:D:134:LEU:HB3	1:D:148:TYR:HB3	1.97	0.47
1:D:134:LEU:CG	1:D:147:ILE:HB	2.44	0.47
1:D:158:ARG:HH22	2:D:899:PO4:P	2.38	0.47
1:D:199:PRO:HD3	1:D:220:ASP:O	2.15	0.47
1:C:126:ARG:HG2	1:C:126:ARG:HH11	1.80	0.47
1:B:141:THR:O	1:B:142:ALA:HB2	2.15	0.47
1:D:85:LYS:HZ1	1:D:87:GLU:HB2	1.80	0.47
1:D:136:GLN:HE21	1:D:136:GLN:HB2	1.49	0.47
1:C:145:LYS:HD2	1:C:145:LYS:N	2.29	0.47
1:A:81:LEU:HB3	1:A:82:PRO:HD2	1.96	0.47
1:A:91:PRO:C	1:A:93:ASP:H	2.23	0.47
1:D:32:ARG:HG2	1:D:33:PHE:CZ	2.50	0.47
1:C:48:MET:CE	1:C:69:LEU:N	2.78	0.47
1:C:126:ARG:NH2	1:B:61:GLU:OE2	2.48	0.47
1:B:52:ILE:O	1:B:52:ILE:HG12	2.14	0.47
1:B:137:ARG:HD3	1:B:142:ALA:O	2.15	0.47
1:C:58:PRO:HG2	1:C:61:GLU:HB2	1.97	0.46
1:C:220:ASP:HB3	1:C:230:VAL:O	2.14	0.46
1:B:90:THR:HB	1:B:94:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:HB3	1:A:85:LYS:H	1.45	0.46
1:D:48:MET:HE2	1:D:69:LEU:N	2.29	0.46
1:D:87:GLU:HB2	1:D:97:HIS:HD2	1.72	0.46
1:D:40:LYS:O	1:D:40:LYS:HG3	2.15	0.46
1:C:40:LYS:O	1:C:45:LEU:HD23	2.16	0.46
1:A:21:GLN:O	1:A:24:SER:OG	2.28	0.46
1:A:165:PRO:HB3	1:A:195:ILE:HD12	1.98	0.46
1:C:169:THR:O	1:C:170:ALA:HB3	2.15	0.46
1:B:54:ASP:OD1	1:B:56:GLU:HB2	2.15	0.46
1:B:73:LEU:O	1:B:76:GLU:HB3	2.15	0.46
1:A:48:MET:HE1	1:A:69:LEU:HA	1.97	0.46
1:A:90:THR:HG23	1:A:91:PRO:CD	2.46	0.46
1:C:26:LEU:O	1:C:29:ILE:HD13	2.16	0.46
1:B:188:GLU:OE1	1:B:211:LYS:NZ	2.30	0.46
1:A:39:MET:HE2	1:A:40:LYS:HD3	1.97	0.46
1:A:84:GLN:HE21	1:A:85:LYS:HD2	1.79	0.46
1:D:90:THR:HG22	1:D:92:LEU:H	1.78	0.46
1:C:203:GLU:HG2	1:C:203:GLU:H	1.64	0.46
1:D:166:MET:HE1	1:D:233:ILE:CG2	2.42	0.46
1:D:166:MET:HE3	3:D:999:URA:N3	2.30	0.46
1:D:170:ALA:N	2:D:799:PO4:O1	2.38	0.46
1:D:181:LEU:HD23	1:D:185:VAL:O	2.15	0.46
1:D:194:ASN:OD1	1:D:214:MET:HE3	2.16	0.46
1:B:104:LYS:HA	4:B:1036:HOH:O	2.15	0.46
1:A:84:GLN:NE2	1:A:85:LYS:CE	2.79	0.46
1:C:117:MET:HE1	1:C:165:PRO:CD	2.45	0.46
1:C:161:MET:HE3	1:C:161:MET:HB3	1.80	0.46
1:A:141:THR:O	1:A:142:ALA:HB3	2.16	0.46
1:A:242:GLY:C	1:A:244:MET:H	2.23	0.46
1:D:23:GLU:OE2	1:D:23:GLU:O	2.33	0.46
