



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 06:52 PM UTC

PDB ID : 1NB6 / pdb_00001nb6
Title : HC-J4 RNA polymerase complexed with UTP
Authors : O'Farrell, D.J.; Trowbridge, R.; Rowlands, D.J.; Jaeger, J.
Deposited on : 2002-12-02
Resolution : 2.60 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

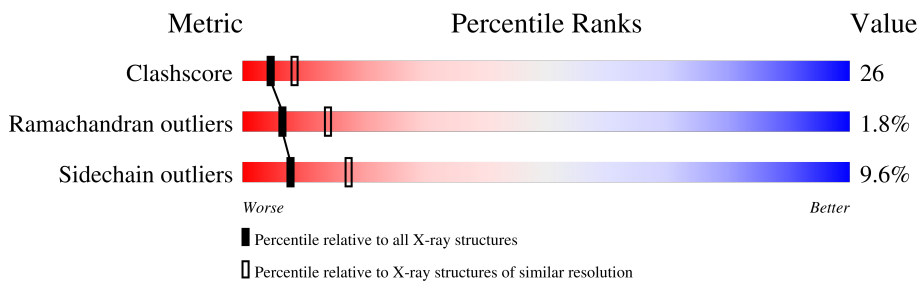
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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	570	 55% 36% 7% ..
1	B	570	 56% 34% 9% ..

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9453 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.

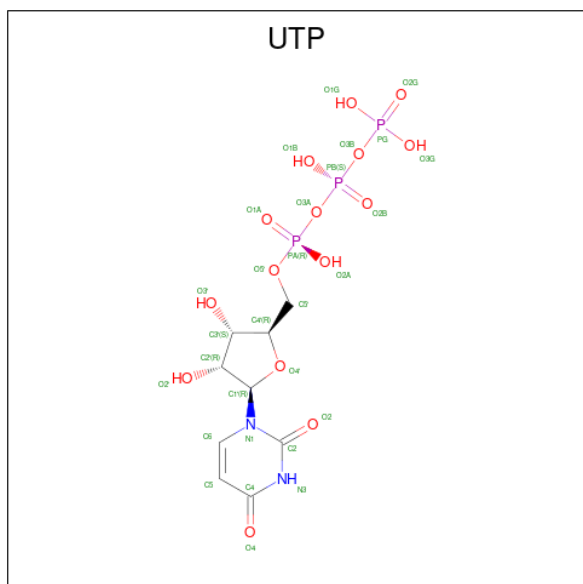
- Molecule 1 is a protein called polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	566	Total	C	N	O	S	0	0	0
			4388	2763	777	816	32			
1	B	565	Total	C	N	O	S	0	0	0
			4381	2758	776	815	32			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		

- Molecule 3 is URIDINE 5'-TRIPHOSPHATE (CCD ID: UTP) (formula: C₉H₁₅N₂O₁₅P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			29	9	2	15	3		
3	B	1	Total	C	N	O	P	0	0
			29	9	2	15	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	270	Total	O	0	0
			270	270		
4	B	352	Total	O	0	0
			352	352		

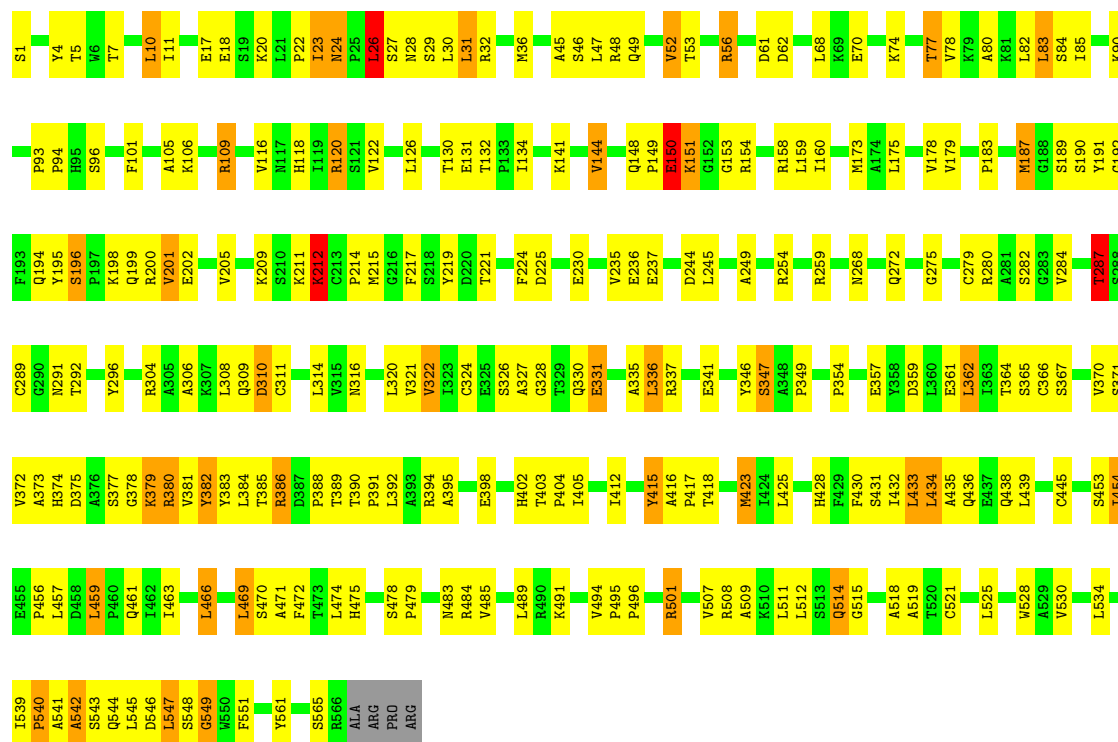
3 Residue-property plots

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.

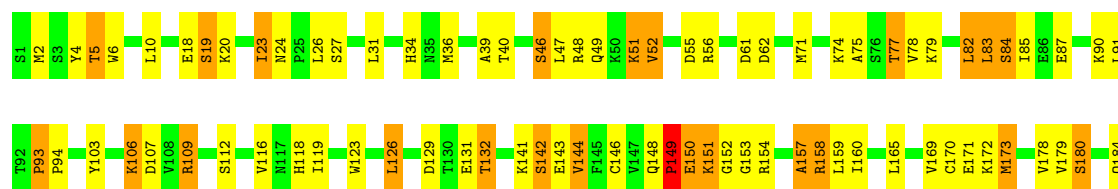
- Molecule 1: polypeptide

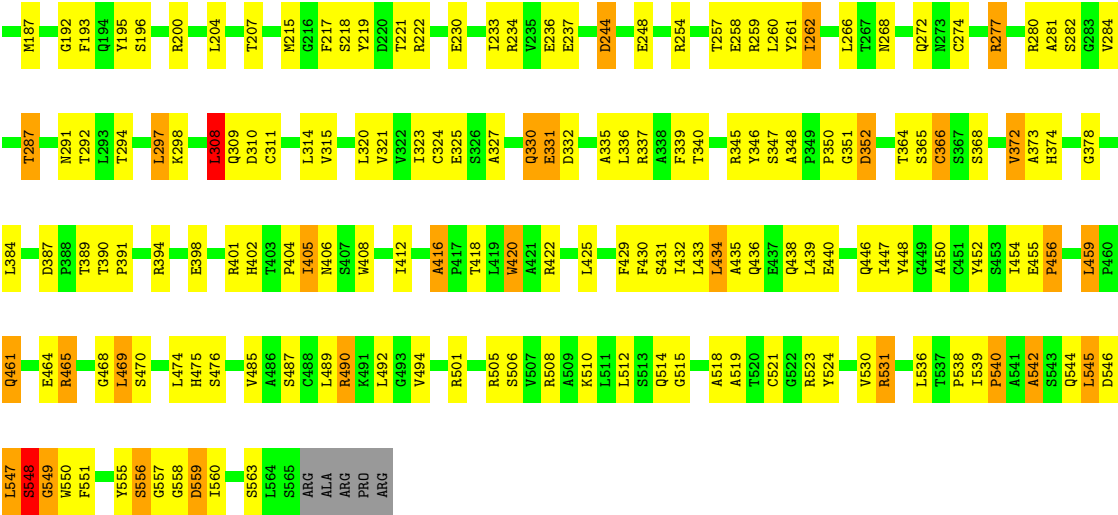
Chain A:  55% 36% 7% ..



