



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:32 PM UTC

PDB ID : 1E9H / pdb_00001e9h
Title : Thr 160 phosphorylated CDK2 - Human cyclin A3 complex with the inhibitor indirubin-5-sulphonate bound
Authors : Davies, T.G.; Tunnah, P.; Noble, M.E.M.; Endicott, J.A.
Deposited on : 2000-10-16
Resolution : 2.50 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

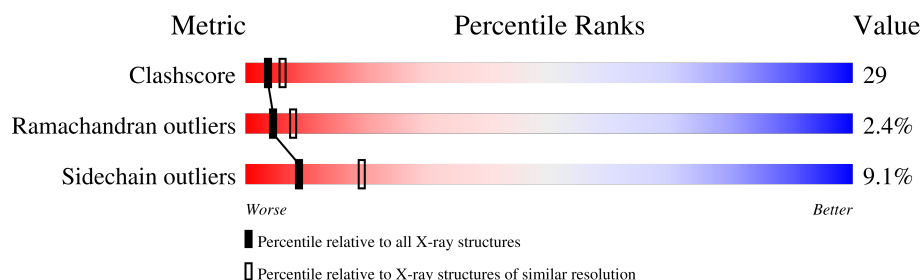
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	297	49% 40% 9% .
1	C	297	49% 40% 9% .
2	B	261	59% 36% . .
2	D	261	44% 46% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9355 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 CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	P	S	0	0	0
			2383	1547	403	424	1	8			
1	C	297	Total	C	N	O	P	S	0	0	0
			2389	1550	404	426	1	8			

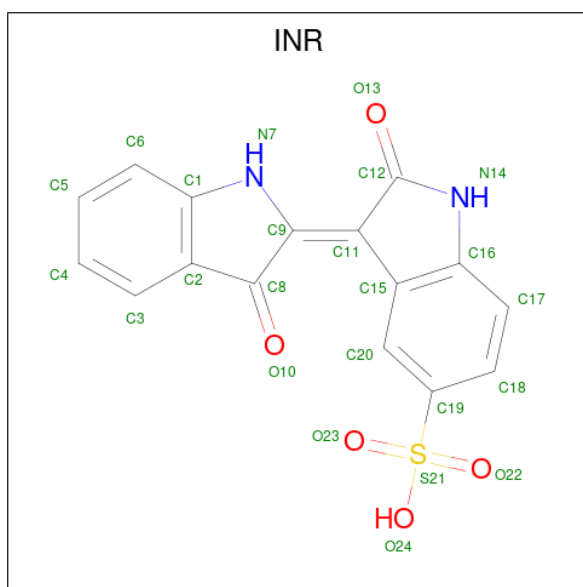
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	160	TPO	THR	modified residue	UNP P20248

- Molecule 2 is a protein called CYCLIN A3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 2',3-DIOXO-1,1',2',3-TETRAHYDRO-2,3'-BIINDOLE-5'-SULFONIC ACID (CCD ID: INR) (formula: C₁₆H₁₀N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	2	5	1		
3	C	1	Total	C	N	O	S	0	0
			24	16	2	5	1		

- Molecule 4 is water.

