



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 PM UTC

PDB ID : 1JST / pdb_00001jst
Title : PHOSPHORYLATED CYCLIN-DEPENDENT KINASE-2 BOUND TO CYCLIN A
Authors : Russo, A.A.; Jeffrey, P.D.; Pavletich, N.P.
Deposited on : 1996-07-03
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

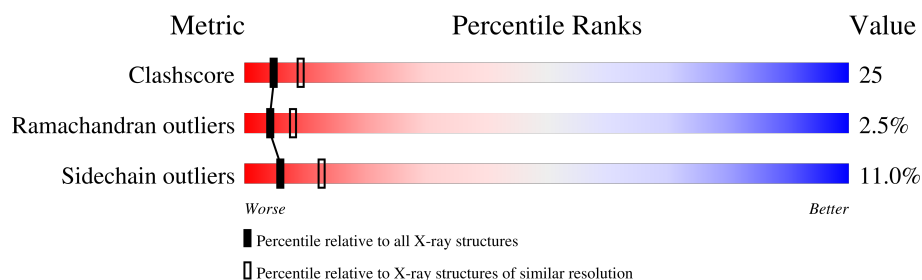
1 Overall quality at a glance

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	298	
1	C	298	
2	B	258	
2	D	258	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9134 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 CYCLIN-DEPENDENT KINASE-2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	P	S	0	0	0
			2402	1559	408	426	1	8			
1	C	298	Total	C	N	O	P	S	0	0	0
			2402	1559	408	426	1	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	TPO	THR	modified residue	UNP P24941
C	160	TPO	THR	modified residue	UNP P24941

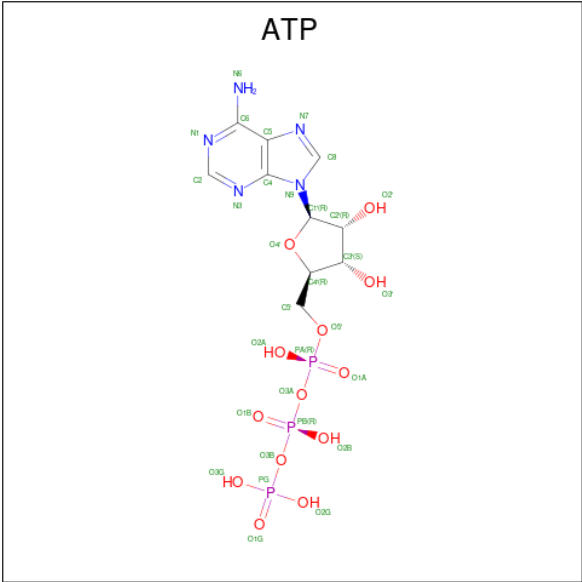
- Molecule 2 is a protein called CYCLIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			
2	D	258	Total	C	N	O	S	0	0	0
			2084	1350	339	384	11			

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

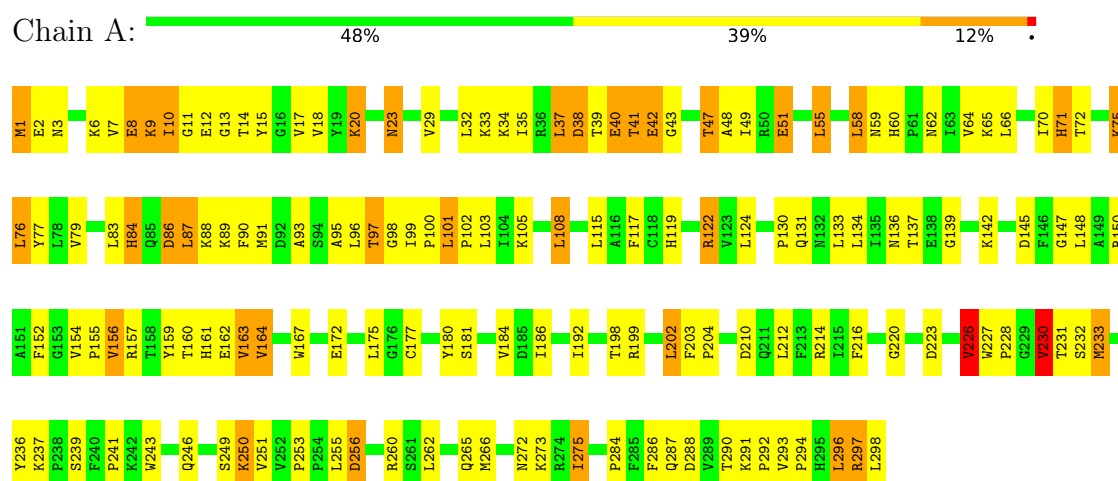
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	24	Total	O	0	0
			24	24		
5	C	20	Total	O	0	0
			20	20		
5	D	16	Total	O	0	0
			16	16		

3 Residue-property plots

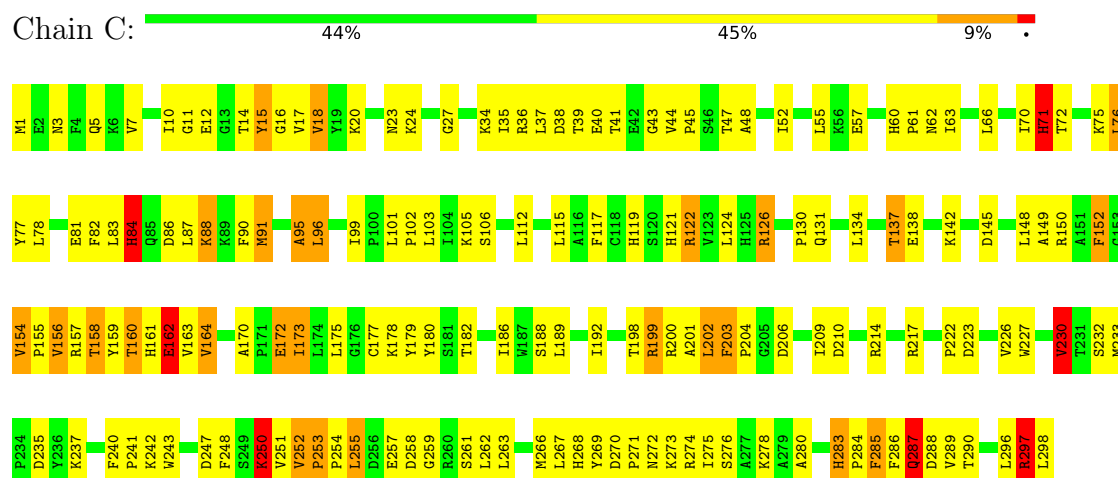
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: CYCLIN-DEPENDENT KINASE-2

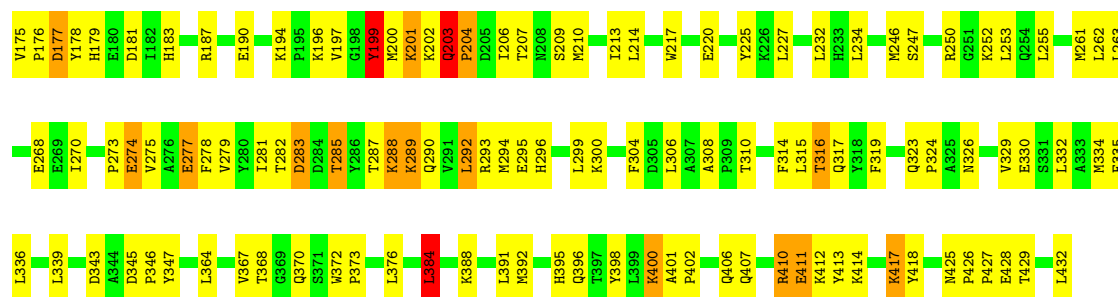


• Molecule 1: CYCLIN-DEPENDENT KINASE-2



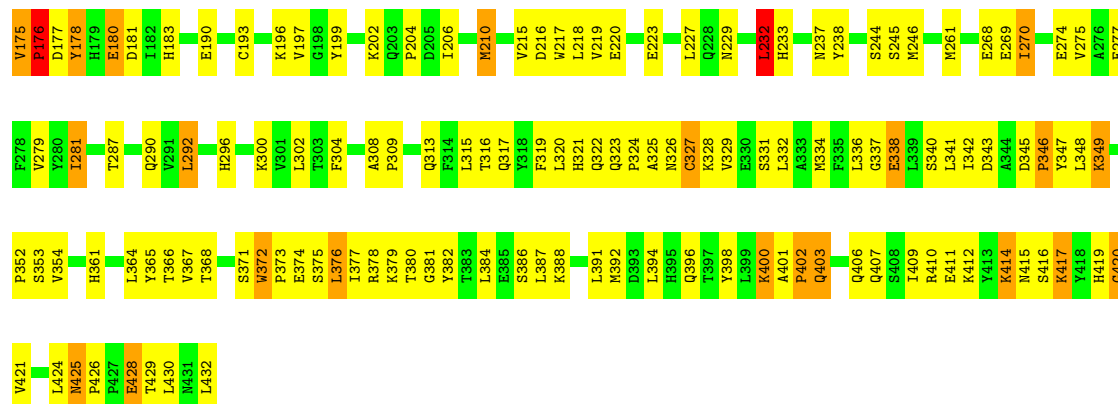
• Molecule 2: CYCLIN A





• Molecule 2: CYCLIN A

Chain D: 48% 43% 8%



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	139.60Å 149.10Å 74.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.60	Depositor
% Data completeness (in resolution range)	98.9 (7.00-2.60)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TPO, MN, ATP