- Molecule 1: polypeptide

Chain B:  56% 34% 9% ..





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.43Å 107.74Å 133.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.00 – 2.60	Depositor
% Data completeness (in resolution range)	95.1 (26.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9453	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: UTP, MN

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	0.78	1/4484 (0.0%)	1.19	37/6087 (0.6%)
1	B	0.83	3/4477 (0.1%)	1.22	41/6077 (0.7%)
All	All	0.81	4/8961 (0.0%)	1.20	78/12164 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	MET	SD-CE	-6.59	1.63	1.79
1	A	187	MET	SD-CE	-6.33	1.63	1.79
1	B	142	SER	CB-OG	5.53	1.53	1.42
1	B	178	VAL	CA-CB	5.40	1.60	1.54

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	11	ILE	N-CA-C	-9.65	94.26	108.54
1	B	475	HIS	N-CA-C	8.97	124.84	114.62
1	B	78	VAL	N-CA-C	8.88	121.29	109.21
1	A	78	VAL	N-CA-C	8.33	121.12	108.71
1	A	24	ASN	N-CA-C	8.15	120.34	110.07
1	A	212	LYS	N-CA-C	-7.92	102.24	111.03
1	B	416	ALA	CA-C-N	-7.64	111.80	121.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	ALA	C-N-CA	-7.64	111.80	121.04
1	B	348	ALA	CA-C-N	7.50	125.06	119.66
1	B	348	ALA	C-N-CA	7.50	125.06	119.66
1	A	287	THR	N-CA-C	7.18	119.97	111.71
1	B	215	MET	N-CA-C	-7.17	98.18	109.50
1	B	51	LYS	N-CA-C	6.89	118.80	111.28
1	A	549	GLY	N-CA-C	-6.89	104.47	115.08
1	A	192	GLY	N-CA-C	6.88	121.57	112.77
1	B	548	SER	N-CA-C	-6.87	96.16	110.80
1	B	352	ASP	N-CA-C	-6.87	100.57	110.40
1	A	466	LEU	N-CA-C	6.59	119.80	111.69
1	A	244	ASP	N-CA-C	-6.56	99.22	109.25
1	B	84	SER	N-CA-C	-6.55	102.08	110.53
1	B	196	SER	N-CA-C	-6.42	100.87	110.24
1	B	308	LEU	N-CA-C	-6.26	101.02	110.28
1	B	560	ILE	N-CA-C	6.25	116.92	108.17
1	A	29	SER	N-CA-C	-6.23	104.59	111.82
1	B	332	ASP	N-CA-C	-6.20	104.60	111.36
1	B	132	THR	CA-C-N	-6.19	113.39	119.76
1	B	132	THR	C-N-CA	-6.19	113.39	119.76
1	B	193	PHE	N-CA-C	6.19	120.55	113.19
1	B	429	PHE	N-CA-C	6.18	119.00	111.82
1	A	454	ILE	N-CA-C	6.05	117.41	108.45
1	B	559	ASP	N-CA-C	-6.05	102.27	110.68
1	A	17	GLU	N-CA-C	6.04	118.24	108.34
1	A	479	PRO	N-CA-C	-6.02	104.86	113.47
1	B	494	VAL	CA-C-N	-5.99	114.21	120.38
1	B	494	VAL	C-N-CA	-5.99	114.21	120.38
1	A	195	TYR	N-CA-C	5.90	118.86	109.24
1	B	420	TRP	N-CA-C	5.87	117.76	111.36
1	A	196	SER	N-CA-C	-5.83	100.43	109.87
1	B	315	VAL	N-CA-C	5.80	117.10	108.46
1	A	150	GLU	N-CA-C	-5.71	106.54	112.93
1	A	53	THR	N-CA-C	5.67	117.90	108.20
1	B	157	ALA	N-CA-C	5.65	118.04	110.35
1	B	387	ASP	N-CA-C	-5.54	101.51	109.48
1	A	175	LEU	N-CA-C	5.50	121.77	114.12
1	B	93	PRO	CA-C-N	5.49	125.84	119.47
1	B	93	PRO	C-N-CA	5.49	125.84	119.47
1	B	536	LEU	N-CA-C	5.45	117.19	108.41
1	A	423	MET	N-CA-C	5.44	118.14	111.82
1	A	131	GLU	N-CA-C	5.43	122.38	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	ASP	N-CA-C	-5.43	100.33	108.96
1	A	178	VAL	CB-CA-C	-5.37	105.10	111.97
1	A	395	ALA	N-CA-C	-5.36	105.43	111.28
1	B	372	VAL	N-CA-C	5.35	117.03	108.89
1	A	62	ASP	N-CA-C	5.34	117.52	111.11
1	A	349	PRO	CA-C-N	5.34	125.31	120.03
1	A	349	PRO	C-N-CA	5.34	125.31	120.03
1	B	389	THR	N-CA-C	5.33	117.53	111.02
1	B	402	HIS	N-CA-C	-5.28	101.83	109.59
1	B	195	TYR	N-CA-C	5.27	117.83	109.24
1	B	230	GLU	N-CA-C	-5.26	105.66	111.71
1	A	214	PRO	N-CA-C	5.26	119.44	111.19
1	A	501	ARG	N-CA-C	-5.25	105.56	111.28
1	A	415	TYR	N-CA-C	5.24	119.36	112.92
1	B	524	TYR	N-CA-C	5.23	119.64	112.68
1	B	218	SER	N-CA-C	-5.20	100.92	109.40
1	A	230	GLU	N-CA-C	-5.17	105.65	111.28
1	B	261	TYR	N-CA-C	5.15	116.89	111.28
1	A	379	LYS	N-CA-C	5.14	117.57	109.39
1	A	475	HIS	N-CA-C	5.12	121.20	114.75
1	B	366	CYS	N-CA-C	-5.12	106.34	112.58
1	A	418	THR	N-CA-C	5.11	117.70	110.50
1	A	547	LEU	N-CA-C	5.10	117.26	110.53
1	A	478	SER	CA-C-N	5.06	124.23	118.97
1	A	478	SER	C-N-CA	5.06	124.23	118.97
1	B	192	GLY	N-CA-C	5.03	118.77	112.73
1	A	101	PHE	N-CA-C	5.03	118.56	112.93
1	B	501	ARG	N-CA-C	-5.01	105.82	111.28
1	A	235	VAL	N-CA-C	-5.01	105.66	110.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	382	TYR	Sidechain

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	4388	0	4383	240	0
1	B	4381	0	4374	218	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	29	0	11	2	0
3	B	29	0	11	2	0
4	A	270	0	0	28	0
4	B	352	0	0	39	0
All	All	9453	0	8779	458	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 26.