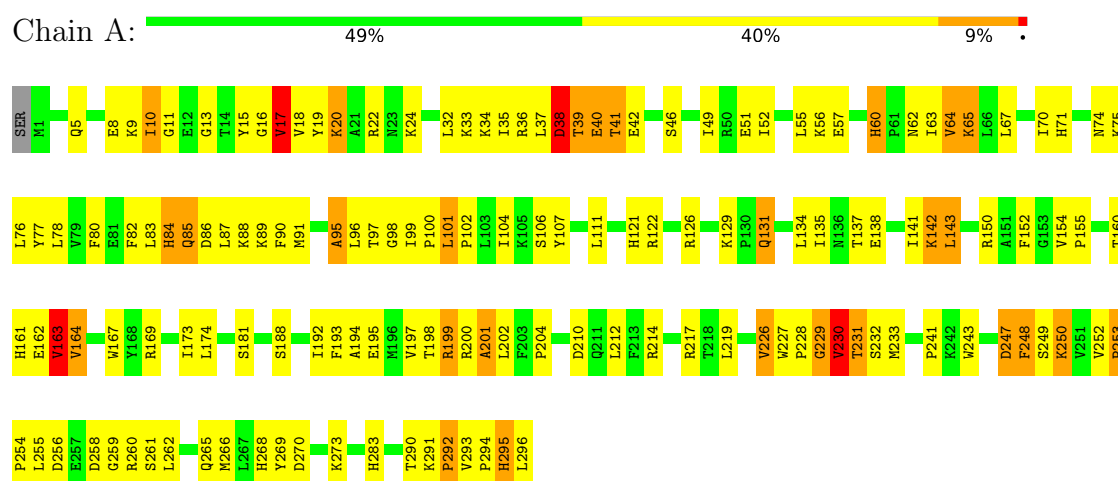
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total	O	0	0
			124	124		
4	B	100	Total	O	0	0
			100	100		
4	C	77	Total	O	0	0
			77	77		
4	D	68	Total	O	0	0
			68	68		

3 Residue-property plots [i](#)

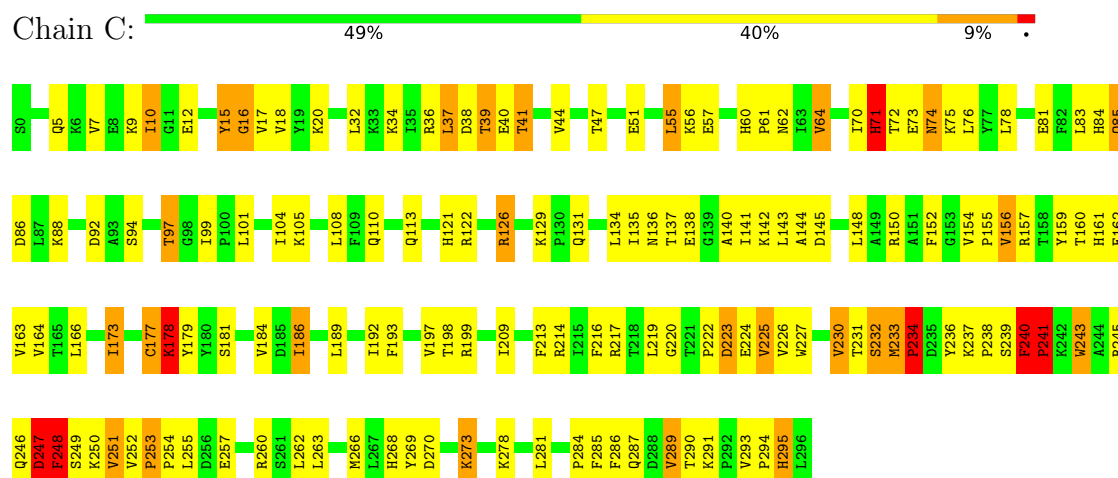
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