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	0.91	3/2452 (0.1%)	1.22	26/3325 (0.8%)
1	C	0.74	0/2452	1.21	25/3325 (0.8%)
2	B	0.86	0/2134	1.32	19/2897 (0.7%)
2	D	0.75	1/2134 (0.0%)	1.21	24/2897 (0.8%)
All	All	0.82	4/9172 (0.0%)	1.24	94/12444 (0.8%)

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
2	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	MET	SD-CE	-7.86	1.59	1.79
2	D	210	MET	SD-CE	-6.05	1.64	1.79
1	A	233	MET	SD-CE	-5.91	1.64	1.79
1	A	226	VAL	CA-CB	5.68	1.61	1.54

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	203	GLN	CA-C-N	16.24	136.13	119.24
2	B	203	GLN	C-N-CA	16.24	136.13	119.24
1	C	17	VAL	N-CA-C	-11.46	102.20	113.20
2	D	414	LYS	N-CA-C	-10.51	99.14	112.90
2	B	345	ASP	N-CA-C	-9.45	94.67	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	425	ASN	CA-C-N	9.31	126.46	119.66
2	B	425	ASN	C-N-CA	9.31	126.46	119.66
2	B	270	ILE	N-CA-C	-8.86	102.20	110.53
1	C	84	HIS	N-CA-C	8.52	121.33	111.11
1	A	293	VAL	CA-C-N	8.07	127.83	119.76
1	A	293	VAL	C-N-CA	8.07	127.83	119.76
1	C	253	PRO	N-CA-C	7.91	120.34	110.70
1	A	84	HIS	N-CA-C	7.88	119.56	110.97
1	C	71	HIS	N-CA-C	7.83	121.36	109.62
1	A	253	PRO	N-CA-C	7.83	120.25	110.70
2	B	199	TYR	N-CA-C	7.74	120.61	111.71
2	B	282	THR	N-CA-C	-7.59	100.13	110.68
2	B	285	THR	N-CA-C	7.54	119.19	110.97
2	D	175	VAL	CA-C-N	7.50	129.22	119.84
2	D	175	VAL	C-N-CA	7.50	129.22	119.84
1	C	95	ALA	N-CA-C	-7.38	99.53	110.23
2	B	347	TYR	N-CA-C	7.23	121.93	113.18
1	C	178	LYS	N-CA-C	7.05	118.97	111.28
1	C	230	VAL	CB-CA-C	-6.88	103.07	111.88
2	D	178	TYR	N-CA-C	6.80	119.53	111.71
2	B	204	PRO	N-CA-C	6.75	124.71	113.78
1	A	40	GLU	N-CA-C	-6.67	102.44	110.44
2	D	425	ASN	CA-C-N	6.57	124.39	119.66
2	D	425	ASN	C-N-CA	6.57	124.39	119.66
1	A	230	VAL	CB-CA-C	-6.54	103.33	111.70
2	D	176	PRO	N-CA-C	6.45	125.75	112.47
2	D	372	TRP	CA-C-N	6.41	126.36	119.76
2	D	372	TRP	C-N-CA	6.41	126.36	119.76
1	C	297	ARG	N-CA-C	-6.40	97.79	109.56
2	B	343	ASP	N-CA-C	6.32	119.51	107.75
1	A	20	LYS	N-CA-C	-6.22	100.05	109.95
2	D	381	GLY	N-CA-C	-6.21	106.13	115.32
2	D	270	ILE	N-CA-C	-6.18	104.26	111.00
2	D	269	GLU	N-CA-C	6.16	119.18	110.50
2	B	414	LYS	N-CA-C	-6.15	105.61	113.23
2	B	289	LYS	N-CA-C	-6.13	104.68	111.36
1	C	66	LEU	N-CA-C	-6.09	99.28	108.96
1	A	101	LEU	CA-C-N	6.02	125.73	119.05
1	A	101	LEU	C-N-CA	6.02	125.73	119.05
1	A	51	GLU	N-CA-C	5.97	117.46	111.07
1	C	250	LYS	N-CA-C	-5.96	104.13	111.40
1	C	126	ARG	N-CA-C	5.91	120.30	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	204	PRO	N-CA-C	5.89	121.29	113.57
2	D	371	SER	N-CA-C	5.87	117.52	109.18
1	A	42	GLU	N-CA-C	5.85	119.24	111.75
2	B	181	ASP	N-CA-C	-5.84	104.99	111.36
1	A	181	SER	CB-CA-C	-5.82	106.08	114.87
2	D	268	GLU	N-CA-C	5.81	120.41	112.04
1	A	72	THR	N-CA-C	-5.79	100.62	109.41
1	C	203	PHE	CA-C-N	5.78	127.07	119.84
1	C	203	PHE	C-N-CA	5.78	127.07	119.84
1	A	86	ASP	N-CA-C	-5.75	100.76	109.85
1	C	63	ILE	N-CA-C	-5.73	99.80	108.17
2	D	386	SER	N-CA-C	-5.72	105.40	112.90
2	B	384	LEU	N-CA-C	-5.72	105.13	111.71
2	D	210	MET	N-CA-C	-5.70	105.14	111.36
2	B	268	GLU	N-CA-C	5.68	120.35	113.41
1	A	231	THR	N-CA-C	5.63	119.63	112.87
2	D	428	GLU	N-CA-C	-5.61	105.16	112.23
2	B	308	ALA	CA-C-N	5.55	125.31	119.76
2	B	308	ALA	C-N-CA	5.55	125.31	119.76
1	C	206	ASP	N-CA-C	-5.55	105.72	112.88
1	A	66	LEU	N-CA-C	-5.50	99.56	108.41
2	D	338	GLU	N-CA-C	-5.48	105.72	112.90
1	A	23	ASN	N-CA-C	-5.45	101.31	109.15
2	D	343	ASP	N-CA-C	5.44	118.12	107.57
1	C	76	LEU	CA-CB-CG	5.42	135.26	116.30
2	D	342	ILE	N-CA-C	5.41	115.62	110.53
1	C	170	ALA	CA-C-N	5.36	125.43	119.32
1	C	170	ALA	C-N-CA	5.36	125.43	119.32
1	C	210	ASP	N-CA-C	-5.36	105.35	111.14
1	C	154	VAL	N-CA-C	5.34	113.76	107.77
1	C	252	VAL	CA-C-N	5.32	125.86	120.38
1	C	252	VAL	C-N-CA	5.32	125.86	120.38
1	C	18	VAL	N-CA-C	5.29	120.35	109.34
1	A	275	ILE	N-CA-C	5.28	117.24	109.63
2	D	345	ASP	N-CA-C	-5.22	101.98	109.24
1	A	230	VAL	N-CA-CB	5.18	116.06	110.62
1	A	250	LYS	N-CA-C	-5.18	106.81	113.23
1	C	152	PHE	N-CA-C	5.18	118.18	110.52
1	A	296	LEU	N-CA-C	5.18	117.54	110.55
1	A	210	ASP	N-CA-C	-5.12	105.70	111.28
1	A	38	ASP	N-CA-C	-5.11	99.92	110.80
1	C	27	GLY	N-CA-C	-5.09	108.60	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	GLN	N-CA-C	5.06	118.29	112.57
1	A	58	LEU	CA-C-N	-5.06	116.26	122.84
1	A	58	LEU	C-N-CA	-5.06	116.26	122.84
1	A	214	ARG	N-CA-C	-5.05	105.48	111.69
2	D	232	LEU	N-CA-C	-5.01	105.71	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	347	TYR	Sidechain

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	2402	0	2449	136	0
1	C	2402	0	2449	145	0
2	B	2084	0	2107	84	0
2	D	2084	0	2107	117	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	31	0	12	8	0
4	C	31	0	12	4	0
5	A	38	0	0	1	0
5	B	24	0	0	1	0
5	C	20	0	0	0	0
5	D	16	0	0	2	0
All	All	9134	0	9136	461	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 25.