All (458) 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:B:109:ARG:NH1	1:B:109:ARG:HB2	1.63	1.12
1:B:141:LYS:NZ	1:B:158:ARG:HH12	1.55	1.04
1:B:148:GLN:HE21	1:B:153:GLY:HA3	1.18	1.03
1:A:547:LEU:HD12	1:A:565:SER:H	1.25	1.01
1:B:277:ARG:HE	1:B:281:ALA:HB2	1.22	0.98
1:B:277:ARG:HH11	1:B:277:ARG:HB3	1.27	0.97
1:B:109:ARG:HB2	1:B:109:ARG:HH11	1.26	0.97
1:A:221:THR:HG1	1:A:224:PHE:HD2	1.01	0.96
1:B:141:LYS:HZ2	1:B:158:ARG:HH12	1.08	0.96
1:A:24:ASN:HD22	1:A:27:SER:H	1.00	0.94
1:A:24:ASN:HD22	1:A:27:SER:N	1.63	0.94
1:B:160:ILE:HD12	1:B:282:SER:OG	1.72	0.90
1:A:141:LYS:HE3	1:A:158:ARG:NH2	1.87	0.89
1:A:327:ALA:O	1:A:331:GLU:HG3	1.72	0.89
1:A:470:SER:O	1:A:474:LEU:HG	1.74	0.88
1:A:132:THR:O	1:A:259:ARG:HD2	1.73	0.87
1:A:93:PRO:HG2	1:A:96:SER:HB2	1.56	0.87
1:A:547:LEU:HD12	1:A:565:SER:N	1.88	0.86
1:B:109:ARG:HH11	1:B:109:ARG:CB	1.89	0.85
1:B:132:THR:O	1:B:259:ARG:HD2	1.76	0.85
1:A:187:MET:HE1	1:A:292:THR:HG22	1.54	0.85
1:B:90:LYS:HG2	4:B:2980:HOH:O	1.77	0.85
1:B:18:GLU:HG2	1:B:401:ARG:CZ	2.06	0.85
1:B:74:LYS:O	1:B:77:THR:HB	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASN:HD21	1:A:272:GLN:HE21	1.20	0.84
1:A:501:ARG:HB3	4:A:1906:HOH:O	1.78	0.83
1:A:337:ARG:O	1:A:341:GLU:HG3	1.79	0.82
1:A:85:ILE:N	1:A:173:MET:HE3	1.95	0.82
1:A:48:ARG:HG2	1:A:159:LEU:HG	1.62	0.81
1:A:187:MET:HE3	1:A:296:TYR:HB2	1.63	0.80
1:A:200:ARG:HH21	1:A:316:ASN:HD21	1.28	0.80
1:A:148:GLN:HB3	1:A:153:GLY:HA3	1.64	0.79
1:B:277:ARG:NE	1:B:281:ALA:HB2	1.97	0.79
1:B:539:ILE:HB	1:B:542:ALA:HB2	1.64	0.78
1:A:148:GLN:HG2	1:A:150:GLU:HG2	1.64	0.77
1:B:131:GLU:HG3	4:B:2910:HOH:O	1.85	0.76
1:B:23:ILE:HB	4:B:2858:HOH:O	1.84	0.76
1:A:398:GLU:HG2	1:A:403:THR:HG21	1.67	0.76
1:B:144:VAL:HG22	1:B:394:ARG:HG2	1.68	0.76
1:B:148:GLN:NE2	1:B:153:GLY:HA3	1.96	0.76
1:B:434:LEU:HD11	1:B:514:GLN:NE2	2.01	0.75
1:B:141:LYS:NZ	1:B:158:ARG:NH1	2.35	0.74
1:A:365:SER:O	1:A:366:CYS:HB2	1.87	0.74
1:A:116:VAL:O	1:A:120:ARG:HG3	1.87	0.74
1:B:152:GLY:HA2	4:B:2774:HOH:O	1.89	0.73
1:A:284:VAL:HG23	1:A:287:THR:HG22	1.72	0.71
1:A:10:LEU:HD12	1:A:10:LEU:N	2.04	0.71
1:B:83:LEU:HB2	1:B:173:MET:HA	1.72	0.71
1:A:179:VAL:HG13	1:A:289:CYS:HB2	1.72	0.71
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.72	0.70
1:A:148:GLN:CD	1:A:150:GLU:HG2	2.16	0.70
1:A:377:SER:HB3	4:A:1885:HOH:O	1.91	0.70
1:A:374:HIS:HA	4:A:1889:HOH:O	1.90	0.70
1:B:222:ARG:HG3	1:B:351:GLY:HA2	1.74	0.70
1:A:56:ARG:NE	4:A:1773:HOH:O	2.24	0.70
1:B:24:ASN:HD22	1:B:27:SER:H	1.36	0.70
1:A:148:GLN:CG	1:A:150:GLU:HG2	2.20	0.70
1:A:336:LEU:HD23	1:A:354:PRO:HB2	1.74	0.70
1:A:511:LEU:O	1:A:519:ALA:HA	1.92	0.70
1:B:476:SER:N	4:B:2898:HOH:O	2.03	0.69
1:B:187:MET:HE1	1:B:292:THR:HG22	1.75	0.69
1:B:18:GLU:HG2	1:B:401:ARG:NH2	2.07	0.69
1:A:90:LYS:HD3	4:A:1880:HOH:O	1.90	0.69
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.58	0.69
1:B:294:THR:HG22	1:B:298:LYS:HE3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ARG:NH2	4:B:2876:HOH:O	2.26	0.68
1:A:24:ASN:HB3	1:A:27:SER:HB3	1.76	0.67
1:A:359:ASP:HB3	1:A:362:LEU:HD22	1.76	0.67
1:B:277:ARG:NE	4:B:2758:HOH:O	2.27	0.67
1:A:268:ASN:ND2	1:A:272:GLN:HE21	1.91	0.67
1:B:346:TYR:O	1:B:347:SER:HB3	1.95	0.67
1:B:547:LEU:HD22	1:B:547:LEU:H	1.60	0.66
1:A:61:ASP:CG	4:A:1836:HOH:O	2.38	0.66
1:B:277:ARG:NH1	4:B:2770:HOH:O	2.29	0.66
1:A:23:ILE:HG23	1:A:23:ILE:O	1.94	0.66
1:A:379:LYS:O	1:A:379:LYS:HD3	1.95	0.66
1:A:26:LEU:CD1	1:A:432:ILE:HD12	2.25	0.66
1:B:464:GLU:OE1	1:B:469:LEU:HD11	1.96	0.65
1:A:200:ARG:HH21	1:A:316:ASN:ND2	1.94	0.65
1:A:4:TYR:CE1	1:A:52:VAL:HG13	2.31	0.65
1:A:346:TYR:O	1:A:347:SER:HB3	1.96	0.64
1:A:10:LEU:HD12	1:A:10:LEU:H	1.60	0.64
1:A:398:GLU:HG2	1:A:403:THR:CG2	2.27	0.64
1:A:187:MET:HE3	1:A:296:TYR:CD1	2.32	0.64
1:A:237:GLU:OE2	1:A:254:ARG:HD2	1.97	0.64
1:B:180:SER:HB3	1:B:555:TYR:OH	1.96	0.64
1:B:325:GLU:HB3	4:B:2836:HOH:O	1.97	0.64
1:A:187:MET:HE3	1:A:296:TYR:CB	2.27	0.64
1:B:248:GLU:HG3	4:B:2708:HOH:O	1.97	0.64
1:B:141:LYS:HD2	1:B:143:GLU:OE1	1.98	0.63
1:B:200:ARG:NH1	4:B:2764:HOH:O	2.30	0.63
1:B:469:LEU:HD12	1:B:469:LEU:H	1.64	0.63
1:A:428:HIS:O	1:A:432:ILE:HG12	1.99	0.63
1:B:84:SER:OG	1:B:87:GLU:HG3	1.98	0.63
1:B:308:LEU:HB3	1:B:311:CYS:SG	2.38	0.63
1:B:79:LYS:HG3	1:B:244:ASP:HB3	1.81	0.63
1:A:337:ARG:HD3	4:A:1815:HOH:O	1.99	0.62
1:A:36:MET:HE2	1:A:491:LYS:O	2.00	0.62
1:A:141:LYS:HE3	1:A:158:ARG:HH21	1.65	0.62
1:A:268:ASN:HD21	1:A:272:GLN:NE2	1.96	0.62
1:B:200:ARG:NE	4:B:2876:HOH:O	2.27	0.62
1:A:547:LEU:CD1	1:A:565:SER:H	2.07	0.62
1:B:260:LEU:O	1:B:277:ARG:NH2	2.33	0.62
1:B:148:GLN:HG3	1:B:149:PRO:HD2	1.81	0.62
1:B:280:ARG:HD2	1:B:291:ASN:OD1	1.99	0.62
1:A:309:GLN:O	1:A:324:CYS:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:NH2	1:B:531:ARG:NE	2.47	0.61
1:A:236:GLU:CD	1:A:280:ARG:HH22	2.07	0.61
1:B:2:MET:HE2	4:B:2775:HOH:O	2.00	0.61
1:B:26:LEU:HD13	1:B:432:ILE:HD12	1.81	0.61
1:B:374:HIS:O	1:B:474:LEU:HA	2.01	0.60
1:B:234:ARG:HG3	1:B:262:ILE:HD11	1.82	0.60
1:B:548:SER:O	1:B:550:TRP:N	2.34	0.60
1:B:34:HIS:HD2	4:B:2906:HOH:O	1.84	0.60
1:A:198:LYS:O	1:A:201:VAL:HG12	2.02	0.60
1:A:361:GLU:HG3	1:A:370:VAL:O	2.01	0.60
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.17	0.60
1:B:109:ARG:NH1	1:B:109:ARG:CB	2.48	0.59
1:A:4:TYR:CE1	1:A:52:VAL:CG1	2.84	0.59
1:B:331:GLU:CD	1:B:331:GLU:H	2.09	0.59
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.84	0.59
1:B:456:PRO:O	1:B:459:LEU:HD22	2.03	0.59
1:A:22:PRO:HB2	4:A:1750:HOH:O	2.02	0.59
1:A:359:ASP:HB3	1:A:362:LEU:CD2	2.33	0.59
1:B:61:ASP:CG	4:B:2719:HOH:O	2.44	0.59
1:B:187:MET:HE1	1:B:292:THR:CG2	2.33	0.59
1:B:434:LEU:HD11	1:B:514:GLN:HE21	1.67	0.59
1:B:277:ARG:CZ	4:B:2758:HOH:O	2.50	0.58
1:B:173:MET:HE2	4:B:2862:HOH:O	2.03	0.58
1:A:1:SER:O	1:A:56:ARG:NH1	2.37	0.58
1:B:19:SER:HA	1:B:39:ALA:HB3	1.86	0.58
1:B:277:ARG:HH11	1:B:277:ARG:CB	2.09	0.58
1:B:222:ARG:HG3	1:B:351:GLY:CA	2.33	0.58
1:A:7:THR:C	4:A:1778:HOH:O	2.46	0.58
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.85	0.58
1:B:85:ILE:HG12	1:B:173:MET:CE	2.34	0.58
1:A:215:MET:HE1	1:A:336:LEU:HD11	1.86	0.58
1:A:24:ASN:ND2	1:A:27:SER:N	2.46	0.57
1:B:447:ILE:HB	1:B:452:TYR:CE1	2.38	0.57
1:A:160:ILE:HD12	1:A:282:SER:OG	2.04	0.57
1:A:83:LEU:HB2	1:A:173:MET:HA	1.86	0.57
1:B:510:LYS:HE2	4:B:3041:HOH:O	2.04	0.56
1:B:24:ASN:HD21	1:B:26:LEU:HB2	1.69	0.56
1:A:542:ALA:C	1:A:544:GLN:H	2.12	0.56
1:B:172:LYS:HZ1	1:B:559:ASP:HB3	1.70	0.56
1:A:361:GLU:HB2	4:A:1955:HOH:O	2.05	0.56
1:A:85:ILE:HD12	1:A:120:ARG:CZ	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:LYS:HB2	1:B:106:LYS:NZ	2.21	0.56
1:B:465:ARG:HH21	1:B:546:ASP:CB	2.18	0.56
1:A:26:LEU:HD13	1:A:432:ILE:HD12	1.88	0.56
1:A:48:ARG:NH1	3:A:1700:UTP:O1G	2.32	0.56
1:B:277:ARG:HB3	1:B:277:ARG:NH1	2.09	0.56
1:A:10:LEU:H	1:A:10:LEU:CD1	2.17	0.56
1:A:379:LYS:C	4:A:1889:HOH:O	2.49	0.56
1:B:277:ARG:HE	1:B:281:ALA:CB	2.08	0.56
1:A:225:ASP:CG	3:A:1700:UTP:H1'	2.32	0.55
1:B:549:GLY:C	4:B:2954:HOH:O	2.48	0.55
1:A:366:CYS:O	1:A:367:SER:HB2	2.06	0.55
1:B:512:LEU:HD21	1:B:523:ARG:HG2	1.88	0.55
1:B:154:ARG:HD3	4:B:3038:HOH:O	2.05	0.55
1:B:434:LEU:C	1:B:436:GLN:H	2.15	0.55
1:B:141:LYS:HZ1	1:B:158:ARG:HH12	1.52	0.55
1:B:294:THR:CG2	1:B:298:LYS:HE3	2.35	0.55
1:A:403:THR:OG1	1:A:404:PRO:HD2	2.08	0.54
1:A:379:LYS:O	1:A:380:ARG:C	2.50	0.54
1:A:31:LEU:O	1:A:31:LEU:HD23	2.07	0.54
1:A:198:LYS:HD3	1:A:466:LEU:O	2.06	0.54
1:A:201:VAL:CG1	1:A:202:GLU:N	2.70	0.54
1:B:200:ARG:CZ	4:B:2876:HOH:O	2.56	0.54
1:B:465:ARG:NH2	1:B:546:ASP:CB	2.70	0.54
1:A:10:LEU:N	1:A:10:LEU:CD1	2.71	0.54
1:A:423:MET:HG2	1:A:528:TRP:CZ3	2.43	0.54
1:A:141:LYS:CE	1:A:158:ARG:NH2	2.68	0.53
1:A:284:VAL:CG2	1:A:287:THR:HG22	2.37	0.53
1:B:284:VAL:O	1:B:287:THR:HG23	2.08	0.53
1:B:447:ILE:HB	1:B:452:TYR:HE1	1.73	0.53
1:B:36:MET:O	1:B:146:CYS:HA	2.08	0.53
1:B:85:ILE:HG12	1:B:173:MET:HE1	1.90	0.53
1:B:106:LYS:HG3	1:B:107:ASP:N	2.24	0.53
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.89	0.53
1:B:51:LYS:CE	1:B:222:ARG:HH22	2.21	0.53
1:A:456:PRO:HA	1:A:459:LEU:HD22	1.91	0.53
1:B:144:VAL:HG22	1:B:394:ARG:CG	2.37	0.53
1:A:154:ARG:HG3	1:A:154:ARG:HH11	1.74	0.53
1:B:366:CYS:HA	4:B:2845:HOH:O	2.07	0.53
1:B:106:LYS:HG3	1:B:107:ASP:H	1.72	0.53
1:B:518:ALA:O	1:B:521:CYS:HB2	2.08	0.53
1:A:336:LEU:CD2	1:A:354:PRO:HB2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:HB2	4:A:1963:HOH:O	2.08	0.53
1:B:237:GLU:O	1:B:237:GLU:HG2	2.09	0.53
1:B:337:ARG:HA	1:B:337:ARG:HE	1.73	0.53
1:A:515:GLY:CA	1:A:519:ALA:HB2	2.38	0.53
1:B:18:GLU:CG	1:B:401:ARG:NH2	2.72	0.53
1:A:85:ILE:HD11	1:A:120:ARG:HG2	1.90	0.52
1:A:461:GLN:HG3	1:A:542:ALA:HB2	1.90	0.52
1:B:132:THR:O	1:B:259:ARG:CD	2.53	0.52
1:B:254:ARG:NH2	1:B:258:GLU:CG	2.73	0.52
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.91	0.52
1:B:446:GLN:C	1:B:447:ILE:HD12	2.34	0.52
1:A:179:VAL:HG12	4:A:1720:HOH:O	2.10	0.52
1:A:26:LEU:HD11	1:A:432:ILE:HD12	1.91	0.52
1:A:132:THR:O	1:A:259:ARG:CD	2.53	0.52
1:A:540:PRO:HG2	1:A:541:ALA:H	1.75	0.52
1:B:490:ARG:HG3	4:B:2985:HOH:O	2.08	0.52
1:A:374:HIS:O	1:A:474:LEU:HA	2.10	0.52
1:B:337:ARG:HD2	4:B:2830:HOH:O	2.10	0.52
1:A:4:TYR:HE1	1:A:52:VAL:HG13	1.73	0.51
1:A:390:THR:HB	1:A:391:PRO:HD3	1.92	0.51
1:B:154:ARG:NH1	4:B:2952:HOH:O	2.41	0.51
1:B:277:ARG:NH2	4:B:2758:HOH:O	2.43	0.51
1:B:284:VAL:CG2	1:B:287:THR:HG22	2.40	0.51
1:B:434:LEU:HD13	1:B:439:LEU:HD22	1.93	0.51
1:A:191:TYR:O	1:A:194:GLN:HG2	2.10	0.51
1:B:390:THR:HB	1:B:391:PRO:HD3	1.91	0.51
1:A:10:LEU:HD13	4:A:1967:HOH:O	2.09	0.51
1:B:24:ASN:ND2	1:B:26:LEU:N	2.59	0.51
1:B:434:LEU:CD1	1:B:514:GLN:NE2	2.73	0.51
1:A:388:PRO:C	1:A:391:PRO:HD2	2.36	0.51
1:B:40:THR:HB	1:B:157:ALA:HB2	1.90	0.51
1:A:336:LEU:HD23	1:A:354:PRO:CB	2.41	0.51
1:A:381:VAL:HG23	4:A:1889:HOH:O	2.10	0.51
1:A:187:MET:HE3	1:A:296:TYR:CG	2.45	0.51
1:B:374:HIS:HD2	1:B:378:GLY:O	1.94	0.51
1:A:485:VAL:O	1:A:489:LEU:HG	2.11	0.51
1:B:365:SER:O	1:B:366:CYS:HB2	2.11	0.51
1:A:215:MET:HB2	1:A:326:SER:HB2	1.93	0.51
1:B:284:VAL:HG22	1:B:287:THR:HG22	1.92	0.51
1:B:508:ARG:NE	4:B:2869:HOH:O	2.19	0.51
1:A:32:ARG:HD2	4:A:1928:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:TYR:O	1:B:558:GLY:N	2.41	0.51
1:A:144:VAL:HG22	1:A:394:ARG:HG3	1.94	0.50
1:A:148:GLN:HB3	1:A:153:GLY:CA	2.38	0.50
1:A:196:SER:OG	1:A:199:GLN:HG3	2.11	0.50
1:B:447:ILE:HD13	1:B:452:TYR:CD1	2.46	0.50
1:A:5:THR:O	1:A:275:GLY:HA3	2.11	0.50
1:B:18:GLU:HG2	1:B:401:ARG:NH1	2.26	0.50