1:D:125:CYS:O	1:D:128:VAL:HG12	2.15	0.46
1:C:145:LYS:N	1:C:145:LYS:CD	2.79	0.46
1:A:109:SER:OG	1:A:118:GLU:OE2	2.31	0.46
1:A:151:LEU:CD1	1:A:183:LEU:HD23	2.46	0.46
1:A:169:THR:O	1:A:170:ALA:HB3	2.16	0.46
1:B:129:ARG:NH1	2:B:899:PO4:O3	2.49	0.45
1:A:113:ALA:HB1	1:A:165:PRO:HG2	1.97	0.45
1:D:51:ILE:CD1	1:D:65:TYR:CD2	3.00	0.45
1:A:33:PHE:HA	1:A:34:PRO:HD2	1.80	0.45
1:C:73:LEU:O	1:C:76:GLU:HB3	2.16	0.45
1:C:231:PRO:CB	1:B:94:VAL:HG22	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:VAL:HG23	1:A:37:VAL:N	2.31	0.45
1:B:244:MET:HG3	1:B:244:MET:H	1.37	0.45
1:A:39:MET:HE3	1:A:76:GLU:HG2	1.97	0.45
1:A:136:GLN:HB2	1:A:147:ILE:HD13	1.99	0.45
1:A:221:ILE:CG1	1:A:222:CYS:N	2.78	0.45
1:D:169:THR:O	1:D:170:ALA:HB3	2.16	0.45
1:B:33:PHE:HB2	1:B:36:VAL:HG12	1.99	0.45
1:C:29:ILE:HD13	1:C:30:ILE:N	2.31	0.45
1:C:145:LYS:NZ	1:C:145:LYS:CA	2.78	0.45
1:C:244:MET:CE	1:C:244:MET:N	2.80	0.45
1:B:148:TYR:OH	1:B:150:LYS:HE3	2.16	0.45
1:C:138:ASP:CG	1:C:141:THR:HB	2.42	0.45
1:A:139:GLU:H	1:A:139:GLU:HG3	1.66	0.45
1:D:156:ARG:HG3	1:D:157:GLU:HG3	1.98	0.45
1:C:26:LEU:HD22	1:C:26:LEU:N	2.21	0.45
1:C:220:ASP:OD2	1:C:231:PRO:HD2	2.16	0.45
1:A:35:ASN:HB2	4:A:1026:HOH:O	2.16	0.45
1:A:138:ASP:CG	1:A:141:THR:HB	2.41	0.45
1:D:39:MET:CE	1:D:76:GLU:HG2	2.46	0.45
1:C:110:ILE:CG2	1:C:135:ILE:HD11	2.47	0.45
1:B:38:LEU:HD23	1:B:216:THR:HG23	1.98	0.45
1:A:141:THR:HG22	1:A:143:GLU:OE2	2.17	0.45
1:D:161:MET:HE3	1:D:161:MET:HB3	1.67	0.44
1:D:231:PRO:HB3	1:A:94:VAL:CG2	2.47	0.44
1:D:111:VAL:HA	1:D:112:ARG:HA	1.48	0.44
1:C:166:MET:CE	3:C:999:URA:C2	3.00	0.44
1:B:53:ARG:NH2	1:B:220:ASP:OD2	2.50	0.44
1:B:200:GLN:HB3	4:B:1057:HOH:O	2.17	0.44
1:A:223:LEU:CD1	1:A:229:ILE:HG12	2.47	0.44
1:D:138:ASP:OD1	1:D:139:GLU:N	2.51	0.44
1:B:137:ARG:HG3	1:B:142:ALA:C	2.42	0.44
1:A:128:VAL:O	1:A:130:ILE:HD13	2.18	0.44
1:A:133:ILE:CG2	1:A:135:ILE:CD1	2.95	0.44
1:A:173:VAL:CG2	1:A:177:ILE:HD11	2.45	0.44
1:D:109:SER:OG	1:D:118:GLU:OE2	2.28	0.44
1:C:230:VAL:HA	1:C:232:GLY:N	2.32	0.44
1:B:154:ASP:CB	1:B:158:ARG:NH1	2.80	0.44