All (461) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:VAL:HA	1:A:233:MET:HE2	1.35	1.08
1:A:15:TYR:HB3	1:A:35:ILE:HG12	1.41	0.99
1:C:60:HIS:HD2	1:C:62:ASN:H	1.06	0.98
1:A:156:VAL:HG22	1:A:159:TYR:CE2	2.04	0.93
1:A:1:MET:CE	1:A:70:ILE:HG13	1.99	0.92
1:A:88:LYS:HD2	1:A:131:GLN:HG2	1.52	0.91
1:A:60:HIS:HD2	1:A:62:ASN:H	1.07	0.91
1:C:154:VAL:O	2:D:316:THR:HG22	1.73	0.87
2:D:373:PRO:HG2	2:D:376:LEU:HB2	1.57	0.87
1:A:60:HIS:CD2	1:A:62:ASN:H	1.93	0.85
1:A:38:ASP:HB3	1:A:43:GLY:H	1.43	0.83
1:C:157:ARG:HG2	1:C:158:THR:H	1.44	0.83
1:C:88:LYS:HD2	1:C:131:GLN:HB3	1.59	0.83
1:C:156:VAL:HG22	1:C:159:TYR:CE2	2.14	0.83
2:D:196:LYS:HD3	2:D:244:SER:HB3	1.60	0.83
2:D:346:PRO:O	2:D:349:LYS:HG3	1.80	0.82
2:D:197:VAL:HG11	2:D:349:LYS:HB3	1.59	0.82
1:C:88:LYS:HZ2	1:C:131:GLN:H	1.24	0.81
1:A:87:LEU:HD13	1:A:91:MET:HE2	1.64	0.81
1:C:202:LEU:HD13	1:C:203:PHE:CE2	2.16	0.81
2:B:407:GLN:O	2:B:411:GLU:HG2	1.80	0.80
1:C:156:VAL:HG22	1:C:159:TYR:HE2	1.47	0.80
1:C:286:PHE:O	1:C:289:VAL:HG23	1.81	0.79
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.63	0.79
1:A:177:CYS:SG	1:A:233:MET:SD	2.81	0.78
2:D:319:PHE:CE2	2:D:334:MET:HE3	2.19	0.78
1:C:60:HIS:HD2	1:C:62:ASN:N	1.81	0.77
1:A:60:HIS:HD2	1:A:62:ASN:N	1.81	0.77
1:C:172:GLU:HB3	1:C:177:CYS:SG	2.25	0.77
1:A:1:MET:HE1	1:A:70:ILE:HG13	1.64	0.77
1:C:83:LEU:HD11	1:C:142:LYS:HD2	1.66	0.76
2:B:289:LYS:O	2:B:293:ARG:HG3	1.86	0.76
1:C:84:HIS:CE1	1:C:298:LEU:HB3	2.20	0.76
1:C:84:HIS:HB3	1:C:298:LEU:HG	1.68	0.75
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.50	0.75
2:D:396:GLN:NE2	2:D:400:LYS:HE3	2.02	0.75
1:C:119:HIS:CD2	1:C:182:THR:HB	2.21	0.75
1:C:200:ARG:HD2	1:C:201:ALA:H	1.50	0.75
1:A:51:GLU:O	1:A:55:LEU:HB2	1.86	0.74
2:D:216:ASP:HB2	2:D:406:GLN:HG3	1.70	0.73
1:A:88:LYS:CD	1:A:131:GLN:HG2	2.17	0.73
1:C:201:ALA:HB3	1:C:204:PRO:HG3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:VAL:HG22	1:A:159:TYR:HE2	1.53	0.73
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.23	0.73
2:B:336:LEU:HD23	2:B:339:LEU:HD12	1.71	0.73
1:C:162:GLU:HG3	1:C:173:ILE:HG22	1.71	0.73
1:A:262:LEU:HG	1:A:266:MET:HE2	1.72	0.71
1:A:10:ILE:HG22	4:A:300:ATP:H1'	1.73	0.71
1:C:160:TPO:O1P	2:D:270:ILE:HA	1.90	0.71
1:C:227:TRP:CZ2	1:C:233:MET:HE1	2.26	0.71
1:C:60:HIS:CD2	1:C:62:ASN:H	1.99	0.71
2:B:209:SER:O	2:B:213:ILE:HG12	1.91	0.70
1:C:268:HIS:HD2	1:C:270:ASP:N	1.87	0.70
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.72	0.70
2:B:288:LYS:HD3	2:B:292:LEU:HD22	1.73	0.70
2:D:287:THR:OG1	2:D:290:GLN:HG3	1.92	0.70
1:A:35:ILE:HG22	1:A:37:LEU:H	1.57	0.69
1:A:108:LEU:HD13	1:A:286:PHE:HZ	1.58	0.69
1:A:202:LEU:HD13	1:A:203:PHE:CE2	2.28	0.69
1:A:227:TRP:O	1:A:230:VAL:HG22	1.92	0.69
1:C:115:LEU:HD22	1:C:189:LEU:HD22	1.75	0.69
1:C:240:PHE:HB2	1:C:242:LYS:HZ3	1.58	0.68
1:A:91:MET:HG2	1:A:99:ILE:HD11	1.75	0.68
1:C:296:LEU:HD13	1:C:298:LEU:HD23	1.76	0.68
2:B:274:GLU:HG3	2:B:277:GLU:HG2	1.75	0.67
1:C:1:MET:HE1	1:C:70:ILE:HG13	1.75	0.67
1:A:38:ASP:CG	1:A:41:THR:HB	2.20	0.66
2:D:417:LYS:NZ	2:D:417:LYS:HB3	2.10	0.66
2:B:213:ILE:HD13	2:B:406:GLN:NE2	2.12	0.65
2:D:274:GLU:HG2	2:D:277:GLU:HG2	1.79	0.65
1:A:7:VAL:O	1:A:8:GLU:HB2	1.95	0.65
1:A:87:LEU:HB3	1:A:130:PRO:HB3	1.79	0.65
1:C:38:ASP:HB2	1:C:43:GLY:H	1.62	0.65
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.78	0.65
2:D:372:TRP:CD1	2:D:377:ILE:HG12	2.32	0.64
1:C:283:HIS:CE1	1:C:284:PRO:HG2	2.33	0.64
1:C:1:MET:HE3	1:C:70:ILE:HG21	1.79	0.64
1:C:15:TYR:HD1	1:C:15:TYR:H	1.44	0.64
1:C:91:MET:HE1	1:C:130:PRO:CG	2.28	0.64
1:C:84:HIS:ND1	1:C:137:THR:HG23	2.13	0.63
2:D:175:VAL:HB	2:D:176:PRO:CD	2.29	0.63
2:D:227:LEU:HD12	2:D:261:MET:HE3	1.79	0.63
1:A:88:LYS:HE3	1:A:131:GLN:N	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:THR:HG22	1:A:147:GLY:O	1.98	0.63
2:D:388:LYS:HG3	2:D:432:LEU:HD12	1.81	0.62
2:D:366:THR:HG21	2:D:398:TYR:OH	1.99	0.62
2:B:202:LYS:HD2	2:B:202:LYS:H	1.63	0.62
2:B:263:LEU:HD21	2:B:295:GLU:HG3	1.81	0.62
2:D:216:ASP:CB	2:D:406:GLN:HG3	2.29	0.62
1:A:88:LYS:CE	1:A:131:GLN:HG2	2.30	0.62
1:C:81:GLU:O	1:C:81:GLU:HG3	1.98	0.62
2:D:417:LYS:HB3	2:D:417:LYS:HZ2	1.66	0.61
2:D:319:PHE:HE2	2:D:334:MET:HE3	1.63	0.61
1:A:99:ILE:HG23	1:A:103:LEU:HD23	1.82	0.61
2:B:202:LYS:HD2	2:B:202:LYS:N	2.15	0.61
2:D:396:GLN:HE21	2:D:400:LYS:HE3	1.66	0.61
1:C:83:LEU:HD11	1:C:142:LYS:CD	2.31	0.60
2:B:202:LYS:O	2:B:204:PRO:HD3	2.02	0.60
1:C:88:LYS:HZ2	1:C:131:GLN:N	1.99	0.60
1:A:58:LEU:HA	1:A:117:PHE:HE2	1.66	0.60
1:A:296:LEU:C	1:A:297:ARG:HD3	2.27	0.60
1:A:64:VAL:HG22	1:A:83:LEU:CD1	2.31	0.60
1:C:84:HIS:ND1	1:C:298:LEU:HB3	2.16	0.60
1:A:71:HIS:HB3	2:B:300:LYS:HE3	1.84	0.59
1:C:160:TPO:HA	2:D:270:ILE:HD13	1.84	0.59
1:C:38:ASP:HB3	1:C:41:THR:OG1	2.02	0.59
2:B:203:GLN:HG2	2:B:206:ILE:HG12	1.83	0.59
2:B:373:PRO:CG	2:B:376:LEU:HD12	2.32	0.59
2:D:377:ILE:HG23	2:D:382:TYR:O	2.02	0.59
2:B:207:THR:OG1	2:B:210:MET:HG3	2.03	0.59
2:D:396:GLN:O	2:D:400:LYS:HD3	2.02	0.59
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.68	0.59
2:B:210:MET:HE1	2:B:250:ARG:CB	2.33	0.59
1:C:240:PHE:HB2	1:C:242:LYS:NZ	2.17	0.59
1:C:160:TPO:OG1	2:D:270:ILE:HG23	2.02	0.59
1:C:1:MET:CE	1:C:70:ILE:HG13	2.32	0.58