1:A:93:PRO:HB3	1:A:561:TYR:HB2	1.93	0.50
1:A:179:VAL:HG13	1:A:289:CYS:CB	2.40	0.50
1:A:364:THR:HG22	4:A:1897:HOH:O	2.11	0.50
1:A:518:ALA:O	1:A:521:CYS:HB2	2.12	0.50
1:B:48:ARG:NH1	3:B:2700:UTP:O2G	2.44	0.50
1:A:306:ALA:HB3	1:A:308:LEU:HD13	1.93	0.50
1:A:183:PRO:HB3	1:A:191:TYR:CE1	2.47	0.50
1:A:187:MET:O	1:A:190:SER:HB2	2.11	0.50
1:A:194:GLN:HA	1:A:551:PHE:O	2.12	0.50
1:B:468:GLY:O	1:B:470:SER:N	2.45	0.50
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.41	0.50
1:B:539:ILE:HB	1:B:542:ALA:CB	2.36	0.50
1:A:74:LYS:O	1:A:77:THR:HB	2.12	0.50
1:B:557:GLY:HA2	3:B:2700:UTP:O4	2.11	0.49
1:A:367:SER:HB2	1:A:386:ARG:HH12	1.77	0.49
1:B:62:ASP:HB2	4:B:2903:HOH:O	2.12	0.49
1:B:237:GLU:OE2	1:B:254:ARG:HD2	2.12	0.49
1:B:82:LEU:HD12	1:B:82:LEU:O	2.13	0.49
1:B:126:LEU:HA	1:B:259:ARG:HH21	1.77	0.49
1:A:105:ALA:O	1:A:109:ARG:HG3	2.11	0.49
1:B:48:ARG:CG	1:B:159:LEU:HG	2.40	0.49
1:B:539:ILE:O	1:B:542:ALA:HB3	2.13	0.49
1:A:148:GLN:HG2	1:A:150:GLU:H	1.77	0.49
1:B:485:VAL:O	1:B:489:LEU:HG	2.11	0.49
1:B:337:ARG:HG3	4:B:2779:HOH:O	2.12	0.49
1:A:56:ARG:NH1	1:A:56:ARG:HB2	2.28	0.49
1:A:539:ILE:HG23	1:A:540:PRO:HD2	1.94	0.49
1:B:75:ALA:C	1:B:77:THR:H	2.21	0.49
1:A:435:ALA:HB3	1:A:436:GLN:OE1	2.13	0.49
1:B:172:LYS:NZ	1:B:559:ASP:HB3	2.26	0.49
1:A:308:LEU:HB3	1:A:311:CYS:SG	2.53	0.48
1:B:366:CYS:C	1:B:368:SER:H	2.20	0.48
1:A:83:LEU:CB	1:A:173:MET:HA	2.44	0.48
1:A:459:LEU:O	1:A:463:ILE:HG13	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PRO:HD2	4:A:1750:HOH:O	2.13	0.48
1:B:330:GLN:HA	1:B:330:GLN:OE1	2.13	0.48
1:B:461:GLN:HB3	1:B:542:ALA:HA	1.94	0.48
1:A:20:LYS:O	1:A:22:PRO:HD3	2.13	0.48
1:A:200:ARG:NH2	1:A:316:ASN:ND2	2.61	0.48
1:B:150:GLU:O	1:B:151:LYS:C	2.57	0.48
1:B:374:HIS:N	4:B:2898:HOH:O	2.40	0.48
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.44	0.48
1:B:103:TYR:CE1	1:B:165:LEU:HD23	2.49	0.48
1:B:505:ARG:HH21	1:B:531:ARG:NE	2.11	0.48
1:A:48:ARG:CG	1:A:159:LEU:HG	2.36	0.48
1:B:433:LEU:CD2	1:B:456:PRO:HG2	2.44	0.48
1:A:30:LEU:O	1:A:494:VAL:HG22	2.14	0.48
1:B:436:GLN:O	1:B:438:GLN:HG2	2.14	0.48
1:A:27:SER:HB3	4:A:1779:HOH:O	2.13	0.48
1:A:327:ALA:O	1:A:331:GLU:CG	2.56	0.48
1:B:447:ILE:HD13	1:B:452:TYR:HD1	1.77	0.48
1:A:453:SER:C	1:A:454:ILE:HG13	2.37	0.47
1:B:51:LYS:HE3	1:B:222:ARG:HH22	1.79	0.47
1:B:24:ASN:ND2	1:B:26:LEU:H	2.12	0.47
1:B:398:GLU:OE2	1:B:408:TRP:HD1	1.97	0.47
1:A:386:ARG:HG3	1:A:386:ARG:HH11	1.78	0.47
1:A:433:LEU:HD12	1:A:438:GLN:HB2	1.97	0.47
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.53	0.47
1:B:171:GLU:OE2	1:B:284:VAL:HB	2.15	0.47
1:B:405:ILE:HG12	1:B:406:ASN:N	2.30	0.47
1:A:70:GLU:CD	1:A:304:ARG:HH22	2.21	0.47
1:A:237:GLU:OE2	1:A:254:ARG:HA	2.15	0.47
1:A:415:TYR:C	1:A:417:PRO:HD2	2.40	0.47
1:B:4:TYR:CE1	1:B:52:VAL:HG13	2.48	0.47
1:B:207:THR:HG22	1:B:323:ILE:HG21	1.96	0.47
1:B:401:ARG:HG2	1:B:401:ARG:HH11	1.80	0.47
1:A:308:LEU:CD1	1:A:335:ALA:HB1	2.45	0.47
1:A:456:PRO:O	1:A:459:LEU:HD22	2.15	0.47
1:B:109:ARG:NE	4:B:3007:HOH:O	2.41	0.47
1:B:217:PHE:CD1	1:B:336:LEU:HD11	2.50	0.47
1:A:189:SER:HA	1:A:194:GLN:HE22	1.80	0.47
1:B:257:THR:HG22	1:B:262:ILE:HD13	1.97	0.47
1:A:150:GLU:N	1:A:150:GLU:CD	2.73	0.47
1:A:215:MET:HE1	1:A:336:LEU:CD1	2.45	0.46
1:A:308:LEU:HD11	1:A:335:ALA:HB1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ASP:OD1	1:B:346:TYR:HE2	1.98	0.46
1:B:46:SER:HA	1:B:49:GLN:HE21	1.80	0.46
1:B:559:ASP:N	4:B:2856:HOH:O	2.34	0.46
1:B:404:PRO:HG2	1:B:405:ILE:H	1.81	0.46
1:B:506:SER:O	1:B:510:LYS:HG3	2.15	0.46
1:A:90:LYS:O	1:A:109:ARG:NH2	2.49	0.46
1:B:109:ARG:NH2	4:B:3007:HOH:O	2.46	0.46
1:B:233:ILE:CG2	1:B:262:ILE:HD12	2.46	0.46
1:A:149:PRO:C	1:A:151:LYS:H	2.23	0.46
1:A:402:HIS:N	4:A:1921:HOH:O	2.49	0.46
1:A:509:ALA:C	1:A:511:LEU:H	2.23	0.46
1:B:5:THR:HG22	4:B:2955:HOH:O	2.16	0.46
1:B:266:LEU:HD21	1:B:277:ARG:HB2	1.98	0.46
1:B:141:LYS:HZ1	1:B:158:ARG:NH1	2.11	0.46
1:A:84:SER:C	1:A:173:MET:HE3	2.41	0.46
1:A:439:LEU:HB3	1:A:457:LEU:HD11	1.97	0.46
1:A:219:TYR:HE2	1:A:221:THR:HG22	1.82	0.45
1:A:436:GLN:OE1	1:A:436:GLN:N	2.49	0.45
1:A:279:CYS:HB3	4:A:1773:HOH:O	2.16	0.45
1:A:469:LEU:C	1:A:471:ALA:N	2.71	0.45
1:A:389:THR:OG1	1:A:491:LYS:NZ	2.48	0.45
1:A:508:ARG:O	1:A:511:LEU:HB2	2.16	0.45
1:B:200:ARG:NH1	1:B:204:LEU:HD11	2.32	0.45
1:A:148:GLN:NE2	1:A:150:GLU:HG2	2.32	0.45
1:A:367:SER:CB	1:A:386:ARG:HH12	2.30	0.45
1:B:24:ASN:ND2	1:B:26:LEU:HB2	2.31	0.45
1:B:490:ARG:HE	1:B:490:ARG:HA	1.82	0.45
1:A:144:VAL:HG22	1:A:394:ARG:CG	2.47	0.45
1:A:314:LEU:HB3	1:A:321:VAL:HG13	1.99	0.45
1:A:495:PRO:HA	1:A:496:PRO:HD3	1.90	0.45
1:A:148:GLN:C	1:A:150:GLU:N	2.74	0.45
1:A:347:SER:O	1:A:347:SER:OG	2.26	0.45
1:B:71:MET:SD	1:B:297:LEU:HB2	2.56	0.45
1:A:308:LEU:CB	1:A:311:CYS:SG	3.04	0.45
1:B:446:GLN:HA	1:B:450:ALA:O	2.17	0.45
1:B:372:VAL:HG12	1:B:373:ALA:N	2.32	0.45
1:B:456:PRO:HA	1:B:459:LEU:HD22	1.99	0.45
1:A:118:HIS:O	1:A:122:VAL:HG23	2.17	0.45
1:A:472:PHE:HE2	1:A:525:LEU:HD23	1.81	0.45
1:A:28:ASN:HB2	4:A:1887:HOH:O	2.17	0.44
1:A:415:TYR:C	1:A:417:PRO:CD	2.91	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:LEU:CD1	1:B:335:ALA:HB1	2.46	0.44
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.85	0.44
1:B:146:CYS:SG	1:B:492:LEU:HD21	2.57	0.44
1:B:455:GLU:HB3	4:B:2934:HOH:O	2.17	0.44
1:A:148:GLN:C	1:A:150:GLU:H	2.24	0.44
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.80	0.44
1:B:327:ALA:O	1:B:331:GLU:CG	2.65	0.44
1:B:436:GLN:C	1:B:438:GLN:H	2.25	0.44
1:A:36:MET:CE	1:A:491:LYS:HG2	2.47	0.44
1:B:434:LEU:C	1:B:436:GLN:N	2.76	0.44
1:A:375:ASP:N	4:A:1889:HOH:O	2.40	0.44
1:A:134:ILE:HG13	1:A:259:ARG:HB3	2.00	0.44
1:B:448:TYR:CE1	1:B:551:PHE:HD2	2.35	0.44
1:A:56:ARG:HB2	1:A:56:ARG:CZ	2.48	0.43
1:A:82:LEU:HD13	1:A:249:ALA:HB2	2.00	0.43
1:A:148:GLN:HG2	1:A:150:GLU:CG	2.43	0.43
1:B:82:LEU:HD12	1:B:82:LEU:C	2.43	0.43
1:A:94:PRO:HA	1:A:109:ARG:HD2	2.00	0.43
1:A:144:VAL:HG13	4:A:1765:HOH:O	2.17	0.43
1:B:412:ILE:O	1:B:416:ALA:HB2	2.18	0.43
1:A:80:ALA:HB3	1:A:245:LEU:HD23	2.00	0.43
1:A:386:ARG:HG3	1:A:386:ARG:NH1	2.34	0.43
1:B:555:TYR:O	1:B:556:SER:C	2.61	0.43
1:A:45:ALA:O	1:A:48:ARG:HB3	2.18	0.43
1:A:224:PHE:O	1:A:225:ASP:C	2.61	0.43
1:A:548:SER:OG	1:A:549:GLY:N	2.51	0.43
1:A:542:ALA:C	1:A:544:GLN:N	2.77	0.43
1:A:56:ARG:NH2	4:A:1773:HOH:O	2.51	0.43
1:A:431:SER:HB3	1:A:507:VAL:CG2	2.48	0.43
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.58	0.43
1:B:31:LEU:C	1:B:31:LEU:HD23	2.43	0.43
1:B:148:GLN:HG2	1:B:150:GLU:OE2	2.19	0.43
1:B:539:ILE:HG23	1:B:540:PRO:HD2	2.01	0.43
1:A:371:SER:HB3	1:A:383:TYR:CE1	2.53	0.43
1:A:433:LEU:HD12	1:A:433:LEU:HA	1.82	0.42
1:A:434:LEU:HD12	1:A:434:LEU:HA	1.87	0.42
1:B:336:LEU:O	1:B:339:PHE:HB3	2.19	0.42
1:B:530:VAL:CG1	4:B:2869:HOH:O	2.66	0.42
1:A:372:VAL:HG12	1:A:373:ALA:N	2.32	0.42
1:A:84:SER:O	1:A:85:ILE:C	2.62	0.42
1:A:280:ARG:HA	4:A:1876:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:GLN:C	1:B:438:GLN:N	2.77	0.42
1:A:254:ARG:HD2	1:A:254:ARG:HA	1.76	0.42
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.33	0.42
1:A:328:GLY:O	1:A:331:GLU:HB2	2.19	0.42
1:A:392:LEU:HD23	1:A:392:LEU:HA	1.90	0.42
1:B:123:TRP:HB2	1:B:170:CYS:SG	2.60	0.42
1:B:544:GLN:O	1:B:545:LEU:C	2.63	0.42
1:A:45:ALA:O	1:A:49:GLN:HG3	2.20	0.42
1:B:309:GLN:O	1:B:324:CYS:HB2	2.19	0.42
1:A:412:ILE:O	1:A:416:ALA:N	2.53	0.42
1:A:512:LEU:C	1:A:514:GLN:H	2.27	0.42
1:B:327:ALA:O	1:B:331:GLU:HG3	2.20	0.42
1:B:418:THR:O	1:B:422:ARG:HG3	2.18	0.42
1:A:483:ASN:HD22	1:A:483:ASN:HA	1.70	0.42
1:B:148:GLN:O	1:B:149:PRO:C	2.62	0.42
1:B:236:GLU:OE1	1:B:280:ARG:NH2	2.36	0.42
1:B:345:ARG:C	1:B:347:SER:H	2.27	0.42
1:B:454:ILE:HG22	1:B:455:GLU:N	2.35	0.42
1:A:209:LYS:C	1:A:211:LYS:N	2.78	0.41
1:A:439:LEU:O	1:A:456:PRO:HG2	2.20	0.41
1:A:544:GLN:C	1:A:546:ASP:H	2.27	0.41
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.87	0.41
1:A:217:PHE:CZ	1:A:322:VAL:HG13	2.55	0.41
1:A:359:ASP:O	1:A:362:LEU:HB2	2.20	0.41
1:B:109:ARG:HB2	1:B:109:ARG:CZ	2.38	0.41
1:A:469:LEU:O	1:A:471:ALA:N	2.54	0.41
1:B:440:GLU:HA	4:B:2934:HOH:O	2.21	0.41
1:B:447:ILE:HD12	1:B:447:ILE:N	2.35	0.41
1:A:221:THR:HG23	4:A:1959:HOH:O	2.20	0.41
1:A:359:ASP:CB	1:A:362:LEU:HD22	2.46	0.41
1:A:430:PHE:O	1:A:434:LEU:HB2	2.21	0.41
1:B:366:CYS:C	1:B:368:SER:N	2.79	0.41
1:A:416:ALA:N	1:A:417:PRO:CD	2.83	0.41
1:B:430:PHE:O	1:B:434:LEU:HB2	2.20	0.41
1:A:385:THR:OG1	1:A:386:ARG:N	2.51	0.41
1:A:309:GLN:O	1:A:310:ASP:C	2.63	0.41
1:A:367:SER:HB2	1:A:386:ARG:NH1	2.35	0.41
1:A:372:VAL:HG22	1:A:382:TYR:CE2	2.56	0.41
1:A:36:MET:HE2	1:A:491:LYS:HG2	2.03	0.41
1:A:366:CYS:O	1:A:367:SER:CB	2.69	0.41
1:A:431:SER:HB3	1:A:507:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TRP:H	1:B:420:TRP:CD1	2.39	0.41
1:B:465:ARG:HE	1:B:546:ASP:CB	2.34	0.41
1:A:362:LEU:HD12	1:A:362:LEU:HA	1.91	0.41
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.51	0.41
1:B:465:ARG:NE	1:B:546:ASP:CB	2.84	0.41
1:A:374:HIS:HB3	1:A:378:GLY:HA2	2.03	0.40
1:B:118:HIS:HE1	4:B:2740:HOH:O	2.04	0.40
1:B:129:ASP:OD2	1:B:129:ASP:C	2.63	0.40
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.51	0.40
1:A:56:ARG:CZ	4:A:1773:HOH:O	2.65	0.40
1:A:217:PHE:CZ	1:A:322:VAL:CG1	3.04	0.40
1:A:336:LEU:HD23	1:A:354:PRO:CG	2.51	0.40
1:A:472:PHE:CE2	1:A:525:LEU:HD23	2.55	0.40
1:B:340:THR:HG23	1:B:350:PRO:HD3	2.03	0.40
1:A:85:ILE:CA	1:A:173:MET:HE3	2.50	0.40
1:A:141:LYS:HE3	1:A:158:ARG:HH22	1.81	0.40
1:A:201:VAL:O	1:A:205:VAL:HG23	2.22	0.40
1:A:212:LYS:HB2	1:A:212:LYS:NZ	2.36	0.40
1:B:6:TRP:HB3	4:B:2809:HOH:O	2.20	0.40
1:A:280:ARG:HD2	1:A:291:ASN:OD1	2.22	0.40
1:B:87:GLU:O	1:B:91:LEU:HG	2.22	0.40
1:B:556:SER:OG	1:B:557:GLY:N	2.55	0.40
1:A:509:ALA:C	1:A:511:LEU:N	2.79	0.40
1:B:508:ARG:CZ	1:B:530:VAL:HG11	2.51	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	564/570 (99%)	517 (92%)	38 (7%)	9 (2%)	7 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	563/570 (99%)	515 (92%)	37 (7%)	11 (2%)	6	12
All	All	1127/1140 (99%)	1032 (92%)	75 (7%)	20 (2%)	6	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LYS
1	A	540	PRO
1	B	469	LEU
1	B	542	ALA
1	B	549	GLY
1	B	556	SER
1	A	380	ARG
1	A	545	LEU
1	B	540	PRO
1	B	563	SER
1	A	26	LEU
1	B	151	LYS
1	A	347	SER
1	A	543	SER
1	B	149	PRO
1	B	545	LEU
1	B	548	SER
1	A	542	ALA
1	B	435	ALA
1	A	23	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	475/485 (98%)	436 (92%)	39 (8%)	10	24
1	B	474/485 (98%)	422 (89%)	52 (11%)	6	13
All	All	949/970 (98%)	858 (90%)	91 (10%)	8	17