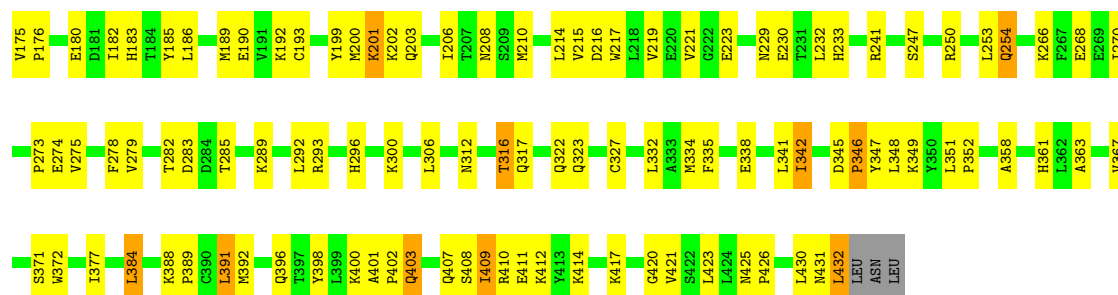


• Molecule 1: CELL DIVISION PROTEIN KINASE 2



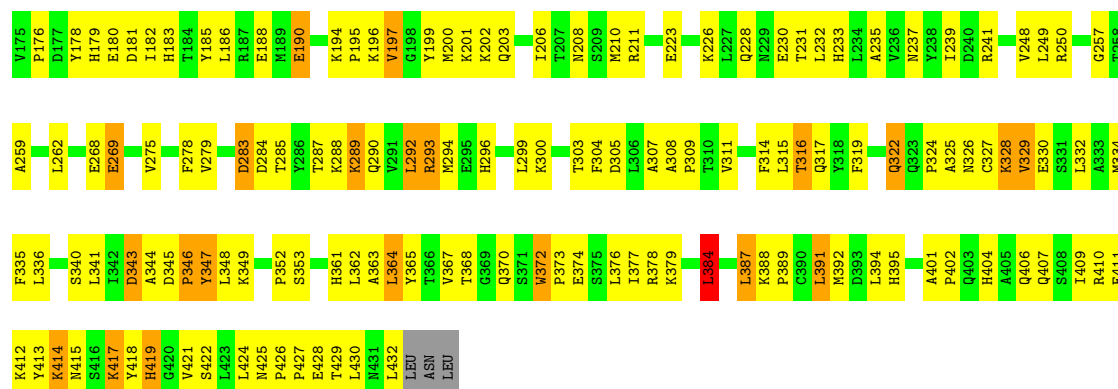
• Molecule 2: CYCLIN A3





• Molecule 2: CYCLIN A3

Chain D: 44% 46% 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	73.80Å 133.80Å 150.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.50	Depositor
% Data completeness (in resolution range)	90.0 (100.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9355	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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: TPO, INR