1:C:198:THR:O	1:C:199:ARG:HG2	2.04	0.58
1:C:296:LEU:HD13	1:C:298:LEU:CD2	2.34	0.58
1:A:83:LEU:HD23	1:A:136:ASN:HB3	1.85	0.58
1:A:145:ASP:HB2	4:A:300:ATP:O2A	2.04	0.58
2:B:288:LYS:HD3	2:B:292:LEU:CD2	2.32	0.58
1:A:265:GLN:NE2	1:A:275:ILE:HD12	2.19	0.58
2:D:217:TRP:CE3	2:D:218:LEU:HD23	2.39	0.58
1:A:83:LEU:CD2	1:A:136:ASN:HB3	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:388:LYS:O	2:B:392:MET:HG2	2.03	0.58
1:C:247:ASP:HB3	1:C:250:LYS:HG2	1.85	0.57
1:A:93:ALA:HB3	1:A:297:ARG:NH2	2.18	0.57
2:B:176:PRO:HA	2:B:179:HIS:CE1	2.39	0.57
1:C:91:MET:HE1	1:C:130:PRO:HG2	1.85	0.57
1:A:297:ARG:N	1:A:297:ARG:HH11	2.02	0.57
2:B:275:VAL:O	2:B:279:VAL:HG23	2.04	0.57
2:B:392:MET:HE2	2:B:392:MET:HA	1.86	0.57
2:D:402:PRO:HG3	2:D:410:ARG:HH12	1.69	0.57
2:B:417:LYS:HE2	2:B:418:TYR:CZ	2.39	0.57
2:B:203:GLN:OE1	2:B:247:SER:HA	2.04	0.57
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.34	0.57
2:B:201:LYS:HD3	2:B:202:LYS:HE3	1.87	0.56
1:A:32:LEU:HD23	1:A:79:VAL:HG22	1.87	0.56
2:D:322:GLN:HG3	2:D:325:ALA:HA	1.86	0.56
1:A:88:LYS:HD2	1:A:131:GLN:CG	2.31	0.56
1:A:297:ARG:HH11	1:A:297:ARG:H	1.54	0.56
1:C:237:LYS:HB2	1:C:240:PHE:CE1	2.41	0.56
1:A:9:LYS:HZ2	1:A:17:VAL:HB	1.71	0.56
1:A:11:GLY:HA3	4:A:300:ATP:O4'	2.05	0.56
2:D:190:GLU:OE1	2:D:352:PRO:HD2	2.06	0.56
1:A:122:ARG:HD2	1:A:122:ARG:O	2.06	0.56
1:C:200:ARG:HD2	1:C:201:ALA:N	2.19	0.56
1:A:10:ILE:HB	1:A:18:VAL:HG12	1.87	0.55
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.88	0.55
2:B:225:TYR:CE2	2:B:277:GLU:HB3	2.41	0.55
1:C:105:LYS:HG3	1:C:285:PHE:CZ	2.41	0.55
1:A:8:GLU:HG2	1:A:9:LYS:H	1.72	0.55
2:B:175:VAL:O	2:B:175:VAL:HG12	2.07	0.55
2:B:278:PHE:O	2:B:281:ILE:HG13	2.06	0.55
1:C:101:LEU:N	1:C:102:PRO:HD2	2.22	0.55
1:A:71:HIS:CD2	2:B:300:LYS:HG3	2.42	0.54
1:C:222:PRO:HD3	1:C:269:TYR:CZ	2.42	0.54
1:C:223:ASP:H	1:C:226:VAL:HG12	1.72	0.54
1:A:9:LYS:NZ	1:A:17:VAL:HB	2.23	0.54
1:A:98:GLY:O	1:A:100:PRO:HD3	2.06	0.54
2:D:332:LEU:O	2:D:336:LEU:HG	2.07	0.54
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.43	0.54
1:C:296:LEU:HD13	1:C:298:LEU:CG	2.37	0.54
1:A:90:PHE:HA	1:A:297:ARG:HH22	1.72	0.54
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:HD3	1:A:297:ARG:N	2.22	0.54
1:C:90:PHE:HD1	1:C:297:ARG:NH2	2.06	0.54
2:D:199:TYR:HE2	2:D:348:LEU:HD21	1.72	0.54
2:B:225:TYR:HE1	2:B:281:ILE:HG21	1.72	0.54
2:D:275:VAL:O	2:D:279:VAL:HG23	2.07	0.54
2:D:277:GLU:O	2:D:281:ILE:HG12	2.08	0.54
1:C:198:THR:C	1:C:199:ARG:HG2	2.33	0.54
2:B:373:PRO:HG2	2:B:376:LEU:HD12	1.88	0.53
2:B:364:LEU:HG	2:B:370:GLN:HB2	1.89	0.53
1:C:268:HIS:CD2	1:C:270:ASP:H	2.26	0.53
1:A:15:TYR:OH	1:A:47:THR:HB	2.08	0.53
1:A:13:GLY:HA3	4:A:300:ATP:PB	2.48	0.53
1:A:249:SER:HA	1:A:260:ARG:HD3	1.90	0.53
1:A:256:ASP:O	1:A:260:ARG:HG3	2.08	0.53
1:C:296:LEU:HD13	1:C:298:LEU:HG	1.91	0.53
2:D:327:CYS:SG	2:D:419:HIS:CE1	3.02	0.53
2:D:219:VAL:HG22	2:D:232:LEU:HD11	1.89	0.52
1:C:38:ASP:HB2	1:C:43:GLY:N	2.24	0.52
1:A:15:TYR:CE1	1:A:48:ALA:HB2	2.45	0.52
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.40	0.52
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.91	0.52
2:D:367:VAL:HG12	2:D:368:THR:HG23	1.91	0.52
1:C:296:LEU:HD22	1:C:298:LEU:HD23	1.92	0.52
1:A:12:GLU:HG2	1:A:17:VAL:HA	1.92	0.52
2:B:395:HIS:HE1	2:B:427:PRO:O	1.93	0.51
1:C:86:ASP:HA	1:C:134:LEU:HA	1.93	0.51
2:D:175:VAL:N	2:D:176:PRO:HD2	2.25	0.51
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.45	0.51
2:D:196:LYS:HD3	2:D:196:LYS:H	1.74	0.51
2:D:319:PHE:O	2:D:322:GLN:HG2	2.11	0.51
2:D:372:TRP:HB3	2:D:384:LEU:HD22	1.92	0.51
1:A:154:VAL:O	2:B:316:THR:HG22	2.10	0.51
1:A:175:LEU:CD1	1:A:233:MET:HE3	2.41	0.51
1:C:162:GLU:HA	1:C:173:ILE:CG2	2.41	0.51
1:C:227:TRP:O	1:C:230:VAL:HG23	2.10	0.51
1:A:1:MET:O	1:A:1:MET:HG3	2.12	0.50
2:D:321:HIS:CE1	2:D:379:LYS:HD2	2.45	0.50
2:D:417:LYS:O	2:D:417:LYS:HG2	2.12	0.50
2:B:388:LYS:HG2	2:B:432:LEU:HD13	1.93	0.50
2:B:395:HIS:CE1	2:B:427:PRO:O	2.65	0.50
2:B:398:TYR:CD2	2:B:426:PRO:HB3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PRO:O	1:C:285:PHE:C	2.53	0.50
2:D:337:GLY:O	2:D:340:SER:OG	2.29	0.50
1:C:105:LYS:HG3	1:C:285:PHE:CE2	2.46	0.50
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.47	0.50
1:C:15:TYR:HE1	4:C:300:ATP:O3B	1.95	0.50
1:C:268:HIS:HD2	1:C:270:ASP:H	1.54	0.50
1:A:9:LYS:HZ3	1:A:12:GLU:HB2	1.76	0.49
1:C:16:GLY:HA3	4:C:300:ATP:O2B	2.11	0.49
2:D:354:VAL:HG13	2:D:387:LEU:HD23	1.92	0.49
1:A:175:LEU:HD13	1:A:233:MET:HE3	1.92	0.49
1:A:296:LEU:HA	1:A:297:ARG:HH11	1.77	0.49
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.93	0.49
1:C:214:ARG:NH1	1:C:214:ARG:HG2	2.27	0.49
1:C:262:LEU:O	1:C:266:MET:HG3	2.12	0.49
1:A:10:ILE:CG2	4:A:300:ATP:H1'	2.41	0.49
1:A:15:TYR:CD1	1:A:48:ALA:HB2	2.47	0.49
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.92	0.49
1:A:93:ALA:HB3	1:A:297:ARG:HH21	1.77	0.49
1:A:64:VAL:HG22	1:A:83:LEU:HD12	1.93	0.49
2:D:196:LYS:HB2	2:D:199:TYR:HB3	1.94	0.49
2:D:196:LYS:H	2:D:196:LYS:CD	2.26	0.49
2:D:365:TYR:HE2	2:D:430:LEU:HA	1.77	0.49
2:B:199:TYR:CD1	2:B:199:TYR:C	2.91	0.49
1:A:119:HIS:HD2	5:A:326:HOH:O	1.94	0.49
1:A:246:GLN:NE2	1:A:251:VAL:HG22	2.28	0.49
1:A:290:THR:OG1	1:A:292:PRO:HD3	2.13	0.49