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	18	GLU
1	A	26	LEU
1	A	31	LEU
1	A	46	SER
1	A	47	LEU
1	A	52	VAL
1	A	56	ARG
1	A	68	LEU
1	A	77	THR
1	A	83	LEU
1	A	106	LYS
1	A	109	ARG
1	A	120	ARG
1	A	126	LEU
1	A	130	THR
1	A	144	VAL
1	A	150	GLU
1	A	201	VAL
1	A	212	LYS
1	A	287	THR
1	A	310	ASP
1	A	322	VAL
1	A	330	GLN
1	A	331	GLU
1	A	336	LEU
1	A	357	GLU
1	A	362	LEU
1	A	384	LEU
1	A	386	ARG
1	A	405	ILE
1	A	425	LEU
1	A	433	LEU
1	A	434	LEU
1	A	459	LEU
1	A	469	LEU
1	A	484	ARG
1	A	514	GLN
1	A	534	LEU
1	B	5	THR
1	B	10	LEU
1	B	19	SER

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Mol	Chain	Res	Type
1	B	20	LYS
1	B	23	ILE
1	B	46	SER
1	B	47	LEU
1	B	52	VAL
1	B	55	ASP
1	B	56	ARG
1	B	77	THR
1	B	82	LEU
1	B	83	LEU
1	B	106	LYS
1	B	109	ARG
1	B	112	SER
1	B	116	VAL
1	B	126	LEU
1	B	142	SER
1	B	144	VAL
1	B	149	PRO
1	B	150	GLU
1	B	158	ARG
1	B	179	VAL
1	B	180	SER
1	B	184	GLN
1	B	221	THR
1	B	262	ILE
1	B	274	CYS
1	B	277	ARG
1	B	287	THR
1	B	297	LEU
1	B	308	LEU
1	B	310	ASP
1	B	330	GLN
1	B	331	GLU
1	B	352	ASP
1	B	364	THR
1	B	384	LEU
1	B	405	ILE
1	B	425	LEU
1	B	431	SER
1	B	434	LEU
1	B	456	PRO
1	B	459	LEU