1:A:129:ARG:NH1	2:A:899:PO4:O4	2.50	0.44
1:C:135:ILE:N	1:C:135:ILE:CD1	2.78	0.44
1:C:165:PRO:HB2	1:C:166:MET:HG2	2.00	0.44
1:B:53:ARG:NH2	1:B:220:ASP:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:TYR:N	1:B:102:TYR:HD1	2.14	0.44
1:C:117:MET:CE	1:C:165:PRO:CD	2.95	0.44
1:B:182:ARG:CG	1:B:182:ARG:NH1	2.80	0.44
1:D:81:LEU:N	1:D:81:LEU:CD2	2.79	0.44
1:A:77:ALA:O	1:A:80:GLU:HB2	2.17	0.44
1:A:213:ARG:CG	1:A:213:ARG:NH1	2.80	0.44
1:C:91:PRO:C	1:C:93:ASP:H	2.25	0.43
1:B:166:MET:HG3	3:B:999:URA:C2	2.53	0.43
1:A:220:ASP:CG	1:A:231:PRO:HD2	2.43	0.43
1:D:81:LEU:HD21	1:D:191:ILE:HD12	1.99	0.43
1:C:26:LEU:H	1:C:26:LEU:CD2	2.23	0.43
1:B:52:ILE:HD12	1:B:52:ILE:HG21	1.79	0.43
1:B:232:GLY:HA3	4:B:1003:HOH:O	2.16	0.43
1:D:81:LEU:N	1:D:81:LEU:HD22	2.32	0.43
1:D:85:LYS:HA	1:D:99:VAL:HG12	2.00	0.43
1:C:90:THR:HG23	1:C:91:PRO:N	2.33	0.43
1:C:188:GLU:HB3	1:C:211:LYS:HE2	1.99	0.43
1:D:90:THR:HG23	1:D:91:PRO:N	2.34	0.43
1:D:231:PRO:HB3	1:A:94:VAL:HG21	1.99	0.43
1:A:90:THR:CG2	1:A:91:PRO:N	2.79	0.43
1:D:39:MET:HE2	1:D:76:GLU:CB	2.48	0.43
1:D:87:GLU:HA	1:D:97:HIS:HA	2.00	0.43
1:C:48:MET:CE	1:C:69:LEU:CA	2.96	0.43
1:C:59:LYS:HE2	1:A:127:GLY:O	2.19	0.43
1:C:84:GLN:HA	1:C:84:GLN:NE2	2.28	0.43
1:B:44:GLN:HG3	4:B:1016:HOH:O	2.19	0.43
1:B:73:LEU:HD21	1:B:194:ASN:O	2.18	0.43
1:B:28:ASP:O	1:B:32:ARG:HB2	2.19	0.43
1:A:45:LEU:HD12	1:A:45:LEU:C	2.44	0.43
1:A:143:GLU:OE1	1:A:145:LYS:HD3	2.18	0.43
1:D:105:ILE:O	1:D:106:CYS:HB3	2.18	0.43
1:C:238:ASP:O	1:C:244:MET:HG3	2.19	0.43
1:B:139:GLU:HB2	1:B:140:THR:H	1.53	0.43
1:B:196:LEU:HD11	1:B:232:GLY:HA2	2.00	0.43
1:A:39:MET:HG2	1:A:217:ALA:HA	2.01	0.43
1:A:66:ALA:O	1:A:70:ILE:HG13	2.19	0.43
1:A:87:GLU:CD	1:A:95:SER:HB2	2.43	0.43
1:D:51:ILE:HG12	1:D:65:TYR:CG	2.54	0.43
1:D:90:THR:HB	1:D:94:VAL:O	2.19	0.43
1:C:94:VAL:CG2	1:B:231:PRO:HA	2.44	0.43
1:A:48:MET:CE	1:A:69:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:PHE:CD1	1:A:83:PHE:C	2.97	0.43
1:A:136:GLN:HB3	1:A:147:ILE:HD11	2.00	0.43
1:D:92:LEU:HD21	1:A:228:TYR:HB3	2.00	0.42
1:C:28:ASP:O	1:C:31:THR:HB	2.19	0.42