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.95	0.49
2:D:326:ASN:OD1	2:D:328:LYS:HB2	2.13	0.49
1:A:6:LYS:HE2	1:A:32:LEU:HD13	1.95	0.48
1:A:157:ARG:HB3	1:A:159:TYR:CE1	2.48	0.48
1:A:223:ASP:H	1:A:226:VAL:HG13	1.78	0.48
2:D:199:TYR:HA	2:D:202:LYS:HE2	1.96	0.48
1:A:1:MET:HA	1:A:1:MET:HE2	1.94	0.48
1:C:95:ALA:O	1:C:96:LEU:HB2	2.13	0.48
1:C:112:LEU:HD22	1:C:280:ALA:HB3	1.95	0.48
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.96	0.48
2:D:183:HIS:HB2	2:D:317:GLN:HE22	1.78	0.48
2:B:332:LEU:O	2:B:335:PHE:HB3	2.14	0.48
1:A:75:LYS:HD2	1:A:77:TYR:OH	2.14	0.48
2:D:206:ILE:HG22	2:D:210:MET:HE1	1.96	0.48
2:D:365:TYR:CD1	2:D:365:TYR:C	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.96	0.48
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.48	0.48
1:C:91:MET:HE1	1:C:130:PRO:CB	2.44	0.48
2:B:187:ARG:O	2:B:190:GLU:HG2	2.14	0.47
1:A:11:GLY:HA3	4:A:300:ATP:C4'	2.43	0.47
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.96	0.47
2:B:274:GLU:HG3	2:B:277:GLU:CG	2.41	0.47
1:C:35:ILE:HD13	1:C:48:ALA:HB2	1.97	0.47
1:C:252:VAL:HG11	1:C:255:LEU:HD22	1.96	0.47
2:D:331:SER:HB2	2:D:421:VAL:HG11	1.97	0.47
2:D:373:PRO:O	2:D:377:ILE:HG13	2.15	0.47
1:A:38:ASP:OD2	1:A:42:GLU:HB3	2.14	0.47
1:A:108:LEU:HD13	1:A:286:PHE:CZ	2.43	0.47
1:A:156:VAL:CG2	1:A:159:TYR:HE2	2.26	0.47
1:C:119:HIS:NE2	1:C:182:THR:HB	2.30	0.47
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.47
1:C:154:VAL:C	2:D:316:THR:HG22	2.38	0.47
2:D:407:GLN:O	2:D:411:GLU:HG2	2.15	0.47
1:C:263:LEU:HG	1:C:267:LEU:HD12	1.97	0.47
1:C:1:MET:HE2	1:C:1:MET:HA	1.97	0.46
1:C:163:VAL:HG23	1:C:164:VAL:HG23	1.97	0.46
2:D:388:LYS:O	2:D:392:MET:HG2	2.16	0.46
1:A:71:HIS:ND1	2:B:296:HIS:HE1	2.13	0.46
1:C:257:GLU:HG3	1:C:258:ASP:N	2.31	0.46
2:B:323:GLN:HA	2:B:324:PRO:HA	1.63	0.46
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.98	0.46
2:D:202:LYS:HB2	2:D:202:LYS:HE3	1.71	0.46
1:A:35:ILE:HD12	1:A:76:LEU:HD13	1.97	0.46
2:B:373:PRO:HG2	2:B:376:LEU:HB2	1.96	0.46
2:B:396:GLN:HE21	2:B:400:LYS:HE3	1.80	0.46
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.84	0.46
2:D:238:TYR:HB3	2:D:302:LEU:HD11	1.98	0.46
2:D:387:LEU:O	2:D:391:LEU:HB2	2.16	0.46
1:A:83:LEU:HD11	1:A:142:LYS:HD2	1.98	0.46
1:C:88:LYS:NZ	1:C:131:GLN:H	2.04	0.46
1:C:71:HIS:NE2	2:D:304:PHE:HE2	2.13	0.46
1:C:84:HIS:CB	1:C:298:LEU:HG	2.42	0.46
2:D:315:LEU:HD13	2:D:334:MET:HE2	1.98	0.46
2:D:329:VAL:HG22	2:D:367:VAL:HB	1.98	0.46
1:A:34:LYS:NZ	1:A:75:LYS:HD3	2.31	0.45
1:A:83:LEU:O	4:A:300:ATP:H2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LYS:CD	2:D:177:ASP:HB3	2.46	0.45
2:D:216:ASP:HB2	2:D:406:GLN:CG	2.44	0.45
1:A:89:LYS:HA	1:A:89:LYS:HD3	1.72	0.45
1:C:156:VAL:CG2	1:C:159:TYR:HE2	2.25	0.45
1:C:288:ASP:OD1	1:C:288:ASP:N	2.50	0.45
2:D:412:LYS:O	2:D:415:ASN:HB3	2.16	0.45
2:B:203:GLN:HG2	2:B:206:ILE:CG1	2.46	0.45
1:A:284:PRO:O	1:A:287:GLN:HG2	2.17	0.45
1:C:34:LYS:HZ1	1:C:36:ARG:HH21	1.63	0.45
2:D:233:HIS:CD2	2:D:341:LEU:HD21	2.51	0.45
2:D:246:MET:HE3	2:D:246:MET:HB3	1.73	0.45
2:D:321:HIS:N	2:D:321:HIS:CD2	2.84	0.45
1:A:227:TRP:HB3	1:A:230:VAL:HG22	1.99	0.45
1:C:91:MET:CE	1:C:130:PRO:HB3	2.46	0.45
1:C:272:ASN:HD22	1:C:273:LYS:NZ	2.14	0.45
1:A:291:LYS:N	1:A:292:PRO:HD3	2.32	0.45
2:B:412:LYS:HE2	2:B:413:TYR:CE1	2.51	0.45
1:C:15:TYR:HE1	4:C:300:ATP:PG	2.40	0.45
1:C:86:ASP:OD2	1:C:88:LYS:HB3	2.17	0.45
1:C:157:ARG:HG2	1:C:158:THR:N	2.23	0.45
1:C:270:ASP:HA	1:C:271:PRO:HD2	1.84	0.45
2:D:327:CYS:SG	2:D:419:HIS:NE2	2.89	0.45
1:C:157:ARG:O	1:C:179:TYR:CD1	2.70	0.45
1:C:241:PRO:HB2	1:C:243:TRP:CZ2	2.51	0.45
2:D:223:GLU:CD	2:D:412:LYS:HB2	2.41	0.45
1:A:13:GLY:HA3	4:A:300:ATP:O1B	2.17	0.44
2:D:315:LEU:HD23	2:D:315:LEU:HA	1.72	0.44
2:D:180:GLU:O	2:D:181:ASP:C	2.60	0.44
1:C:124:LEU:O	1:C:149:ALA:HA	2.18	0.44
1:C:161:HIS:O	1:C:162:GLU:C	2.61	0.44
1:A:3:ASN:O	1:A:23:ASN:HA	2.17	0.44
1:C:287:GLN:HG2	1:C:288:ASP:OD1	2.17	0.44
2:D:229:ASN:ND2	2:D:338:GLU:OE1	2.50	0.44
2:D:414:LYS:HA	2:D:420:GLY:HA2	1.99	0.44
2:B:217:TRP:O	2:B:220:GLU:HB2	2.18	0.44
2:B:368:THR:C	2:B:370:GLN:H	2.25	0.44
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.76	0.44
1:C:105:LYS:NZ	1:C:285:PHE:O	2.50	0.44
2:D:275:VAL:HG21	2:D:292:LEU:HD11	1.99	0.44
2:B:201:LYS:HD3	2:B:202:LYS:CE	2.47	0.44
1:C:172:GLU:CB	1:C:177:CYS:SG	3.03	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:LEU:HA	1:C:235:ASP:HB2	2.00	0.44
1:C:278:LYS:HD3	2:D:177:ASP:HB3	2.00	0.44
1:A:89:LYS:NZ	1:A:131:GLN:OE1	2.51	0.44
1:C:95:ALA:O	1:C:96:LEU:CB	2.66	0.44
2:D:199:TYR:CE2	2:D:348:LEU:HD21	2.50	0.44
2:B:293:ARG:HD2	1:C:24:LYS:NZ	2.33	0.44
1:C:268:HIS:CD2	1:C:270:ASP:N	2.75	0.44
2:D:419:HIS:O	2:D:421:VAL:N	2.50	0.44
1:A:108:LEU:HD23	1:A:108:LEU:HA	1.76	0.43
2:B:329:VAL:HG22	2:B:367:VAL:HB	2.00	0.43
2:B:372:TRP:HB3	2:B:384:LEU:HD13	2.00	0.43
1:A:1:MET:HE3	1:A:70:ILE:HG13	1.93	0.43
1:A:20:LYS:HE3	1:A:29:VAL:HG11	2.00	0.43
1:A:84:HIS:ND1	1:A:84:HIS:N	2.66	0.43
1:A:212:LEU:HA	1:A:212:LEU:HD23	1.82	0.43
1:A:272:ASN:C	1:A:273:LYS:HD3	2.43	0.43
2:D:237:ASN:ND2	2:D:308:ALA:HB1	2.34	0.43
1:A:8:GLU:HG2	1:A:9:LYS:N	2.33	0.43
1:C:126:ARG:NH1	1:C:180:TYR:OH	2.50	0.43
2:B:262:LEU:HD13	2:B:278:PHE:CD2	2.53	0.43