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Mol	Chain	Res	Type
1	B	461	GLN
1	B	465	ARG
1	B	487	SER
1	B	490	ARG
1	B	531	ARG
1	B	538	PRO
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	33	HIS
1	A	35	ASN
1	A	49	GLN
1	A	63	HIS
1	A	117	ASN
1	A	194	GLN
1	A	206	ASN
1	A	272	GLN
1	A	309	GLN
1	A	316	ASN
1	A	428	HIS
1	A	446	GLN
1	A	483	ASN
1	A	514	GLN
1	A	562	HIS
1	B	24	ASN
1	B	34	HIS
1	B	35	ASN
1	B	49	GLN
1	B	148	GLN
1	B	206	ASN
1	B	273	ASN
1	B	316	ASN
1	B	355	GLN
1	B	374	HIS
1	B	461	GLN
1	B	483	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	UTP	B	2700	2	29,30,30	4.18	6 (20%)	43,47,47	1.84	8 (18%)
3	UTP	A	1700	2	29,30,30	3.04	6 (20%)	43,47,47	2.12	11 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	UTP	B	2700	2	-	7/22/38/38	0/2/2/2
3	UTP	A	1700	2	-	7/22/38/38	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2700	UTP	PA-O3A	17.56	1.78	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1700	UTP	PB-O3A	12.52	1.73	1.59
3	B	2700	UTP	PB-O3A	10.45	1.70	1.59
3	B	2700	UTP	PB-O3B	6.72	1.66	1.59
3	A	1700	UTP	PA-O3A	5.75	1.65	1.59
3	A	1700	UTP	PB-O3B	-5.43	1.53	1.59
3	A	1700	UTP	PG-O3G	4.04	1.69	1.54
3	B	2700	UTP	O3'-C3'	3.41	1.51	1.43
3	A	1700	UTP	PG-O1G	-2.30	1.46	1.54
3	A	1700	UTP	O3'-C3'	2.20	1.48	1.43
3	B	2700	UTP	C2-N1	2.12	1.41	1.38
3	B	2700	UTP	O4'-C4'	-2.02	1.40	1.45