1:A:223:LEU:HD12	1:A:229:ILE:HA	2.00	0.42
1:D:32:ARG:CG	1:D:33:PHE:CE1	3.02	0.42
1:D:48:MET:HE2	1:D:69:LEU:CB	2.48	0.42
1:D:57:THR:HA	1:D:58:PRO:HD3	1.80	0.42
1:B:26:LEU:C	1:B:30:ILE:HD12	2.44	0.42
1:C:33:PHE:HA	1:C:34:PRO:HD2	1.94	0.42
1:B:32:ARG:HG2	1:B:32:ARG:NH1	2.32	0.42
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.85	0.42
1:C:87:GLU:HB2	1:C:97:HIS:HD2	1.84	0.42
1:D:176:ALA:O	1:D:180:LEU:HD22	2.19	0.42
1:C:188:GLU:HB3	1:C:211:LYS:CE	2.50	0.42
1:B:186:LYS:HB2	1:B:189:ARG:HG3	2.01	0.42
1:A:136:GLN:CB	1:A:147:ILE:HD13	2.49	0.42
1:D:48:MET:HE3	1:D:68:ARG:CG	2.50	0.42
1:D:81:LEU:CD2	1:D:191:ILE:HD12	2.49	0.42
1:D:99:VAL:H	1:A:50:THR:HG21	1.85	0.42
1:D:226:ARG:C	1:D:227:TYR:CD2	2.97	0.42
1:C:94:VAL:HG21	1:B:230:VAL:HG23	2.02	0.42
1:C:163:LEU:HD12	1:C:193:VAL:HB	2.02	0.42
1:B:137:ARG:HE	1:B:137:ARG:HB2	1.61	0.42
1:D:25:ILE:O	1:D:29:ILE:HG12	2.20	0.42
1:B:90:THR:CG2	1:B:92:LEU:HG	2.49	0.42
1:A:85:LYS:N	1:A:85:LYS:CD	2.78	0.42
1:D:33:PHE:HA	1:D:34:PRO:HD2	1.86	0.42
1:A:90:THR:HG23	1:A:91:PRO:N	2.35	0.42
1:D:71:ARG:HH11	1:D:71:ARG:HG3	1.85	0.41
1:D:102:TYR:O	1:D:102:TYR:CG	2.73	0.41
1:A:150:LYS:HA	1:A:150:LYS:NZ	2.33	0.41
1:D:115:GLU:OE1	1:B:132:LYS:NZ	2.29	0.41
1:D:221:ILE:HD13	1:D:221:ILE:HA	1.62	0.41
1:B:84:GLN:N	1:B:100:SER:O	2.37	0.41
1:A:138:ASP:HB3	1:A:143:GLU:OE2	2.20	0.41
1:B:87:GLU:OE2	1:B:95:SER:HB2	2.19	0.41
1:B:186:LYS:H	1:B:186:LYS:HG2	1.74	0.41
1:A:48:MET:CE	1:A:69:LEU:CA	2.98	0.41
1:A:71:ARG:NE	4:A:1008:HOH:O	2.25	0.41
1:A:183:LEU:HD12	1:A:183:LEU:HA	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:CD1	1:D:83:PHE:C	2.98	0.41
1:C:53:ARG:NH2	1:C:231:PRO:HG2	2.36	0.41
1:C:117:MET:CE	1:C:165:PRO:CG	2.98	0.41
1:C:188:GLU:HB3	1:C:211:LYS:NZ	2.35	0.41
1:B:177:ILE:O	1:B:181:LEU:HD22	2.20	0.41
1:A:23:GLU:OE1	1:A:23:GLU:O	2.38	0.41
1:A:224:ASN:ND2	1:A:224:ASN:C	2.78	0.41
1:A:224:ASN:HD22	1:A:224:ASN:C	2.28	0.41
1:C:143:GLU:HA	1:C:144:PRO:HD3	1.76	0.41
1:C:166:MET:HE3	3:C:999:URA:C2	2.56	0.41
1:D:199:PRO:HA	1:D:202:ILE:HG13	2.03	0.41