1:A:97:THR:HG22	1:A:98:GLY:O	2.19	0.43
1:C:60:HIS:CD2	1:C:61:PRO:N	2.87	0.43
1:A:38:ASP:HB3	1:A:43:GLY:N	2.22	0.43
1:A:9:LYS:HZ2	1:A:18:VAL:H	1.66	0.43
1:A:9:LYS:NZ	1:A:12:GLU:HB2	2.33	0.43
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.54	0.43
2:B:183:HIS:CE1	5:B:28:HOH:O	2.71	0.43
2:B:246:MET:HE3	2:B:246:MET:HB3	1.95	0.43
2:B:372:TRP:CB	2:B:384:LEU:HD13	2.48	0.43
1:A:64:VAL:HG21	1:A:134:LEU:HD12	2.01	0.43
1:A:65:LYS:HE2	1:A:65:LYS:HB3	1.91	0.43
2:B:417:LYS:HE2	2:B:418:TYR:CE2	2.54	0.43
1:C:198:THR:HG23	1:C:252:VAL:HG13	2.00	0.43
1:C:214:ARG:HG2	1:C:214:ARG:HH11	1.83	0.43
1:A:34:LYS:HZ2	1:A:75:LYS:HD3	1.83	0.43
1:A:139:GLY:HA2	1:A:294:PRO:HD2	2.00	0.43
2:B:315:LEU:HD23	2:B:315:LEU:HA	1.75	0.43
1:A:105:LYS:HE3	1:A:105:LYS:HB2	1.86	0.42
1:A:186:ILE:HD12	1:A:186:ILE:HG23	1.73	0.42
1:A:216:PHE:O	1:A:220:GLY:N	2.51	0.42
2:B:255:LEU:HD23	2:B:294:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:410:ARG:HH11	2:B:410:ARG:HG2	1.84	0.42
1:C:155:PRO:HD3	2:D:320:LEU:HD21	2.00	0.42
1:A:42:GLU:O	1:A:42:GLU:HG2	2.18	0.42
1:C:48:ALA:O	1:C:52:ILE:HG13	2.19	0.42
2:D:375:SER:HA	2:D:378:ARG:NH2	2.35	0.42
1:A:18:VAL:HG22	1:A:33:LYS:HG3	2.01	0.42
1:C:186:ILE:HD13	1:C:186:ILE:HA	1.95	0.42
2:D:309:PRO:HA	2:D:313:GLN:NE2	2.34	0.42
1:A:95:ALA:O	1:A:97:THR:N	2.52	0.42
2:D:402:PRO:HB2	2:D:403:GLN:OE1	2.20	0.42
1:A:1:MET:HE3	1:A:70:ILE:HG21	2.00	0.42
1:A:163:VAL:O	1:A:164:VAL:HB	2.19	0.42
2:B:417:LYS:HE2	2:B:418:TYR:OH	2.19	0.42
1:C:101:LEU:O	1:C:101:LEU:HG	2.15	0.42
1:C:126:ARG:HD2	1:C:163:VAL:HG21	2.01	0.42
1:C:209:ILE:HD12	1:C:209:ILE:HA	1.86	0.42
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.48	0.42
1:A:133:LEU:HD11	1:A:192:ILE:HD13	2.00	0.42
1:A:227:TRP:CE3	1:A:230:VAL:HG13	2.53	0.42
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.54	0.42
1:A:175:LEU:HD23	1:A:175:LEU:HA	1.82	0.42
1:C:44:VAL:HA	1:C:45:PRO:HD3	1.86	0.42
2:D:402:PRO:HA	2:D:410:ARG:CZ	2.50	0.42
1:A:297:ARG:H	1:A:297:ARG:NH1	2.17	0.42
2:B:194:LYS:HE3	2:B:197:VAL:CG2	2.49	0.42
1:C:3:ASN:O	1:C:23:ASN:HA	2.20	0.42
1:C:289:VAL:HG12	1:C:290:THR:N	2.35	0.42
1:C:55:LEU:C	1:C:57:GLU:H	2.28	0.42
1:C:227:TRP:O	1:C:230:VAL:CG2	2.68	0.42
1:A:236:TYR:C	1:A:237:LYS:HD3	2.45	0.41
1:C:188:SER:O	1:C:192:ILE:HG13	2.20	0.41
2:D:424:LEU:HB2	5:D:99:HOH:O	2.20	0.41
1:A:10:ILE:HG22	1:A:11:GLY:N	2.34	0.41
2:B:176:PRO:O	2:B:178:TYR:N	2.53	0.41
2:B:426:PRO:HA	2:B:427:PRO:HD3	1.89	0.41
2:D:215:VAL:O	2:D:219:VAL:HG23	2.19	0.41
1:A:124:LEU:HG	1:A:152:PHE:CD1	2.55	0.41
2:B:252:LYS:HD3	2:B:252:LYS:HA	1.66	0.41
2:B:287:THR:OG1	2:B:290:GLN:HB2	2.21	0.41
2:B:326:ASN:O	2:B:330:GLU:HG3	2.20	0.41
1:C:7:VAL:HB	1:C:20:LYS:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:196:LYS:O	2:D:199:TYR:HD2	2.04	0.41
2:D:327:CYS:HG	2:D:419:HIS:CE1	2.38	0.41
2:D:338:GLU:HG2	2:D:409:ILE:HD13	2.01	0.41
1:C:90:PHE:CE2	1:C:99:ILE:HG12	2.55	0.41
2:D:328:LYS:HB2	2:D:328:LYS:HE3	1.89	0.41
2:D:332:LEU:HD22	2:D:424:LEU:HD12	2.02	0.41
1:A:71:HIS:CE1	2:B:296:HIS:CE1	3.08	0.41
2:B:197:VAL:O	2:B:197:VAL:HG12	2.21	0.41
1:C:84:HIS:CG	1:C:298:LEU:HG	2.55	0.41
2:D:178:TYR:HA	2:D:181:ASP:OD1	2.20	0.41
2:D:365:TYR:C	2:D:365:TYR:HD1	2.28	0.41
2:D:380:THR:HB	2:D:382:TYR:CD2	2.55	0.41
2:B:234:LEU:HD23	2:B:310:THR:CG2	2.50	0.41
2:B:292:LEU:HD12	2:B:292:LEU:HA	1.79	0.41
2:D:364:LEU:HD12	2:D:368:THR:OG1	2.20	0.41
2:D:394:LEU:HD12	2:D:394:LEU:HA	1.63	0.41
1:A:71:HIS:CE1	2:B:296:HIS:HE1	2.39	0.41
2:B:314:PHE:O	2:B:315:LEU:C	2.60	0.41
1:C:57:GLU:OE1	1:C:122:ARG:NH2	2.54	0.41
1:C:103:LEU:O	1:C:106:SER:HB3	2.21	0.41
2:D:217:TRP:O	2:D:220:GLU:HB3	2.20	0.41
2:D:425:ASN:HA	2:D:426:PRO:HD2	1.91	0.41
1:C:286:PHE:O	1:C:288:ASP:N	2.54	0.41
2:D:206:ILE:HA	2:D:210:MET:CE	2.50	0.41
2:B:299:LEU:HD13	2:B:304:PHE:CZ	2.56	0.40
2:B:376:LEU:HD23	2:B:376:LEU:HA	1.73	0.40
1:C:15:TYR:CD1	1:C:15:TYR:N	2.87	0.40
1:C:82:PHE:CD2	1:C:82:PHE:C	2.99	0.40
1:C:258:ASP:O	1:C:261:SER:HB3	2.21	0.40
2:D:407:GLN:HA	5:D:98:HOH:O	2.20	0.40
1:A:180:TYR:HB2	1:A:184:VAL:HG11	2.03	0.40
1:C:117:PHE:CZ	1:C:121:HIS:NE2	2.89	0.40
1:C:186:ILE:HG21	1:C:274:ARG:HG2	2.03	0.40
2:D:323:GLN:HA	2:D:324:PRO:HA	1.87	0.40
2:D:365:TYR:CE2	2:D:430:LEU:HA	2.55	0.40
1:A:101:LEU:N	1:A:102:PRO:CD	2.83	0.40
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.40
1:C:119:HIS:CG	1:C:182:THR:HB	2.57	0.40
2:D:372:TRP:HA	2:D:373:PRO:HD2	1.82	0.40
2:D:374:GLU:O	2:D:378:ARG:HG3	2.21	0.40
1:C:287:GLN:HG2	1:C:288:ASP:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:VAL:CB	2:D:176:PRO:CD	2.96	0.40
1:A:86:ASP:OD1	1:A:88:LYS:HB3	2.21	0.40
1:A:198:THR:O	1:A:199:ARG:HB2	2.21	0.40
2:B:214:LEU:HD22	2:B:253:LEU:HG	2.02	0.40
1:C:15:TYR:HE1	4:C:300:ATP:O1G	2.05	0.40
2:D:232:LEU:HD13	2:D:341:LEU:CD1	2.51	0.40
2:D:375:SER:HA	2:D:378:ARG:HH21	1.87	0.40
2:D:402:PRO:HA	2:D:410:ARG:NH1	2.37	0.40
2:D:417:LYS:HZ2	2:D:417:LYS:CB	2.34	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	295/298 (99%)	264 (90%)	21 (7%)	10 (3%)	3	4
1	C	295/298 (99%)	258 (88%)	24 (8%)	13 (4%)	2	2
2	B	256/258 (99%)	241 (94%)	12 (5%)	3 (1%)	10	23
2	D	256/258 (99%)	241 (94%)	13 (5%)	2 (1%)	16	34
All	All	1102/1112 (99%)	1004 (91%)	70 (6%)	28 (2%)	4	8