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2700	UTP	O3A-PA-O1A	-6.70	90.56	110.70
3	A	1700	UTP	O3G-PG-O2G	-5.53	89.30	110.83
3	A	1700	UTP	O3G-PG-O3B	-4.71	88.83	104.64
3	B	2700	UTP	O2A-PA-O3A	-4.49	95.15	107.27
3	A	1700	UTP	O2A-PA-O3A	-4.44	95.27	107.27
3	A	1700	UTP	O3G-PG-O1G	-4.36	91.47	107.80
3	A	1700	UTP	O1G-PG-O2G	4.22	127.27	110.83
3	A	1700	UTP	O5'-C5'-C4'	-3.93	95.61	108.99
3	A	1700	UTP	O2A-PA-O5'	3.90	125.26	107.57
3	B	2700	UTP	O5'-PA-O1A	3.58	123.14	108.94
3	A	1700	UTP	O3A-PA-O1A	-3.25	100.92	110.70
3	B	2700	UTP	O2A-PA-O1A	3.17	127.19	112.44
3	A	1700	UTP	O1G-PG-O3B	3.04	114.83	104.64
3	A	1700	UTP	O2A-PA-O1A	2.94	126.14	112.44
3	B	2700	UTP	O3A-PB-O2B	-2.55	103.05	110.70
3	B	2700	UTP	O4'-C1'-N1	2.39	113.77	108.36
3	A	1700	UTP	C5'-C4'-C3'	-2.35	106.75	115.21
3	B	2700	UTP	O5'-C5'-C4'	-2.02	102.10	108.99
3	B	2700	UTP	N3-C2-N1	-2.00	112.29	114.89