1:C:145:LYS:HE3	1:C:145:LYS:HB3	1.74	0.41
1:A:143:GLU:HA	1:A:144:PRO:HD3	1.69	0.41
1:D:32:ARG:HG2	1:D:33:PHE:CE1	2.55	0.41
1:C:154:ASP:OD1	1:C:154:ASP:N	2.50	0.41
1:B:194:ASN:O	1:B:216:THR:HA	2.21	0.41
1:A:129:ARG:H	1:A:129:ARG:HG3	1.57	0.41
1:A:143:GLU:HB2	1:A:144:PRO:HD2	2.01	0.41
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.94	0.41
1:D:84:GLN:CA	1:D:84:GLN:NE2	2.79	0.41
1:C:137:ARG:HA	1:C:144:PRO:HA	2.03	0.41
1:D:39:MET:HE2	1:D:76:GLU:HB2	2.03	0.41
1:D:173:VAL:HG13	1:D:174:CYS:N	2.35	0.41
1:C:105:ILE:HG22	1:C:159:TRP:HB2	2.03	0.41
1:B:187:GLU:CB	1:B:211:LYS:HD2	2.45	0.41
1:B:188:GLU:HA	1:B:211:LYS:O	2.21	0.41
1:B:229:ILE:O	1:B:232:GLY:HA3	2.20	0.41
1:A:91:PRO:C	1:A:93:ASP:N	2.78	0.41
1:A:133:ILE:HG21	1:A:135:ILE:CD1	2.51	0.41
1:A:136:GLN:CB	1:A:147:ILE:CD1	2.99	0.41
1:D:188:GLU:H	1:D:188:GLU:HG3	0.97	0.41
1:C:79:ASN:HD21	1:B:44:GLN:H	1.68	0.41
1:C:105:ILE:HG13	1:C:106:CYS:N	2.33	0.41
1:B:102:TYR:HD1	1:B:102:TYR:H	1.69	0.41
1:A:53:ARG:NH2	4:A:1042:HOH:O	2.51	0.41
1:A:72:LEU:HA	1:A:72:LEU:HD23	1.64	0.41
1:A:88:VAL:HG23	1:A:96:TYR:HB3	2.03	0.41
1:D:140:THR:HB	1:D:141:THR:H	1.69	0.40
1:C:143:GLU:HG2	1:C:145:LYS:HE2	2.02	0.40
1:B:117:MET:CE	1:B:165:PRO:N	2.84	0.40
1:B:220:ASP:OD2	1:B:231:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:223:LEU:HD23	1:C:229:ILE:CA	2.44	0.40
1:A:71:ARG:NH2	4:A:1008:HOH:O	2.47	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	222/243 (91%)	209 (94%)	11 (5%)	2 (1%)	14	14
1	B	222/243 (91%)	207 (93%)	11 (5%)	4 (2%)	6	4
1	C	222/243 (91%)	209 (94%)	11 (5%)	2 (1%)	14	14
1	D	222/243 (91%)	208 (94%)	11 (5%)	3 (1%)	9	7
All	All	888/972 (91%)	833 (94%)	44 (5%)	11 (1%)	10	8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	142	ALA
1	C	22	GLU
1	B	142	ALA
1	D	221	ILE
1	B	139	GLU
1	A	84	GLN
1	D	103	SER
1	B	102	TYR
1	B	140	THR
1	C	25	ILE
1	A	221	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/212 (92%)	137 (70%)	59 (30%)	0	0
1	B	196/212 (92%)	124 (63%)	72 (37%)	0	0
1	C	196/212 (92%)	131 (67%)	65 (33%)	0	0
1	D	196/212 (92%)	128 (65%)	68 (35%)	0	0