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	18	VAL
1	C	162	GLU
1	C	164	VAL
1	C	287	GLN
2	D	176	PRO
1	A	10	ILE

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Mol	Chain	Res	Type
1	A	14	THR
1	A	97	THR
1	A	164	VAL
2	B	177	ASP
2	B	283	ASP
1	C	11	GLY
2	D	420	GLY
1	A	8	GLU
1	A	162	GLU
1	C	96	LEU
1	A	37	LEU
1	A	39	THR
2	B	319	PHE
1	C	10	ILE
1	C	14	THR
1	C	275	ILE
1	C	283	HIS
1	C	285	PHE
1	A	96	LEU
1	C	145	ASP
1	A	228	PRO
1	C	251	VAL

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	262/262 (100%)	230 (88%)	32 (12%)	5	10
1	C	262/262 (100%)	225 (86%)	37 (14%)	3	6
2	B	232/232 (100%)	208 (90%)	24 (10%)	7	15
2	D	232/232 (100%)	216 (93%)	16 (7%)	14	32
All	All	988/988 (100%)	879 (89%)	109 (11%)	6	13

All (109) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	9	LYS
1	A	40	GLU
1	A	41	THR
1	A	47	THR
1	A	55	LEU
1	A	59	ASN
1	A	71	HIS
1	A	75	LYS
1	A	76	LEU
1	A	87	LEU
1	A	108	LEU
1	A	115	LEU
1	A	122	ARG
1	A	137	THR
1	A	148	LEU
1	A	150	ARG
1	A	156	VAL
1	A	161	HIS
1	A	163	VAL
1	A	172	GLU
1	A	202	LEU
1	A	226	VAL
1	A	230	VAL
1	A	232	SER
1	A	239	SER
1	A	250	LYS
1	A	255	LEU
1	A	256	ASP
1	A	288	ASP
1	A	297	ARG
1	A	298	LEU
2	B	177	ASP
2	B	196	LYS
2	B	199	TYR
2	B	200	MET
2	B	201	LYS
2	B	203	GLN
2	B	232	LEU
2	B	274	GLU
2	B	277	GLU
2	B	283	ASP
2	B	285	THR

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Mol	Chain	Res	Type
2	B	288	LYS
2	B	292	LEU
2	B	316	THR
2	B	334	MET
2	B	346	PRO
2	B	384	LEU
2	B	391	LEU
2	B	400	LYS
2	B	410	ARG
2	B	411	GLU
2	B	417	LYS
2	B	428	GLU
2	B	429	THR
1	C	5	GLN
1	C	12	GLU
1	C	15	TYR
1	C	39	THR
1	C	40	GLU
1	C	47	THR
1	C	71	HIS
1	C	72	THR
1	C	75	LYS
1	C	76	LEU
1	C	77	TYR
1	C	78	LEU
1	C	84	HIS
1	C	87	LEU
1	C	88	LYS
1	C	91	MET
1	C	122	ARG
1	C	137	THR
1	C	138	GLU
1	C	148	LEU
1	C	150	ARG
1	C	156	VAL
1	C	158	THR
1	C	162	GLU
1	C	172	GLU
1	C	173	ILE
1	C	199	ARG
1	C	202	LEU
1	C	217	ARG

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Mol	Chain	Res	Type
1	C	230	VAL
1	C	232	SER
1	C	248	PHE
1	C	250	LYS
1	C	255	LEU
1	C	276	SER
1	C	287	GLN
1	C	297	ARG
2	D	180	GLU
2	D	193	CYS
2	D	232	LEU
2	D	245	SER
2	D	281	ILE
2	D	292	LEU
2	D	300	LYS
2	D	327	CYS
2	D	346	PRO
2	D	349	LYS
2	D	353	SER
2	D	376	LEU
2	D	400	LYS
2	D	402	PRO
2	D	416	SER
2	D	417	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	59	ASN
1	A	60	HIS
1	A	71	HIS
1	A	119	HIS
1	A	246	GLN
1	A	265	GLN
1	A	272	ASN
2	B	183	HIS
2	B	228	GLN
2	B	296	HIS
2	B	313	GLN
2	B	317	GLN
2	B	370	GLN

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Mol	Chain	Res	Type
2	B	395	HIS
2	B	396	GLN
1	C	59	ASN
1	C	119	HIS
1	C	268	HIS
1	C	272	ASN
2	D	179	HIS
2	D	233	HIS
2	D	313	GLN
2	D	317	GLN
2	D	321	HIS
2	D	361	HIS
2	D	406	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TPO	C	160	1	8,10,11	1.76	1 (12%)	10,14,16	1.48	2 (20%)
1	TPO	A	160	1	8,10,11	1.12	1 (12%)	10,14,16	1.24	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
1	TPO	C	160	1	-	1/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	160	1	-	2/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	TPO	P-OG1	-4.33	1.51	1.59
1	A	160	TPO	P-O3P	-2.06	1.47	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	OG1-P-O1P	-2.46	100.56	109.33
1	C	160	TPO	O3P-P-O2P	2.01	115.34	107.80

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	C-CA-CB-CG2
1	A	160	TPO	CB-OG1-P-O3P
1	A	160	TPO	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	160	TPO	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ATP	C	300	3	32,33,33	1.80	4 (12%)	48,52,52	2.08	13 (27%)
4	ATP	A	300	3	32,33,33	2.94	5 (15%)	48,52,52	1.46	6 (12%)

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
4	ATP	C	300	3	-	5/22/38/38	0/3/3/3
4	ATP	A	300	3	-	7/22/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	300	ATP	PB-O3B	10.15	1.70	1.59
4	A	300	ATP	PB-O3A	9.78	1.70	1.59
4	C	300	ATP	PB-O3A	7.32	1.67	1.59
4	A	300	ATP	PA-O3A	5.46	1.65	1.59
4	C	300	ATP	PB-O3B	-3.77	1.55	1.59
4	A	300	ATP	PA-O5'	2.91	1.70	1.59
4	C	300	ATP	PA-O3A	2.53	1.62	1.59
4	A	300	ATP	C4-N9	2.17	1.42	1.37
4	C	300	ATP	PA-O2A	-2.12	1.45	1.55

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	300	ATP	O5'-C5'-C4'	6.23	130.21	108.99
4	C	300	ATP	C2'-C1'-N9	-5.41	99.87	113.30
4	C	300	ATP	O4'-C1'-N9	5.09	117.87	108.09
4	A	300	ATP	O4'-C1'-N9	4.39	116.52	108.09
4	A	300	ATP	C2'-C1'-N9	-3.79	103.88	113.30
4	C	300	ATP	O2B-PB-O3A	3.76	117.44	107.27
4	C	300	ATP	C4'-O4'-C1'	-3.73	101.22	109.47
4	C	300	ATP	O4'-C4'-C3'	3.55	112.19	105.15
4	A	300	ATP	PA-O5'-C5'	3.40	140.84	121.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	300	ATP	O2A-PA-O5'	-3.04	93.80	107.57
4	C	300	ATP	O2B-PB-O1B	2.86	125.76	112.44
4	A	300	ATP	C3'-C2'-C1'	2.63	106.44	101.46
4	C	300	ATP	PA-O5'-C5'	-2.60	106.44	121.35
4	C	300	ATP	C1'-N9-C8	2.46	132.55	127.09
4	A	300	ATP	O2A-PA-O3A	2.14	113.06	107.27
4	C	300	ATP	C5'-C4'-C3'	-2.13	107.54	115.21
4	C	300	ATP	O2A-PA-O1A	2.06	122.02	112.44
4	C	300	ATP	O3G-PG-O2G	2.06	115.51	107.80
4	C	300	ATP	O4'-C1'-C2'	2.05	111.01	106.62