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1700	UTP	C5'-O5'-PA-O2A
3	A	1700	UTP	O4'-C1'-N1-C2
3	A	1700	UTP	C2'-C1'-N1-C6

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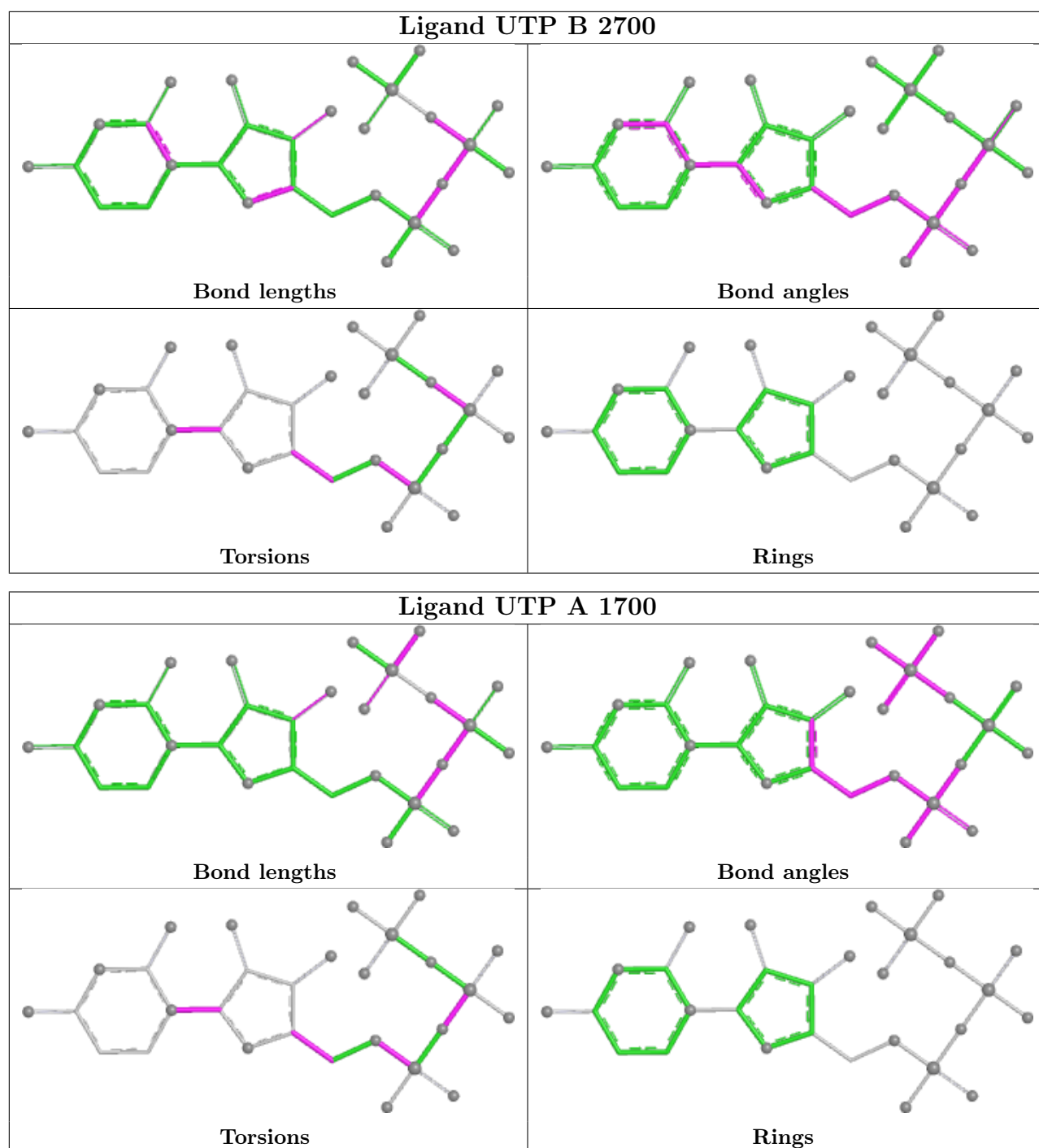
Mol	Chain	Res	Type	Atoms
3	A	1700	UTP	C2'-C1'-N1-C2
3	B	2700	UTP	C2'-C1'-N1-C6
3	B	2700	UTP	C2'-C1'-N1-C2
3	A	1700	UTP	O4'-C1'-N1-C6
3	A	1700	UTP	O4'-C4'-C5'-O5'
3	B	2700	UTP	C5'-O5'-PA-O1A
3	A	1700	UTP	PA-O3A-PB-O1B
3	B	2700	UTP	O4'-C1'-N1-C6
3	B	2700	UTP	O4'-C1'-N1-C2
3	B	2700	UTP	PG-O3B-PB-O1B
3	B	2700	UTP	O4'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2700	UTP	2	0
3	A	1700	UTP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

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.