All	All	784/848 (92%)	520 (66%)	264 (34%)	0	0

All (264) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	24	SER
1	D	25	ILE
1	D	26	LEU
1	D	30	ILE
1	D	31	THR
1	D	32	ARG
1	D	36	VAL
1	D	37	VAL
1	D	40	LYS
1	D	46	ARG
1	D	50	THR
1	D	51	ILE
1	D	52	ILE
1	D	56	GLU
1	D	60	GLU
1	D	63	VAL
1	D	68	ARG
1	D	69	LEU
1	D	71	ARG
1	D	74	ILE
1	D	84	GLN
1	D	85	LYS
1	D	87	GLU
1	D	90	THR

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Mol	Chain	Res	Type
1	D	94	VAL
1	D	95	SER
1	D	103	SER
1	D	104	LYS
1	D	105	ILE
1	D	112	ARG
1	D	118	GLU
1	D	119	SER
1	D	124	VAL
1	D	126	ARG
1	D	129	ARG
1	D	130	ILE
1	D	132	LYS
1	D	135	ILE
1	D	136	GLN
1	D	137	ARG
1	D	139	GLU
1	D	141	THR
1	D	143	GLU
1	D	156	ARG
1	D	163	LEU
1	D	172	SER
1	D	175	LYS
1	D	179	VAL
1	D	180	LEU
1	D	183	LEU
1	D	186	LYS
1	D	188	GLU
1	D	190	ILE
1	D	196	LEU
1	D	200	GLN
1	D	202	ILE
1	D	204	ARG
1	D	205	VAL
1	D	207	LYS
1	D	211	LYS
1	D	212	VAL
1	D	213	ARG
1	D	221	ILE
1	D	223	LEU
1	D	226	ARG
1	D	230	VAL

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Mol	Chain	Res	Type
1	D	233	ILE
1	D	244	MET
1	C	23	GLU
1	C	25	ILE
1	C	27	GLN
1	C	29	ILE
1	C	30	ILE
1	C	32	ARG
1	C	36	VAL
1	C	44	GLN
1	C	45	LEU
1	C	46	ARG
1	C	51	ILE
1	C	52	ILE
1	C	57	THR
1	C	59	LYS
1	C	60	GLU
1	C	63	VAL
1	C	72	LEU
1	C	73	LEU
1	C	79	ASN
1	C	81	LEU
1	C	84	GLN
1	C	85	LYS
1	C	88	VAL
1	C	89	THR
1	C	90	THR
1	C	92	LEU
1	C	95	SER
1	C	104	LYS
1	C	109	SER
1	C	112	ARG
1	C	126	ARG
1	C	128	VAL
1	C	130	ILE
1	C	132	LYS
1	C	135	ILE
1	C	136	GLN
1	C	139	GLU
1	C	141	THR
1	C	145	LYS
1	C	146	LEU

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Mol	Chain	Res	Type
1	C	147	ILE
1	C	150	LYS
1	C	151	LEU
1	C	156	ARG
1	C	160	VAL
1	C	161	MET
1	C	163	LEU
1	C	175	LYS
1	C	179	VAL
1	C	182	ARG
1	C	185	VAL
1	C	186	LYS
1	C	188	GLU
1	C	196	LEU
1	C	203	GLU
1	C	204	ARG
1	C	205	VAL
1	C	208	GLU
1	C	211	LYS
1	C	219	VAL
1	C	221	ILE
1	C	226	ARG
1	C	230	VAL
1	C	233	ILE
1	C	244	MET
1	B	21	GLN
1	B	26	LEU
1	B	28	ASP
1	B	29	ILE
1	B	31	THR
1	B	32	ARG
1	B	36	VAL
1	B	37	VAL
1	B	38	LEU
1	B	45	LEU