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	300	ATP	C5'-O5'-PA-O1A
4	A	300	ATP	C5'-O5'-PA-O2A
4	A	300	ATP	C5'-O5'-PA-O3A
4	C	300	ATP	PB-O3B-PG-O2G
4	A	300	ATP	C3'-C4'-C5'-O5'
4	A	300	ATP	PB-O3A-PA-O5'
4	A	300	ATP	O4'-C4'-C5'-O5'
4	C	300	ATP	C4'-C5'-O5'-PA
4	C	300	ATP	O4'-C4'-C5'-O5'
4	C	300	ATP	PB-O3B-PG-O1G
4	C	300	ATP	PB-O3B-PG-O3G
4	A	300	ATP	PA-O3A-PB-O2B

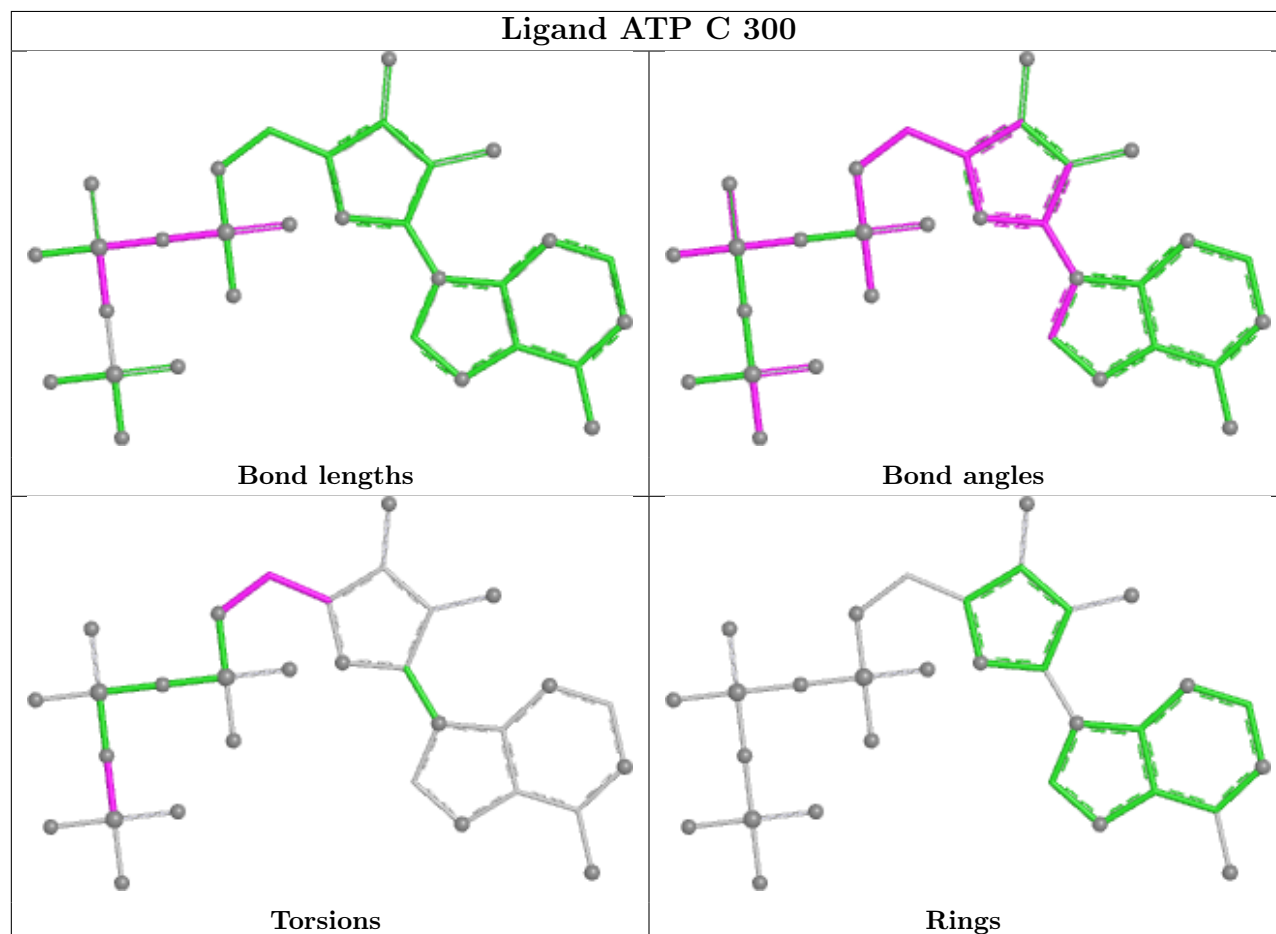
There are no ring outliers.

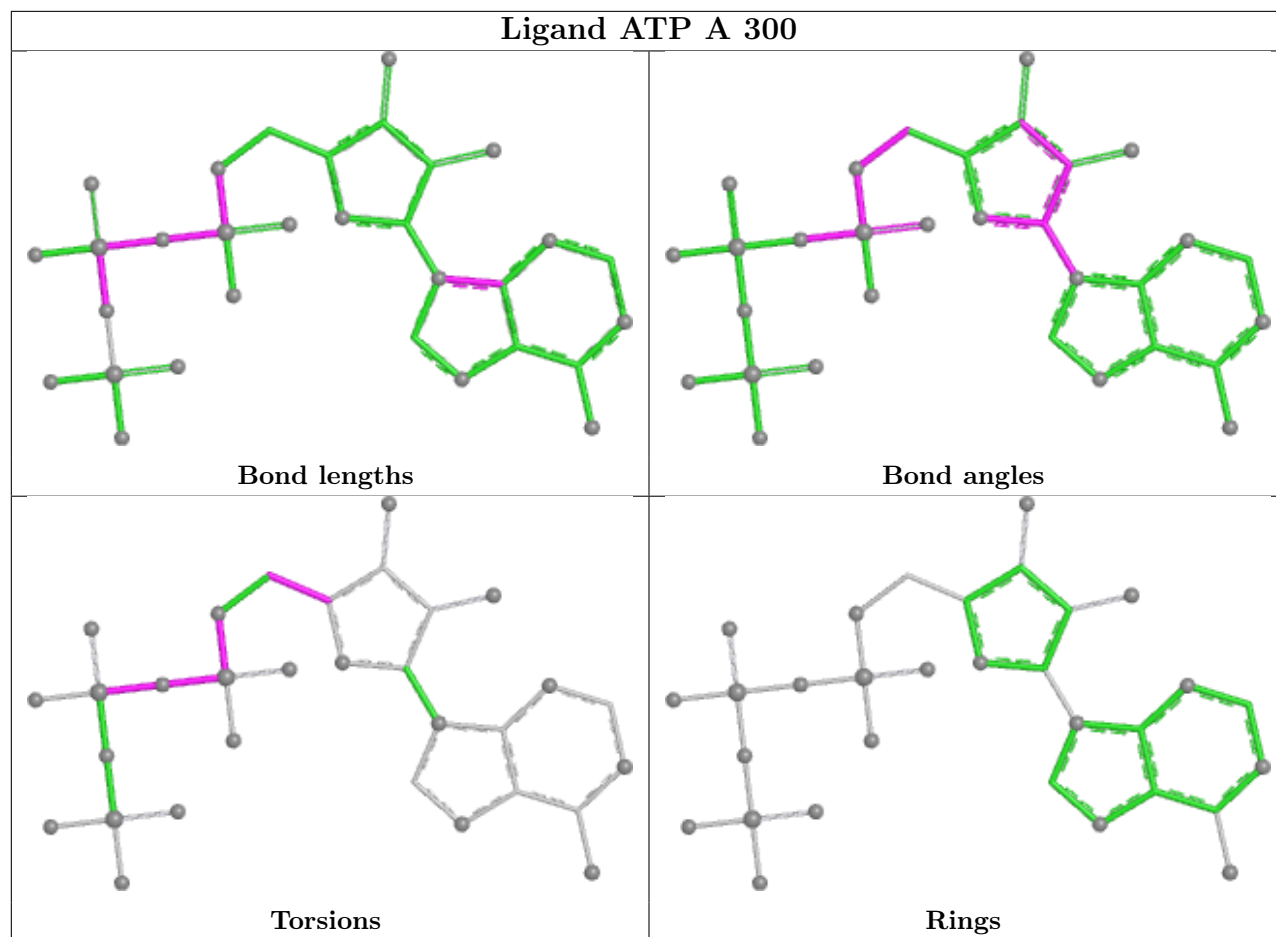
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	300	ATP	4	0
4	A	300	ATP	8	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 [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.