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	0.56	1/2433 (0.0%)	1.10	22/3300 (0.7%)
1	C	0.44	0/2439	1.15	17/3308 (0.5%)
2	B	0.46	0/2133	0.99	10/2897 (0.3%)
2	D	0.41	0/2133	1.00	13/2897 (0.4%)
All	All	0.47	1/9138 (0.0%)	1.07	62/12402 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	230	VAL	CA-CB	5.16	1.59	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	240	PHE	CA-C-N	18.50	142.97	119.84
1	C	240	PHE	C-N-CA	18.50	142.97	119.84
2	D	285	THR	N-CA-C	-9.90	101.33	113.41
2	B	347	TYR	N-CA-C	9.60	124.09	112.38
1	C	241	PRO	N-CA-C	8.51	129.99	112.47
1	A	248	PHE	N-CA-C	8.25	122.31	111.75
1	A	253	PRO	N-CA-C	8.18	120.67	110.70
2	B	285	THR	N-CA-C	-7.89	103.10	112.89
1	C	173	ILE	N-CA-C	-7.71	105.18	111.81
1	A	87	LEU	N-CA-C	7.55	119.51	111.28
1	A	295	HIS	N-CA-C	7.38	121.60	112.59
1	C	233	MET	CA-C-N	7.06	128.67	119.84
1	C	233	MET	C-N-CA	7.06	128.67	119.84
1	A	163	VAL	N-CA-C	7.03	118.85	108.45
1	A	84	HIS	N-CA-C	6.91	119.66	111.71
2	D	268	GLU	N-CA-C	6.85	121.97	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	GLY	N-CA-C	6.84	122.99	114.37
1	A	142	LYS	N-CA-C	6.70	119.61	109.23
2	D	329	VAL	N-CA-C	-6.65	103.83	110.62
1	C	247	ASP	N-CA-C	-6.65	100.86	110.24
1	C	248	PHE	N-CA-C	6.54	120.12	111.75
2	B	414	LYS	N-CA-C	-6.54	105.46	113.50
2	B	268	GLU	N-CA-C	6.50	121.42	112.90
2	D	372	TRP	CA-C-N	6.45	127.91	119.84
2	D	372	TRP	C-N-CA	6.45	127.91	119.84
2	D	414	LYS	N-CA-C	-6.42	106.17	112.97
1	A	126	ARG	N-CA-C	6.42	120.69	112.86
1	C	193	PHE	N-CA-C	-6.26	104.38	111.14
1	C	97	THR	N-CA-C	6.14	118.76	111.33
1	C	81	GLU	N-CA-C	-6.07	101.50	110.48
1	C	253	PRO	N-CA-C	6.02	118.05	110.70
2	B	270	ILE	N-CA-C	-5.95	104.52	111.00
1	C	126	ARG	N-CA-C	5.93	120.46	113.23
1	A	38	ASP	N-CA-C	5.93	123.42	110.80
2	D	197	VAL	N-CA-C	5.92	121.66	109.34
2	B	342	ILE	N-CA-C	5.90	118.46	111.09
2	D	269	GLU	N-CA-C	5.85	118.74	110.50
1	A	13	GLY	N-CA-C	-5.80	103.26	112.66
2	B	377	ILE	N-CA-C	-5.80	104.86	110.72
2	D	181	ASP	N-CA-C	-5.78	104.89	111.07
2	B	367	VAL	N-CA-C	5.75	117.26	111.00
2	B	279	VAL	N-CA-C	-5.63	104.86	111.00
1	A	193	PHE	N-CA-C	-5.63	105.05	111.07
2	D	384	LEU	N-CA-C	-5.63	105.67	112.54
1	C	71	HIS	N-CA-C	5.61	117.87	107.99
1	A	20	LYS	N-CA-C	-5.60	100.86	109.76
1	A	226	VAL	N-CA-C	5.56	116.33	110.72
2	B	384	LEU	N-CA-C	-5.54	105.24	111.28
1	C	257	GLU	N-CA-C	5.48	117.69	111.11
1	A	173	ILE	N-CA-C	-5.44	106.39	111.45
1	C	138	GLU	N-CA-C	5.40	119.85	112.88
2	D	279	VAL	N-CA-C	-5.39	105.59	110.82
1	A	283	HIS	CA-C-N	5.38	125.71	119.47
1	A	283	HIS	C-N-CA	5.38	125.71	119.47
1	C	178	LYS	N-CA-C	5.31	117.75	111.33
1	A	24	LYS	N-CA-C	5.28	117.03	111.28
1	A	295	HIS	O-C-N	5.15	128.59	122.26
2	D	425	ASN	N-CA-C	5.15	116.86	109.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	VAL	CB-CA-C	-5.09	105.19	111.70
1	A	60	HIS	CA-C-N	5.08	124.74	119.56
1	A	60	HIS	C-N-CA	5.08	124.74	119.56
2	D	343	ASP	N-CA-C	5.03	117.33	107.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2383	0	2425	143	0
1	C	2389	0	2430	179	0
2	B	2083	0	2107	81	0
2	D	2083	0	2107	145	0
3	A	24	0	10	2	0
3	C	24	0	10	0	0
4	A	124	0	0	11	0
4	B	100	0	0	8	0
4	C	77	0	0	8	0
4	D	68	0	0	7	0
All	All	9355	0	9089	524	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 29.