1	B	51	ILE
1	B	52	ILE
1	B	55	LYS
1	B	56	GLU
1	B	57	THR
1	B	59	LYS
1	B	60	GLU

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Mol	Chain	Res	Type
1	B	63	VAL
1	B	69	LEU
1	B	71	ARG
1	B	84	GLN
1	B	85	LYS
1	B	87	GLU
1	B	89	THR
1	B	90	THR
1	B	92	LEU
1	B	94	VAL
1	B	95	SER
1	B	102	TYR
1	B	103	SER
1	B	112	ARG
1	B	115	GLU
1	B	118	GLU
1	B	124	VAL
1	B	126	ARG
1	B	133	ILE
1	B	134	LEU
1	B	135	ILE
1	B	136	GLN
1	B	137	ARG
1	B	140	THR
1	B	141	THR
1	B	143	GLU
1	B	147	ILE
1	B	150	LYS
1	B	156	ARG
1	B	157	GLU
1	B	160	VAL
1	B	162	LEU
1	B	163	LEU
1	B	166	MET
1	B	172	SER
1	B	179	VAL
1	B	180	LEU
1	B	181	LEU
1	B	182	ARG
1	B	183	LEU
1	B	196	LEU
1	B	200	GLN

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Mol	Chain	Res	Type
1	B	202	ILE
1	B	204	ARG
1	B	205	VAL
1	B	207	LYS
1	B	208	GLU
1	B	209	TYR
1	B	213	ARG
1	B	221	ILE
1	B	224	ASN
1	B	226	ARG
1	B	230	VAL
1	B	233	ILE
1	B	244	MET
1	A	21	GLN
1	A	23	GLU
1	A	24	SER
1	A	25	ILE
1	A	29	ILE
1	A	30	ILE
1	A	36	VAL
1	A	37	VAL
1	A	40	LYS
1	A	50	THR
1	A	56	GLU
1	A	59	LYS
1	A	60	GLU
1	A	63	VAL
1	A	69	LEU
1	A	71	ARG
1	A	73	LEU
1	A	80	GLU
1	A	84	GLN
1	A	85	LYS
1	A	87	GLU
1	A	89	THR
1	A	90	THR
1	A	92	LEU
1	A	93	ASP
1	A	100	SER
1	A	104	LYS
1	A	110	ILE
1	A	119	SER

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Mol	Chain	Res	Type
1	A	126	ARG
1	A	130	ILE
1	A	135	ILE
1	A	136	GLN
1	A	139	GLU
1	A	143	GLU
1	A	145	LYS
1	A	150	LYS
1	A	161	MET
1	A	163	LEU
1	A	166	MET
1	A	172	SER
1	A	175	LYS
1	A	179	VAL
1	A	180	LEU
1	A	183	LEU
1	A	185	VAL
1	A	186	LYS
1	A	196	LEU
1	A	202	ILE
1	A	203	GLU
1	A	207	LYS
1	A	213	ARG
1	A	221	ILE
1	A	223	LEU
1	A	224	ASN
1	A	225	SER
1	A	226	ARG
1	A	230	VAL
1	A	233	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	79	ASN
1	D	84	GLN
1	D	97	HIS
1	D	136	GLN
1	D	200	GLN
1	C	44	GLN
1	C	79	ASN
1	C	84	GLN

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Mol	Chain	Res	Type
1	C	97	HIS
1	C	136	GLN
1	B	27	GLN
1	B	35	ASN
1	B	79	ASN
1	B	97	HIS
1	B	200	GLN
1	A	21	GLN
1	A	35	ASN
1	A	44	GLN
1	A	79	ASN
1	A	84	GLN
1	A	136	GLN
1	A	224	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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
3	URA	A	999	-	8,8,8	1.23	2 (25%)	10,10,10	1.04	0
3	URA	C	999	-	8,8,8	0.92	0	10,10,10	1.00	1 (10%)
2	PO4	B	799	-	4,4,4	2.70	2 (50%)	6,6,6	0.72	0
2	PO4	C	799	-	4,4,4	2.62	3 (75%)	6,6,6	0.75	0
2	PO4	B	899	-	4,4,4	2.87	3 (75%)	6,6,6	0.38	0
2	PO4	D	899	-	4,4,4	1.60	1 (25%)	6,6,6	0.70	0
3	URA	D	999	-	8,8,8	0.95	0	10,10,10	1.73	3 (30%)
3	URA	B	999	-	8,8,8	0.75	0	10,10,10	0.95	0
2	PO4	D	799	-	4,4,4	2.40	2 (50%)	6,6,6	0.39	0
2	PO4	A	799	-	4,4,4	2.47	3 (75%)	6,6,6	0.94	0
2	PO4	A	899	-	4,4,4	1.61	2 (50%)	6,6,6	0.62	0
2	PO4	C	899	-	4,4,4	2.30	2 (50%)	6,6,6	0.85	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	A	999	-	-	-	0/1/1/1
3	URA	D	999	-	-	-	0/1/1/1
3	URA	B	999	-	-	-	0/1/1/1
3	URA	C	999	-	-	-	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	799	PO4	P-O4	-4.48	1.41	1.54
2	D	799	PO4	P-O4	-4.02	1.42	1.54
2	B	899	PO4	P-O4	-3.95	1.43	1.54
2	A	799	PO4	P-O4	-3.53	1.44	1.54
2	C	799	PO4	P-O3	-3.31	1.45	1.54
2	C	899	PO4	P-O3	-3.07	1.45	1.54
2	C	799	PO4	P-O2	-2.89	1.46	1.54
2	B	899	PO4	P-O3	-2.79	1.46	1.54
2	D	899	PO4	P-O2	-2.54	1.47	1.54
3	A	999	URA	C2-N1	2.52	1.40	1.36
2	C	899	PO4	P-O1	-2.39	1.45	1.50
2	B	899	PO4	P-O2	-2.39	1.47	1.54
2	B	799	PO4	P-O3	-2.27	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	799	PO4	P-O1	-2.17	1.45	1.50
2	A	899	PO4	P-O2	-2.12	1.48	1.54
3	A	999	URA	C6-N1	2.12	1.39	1.36
2	A	799	PO4	P-O2	-2.11	1.48	1.54
2	A	899	PO4	P-O4	-2.09	1.48	1.54
2	C	799	PO4	P-O4	-2.08	1.48	1.54
2	D	799	PO4	P-O2	-2.05	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	999	URA	C4-N3-C2	3.13	128.58	125.55
3	D	999	URA	O2-C2-N1	2.94	125.82	122.79
3	D	999	URA	C6-C5-C4	-2.38	117.21	119.30
3	C	999	URA	C6-N1-C2	-2.07	121.13	122.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	URA	6	0
2	B	799	PO4	1	0
2	B	899	PO4	1	0
2	D	899	PO4	2	0
3	D	999	URA	3	0
3	B	999	URA	2	0
2	D	799	PO4	3	0
2	A	899	PO4	1	0
2	C	899	PO4	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.