All (524) 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:41:THR:HG23	1:A:42:GLU:H	1.13	1.14
1:A:227:TRP:O	4:A:2094:HOH:O	1.73	1.07
1:A:39:THR:HG22	1:A:40:GLU:H	1.13	1.06
1:A:293:VAL:HG22	1:A:294:PRO:HD2	1.42	1.02
1:A:262:LEU:HG	1:A:266:MET:HE2	1.45	0.95
2:D:346:PRO:HB2	2:D:349:LYS:NZ	1.85	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.53	0.90
1:C:213:PHE:O	1:C:217:ARG:HG3	1.71	0.90
1:A:85:GLN:OE1	1:A:89:LYS:HB3	1.72	0.89
1:A:41:THR:HG23	1:A:42:GLU:N	1.86	0.89
1:C:217:ARG:HG2	1:C:243:TRP:NE1	1.89	0.87
2:D:210:MET:HE1	2:D:250:ARG:HB2	1.55	0.87
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.56	0.86
2:D:197:VAL:HA	4:D:2054:HOH:O	1.74	0.86
2:D:201:LYS:HZ2	2:D:202:LYS:HE3	1.38	0.85
1:A:290:THR:O	1:A:292:PRO:HD3	1.76	0.85
1:A:39:THR:HG22	1:A:40:GLU:N	1.92	0.83
1:C:7:VAL:HB	1:C:20:LYS:O	1.77	0.83
1:C:60:HIS:HD2	1:C:62:ASN:H	1.26	0.83
1:A:39:THR:HG21	2:B:289:LYS:HZ3	1.45	0.82
1:C:155:PRO:HD2	2:D:316:THR:HG23	1.62	0.82
1:A:39:THR:HG21	2:B:289:LYS:NZ	1.94	0.81
2:B:175:VAL:HA	4:B:2017:HOH:O	1.80	0.81
1:A:41:THR:HG22	4:A:2017:HOH:O	1.80	0.80
2:B:338:GLU:HG3	4:B:2072:HOH:O	1.81	0.80
1:C:284:PRO:O	1:C:287:GLN:HG2	1.82	0.79
1:C:88:LYS:HD2	1:C:131:GLN:HG3	1.64	0.79
2:D:404:HIS:CE1	2:D:406:GLN:HG2	2.17	0.79
1:C:39:THR:HG22	1:C:40:GLU:H	1.48	0.78
1:A:229:GLY:N	4:A:2094:HOH:O	2.15	0.78
1:C:60:HIS:CD2	1:C:62:ASN:H	2.01	0.78
2:D:372:TRP:HB3	2:D:384:LEU:HD21	1.65	0.78
2:D:210:MET:HE1	2:D:250:ARG:HD3	1.64	0.77
2:D:374:GLU:HG3	2:D:378:ARG:HH11	1.50	0.77
1:C:262:LEU:HG	1:C:266:MET:HE3	1.66	0.77
2:B:289:LYS:HE2	2:B:293:ARG:NH2	2.01	0.76
1:C:240:PHE:HB2	1:C:241:PRO:HD2	1.67	0.76
1:A:198:THR:O	1:A:199:ARG:HB2	1.85	0.75
1:C:88:LYS:HE3	1:C:131:GLN:HE21	1.49	0.75
2:D:322:GLN:NE2	2:D:326:ASN:H	1.85	0.74
1:A:85:GLN:HG3	1:A:86:ASP:N	2.03	0.74
1:A:129:LYS:HD2	1:A:131:GLN:HG2	1.70	0.74
1:C:154:VAL:O	2:D:316:THR:HG22	1.87	0.74
1:A:39:THR:CG2	1:A:40:GLU:H	1.96	0.73
1:A:98:GLY:N	1:A:199:ARG:HH11	1.85	0.73
2:D:326:ASN:OD1	2:D:329:VAL:HG23	1.88	0.73
1:A:60:HIS:CD2	1:A:62:ASN:H	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:LYS:NZ	2:D:348:LEU:O	2.22	0.73
2:D:364:LEU:HD23	2:D:365:TYR:H	1.54	0.73
1:A:41:THR:CG2	1:A:42:GLU:H	1.98	0.72
1:C:240:PHE:CB	1:C:241:PRO:HD2	2.19	0.72
1:A:230:VAL:HA	1:A:233:MET:HE2	1.72	0.72
2:D:329:VAL:HG22	2:D:364:LEU:HA	1.72	0.72
1:A:60:HIS:HD2	1:A:62:ASN:H	1.37	0.71
1:C:199:ARG:HH21	1:C:199:ARG:HG3	1.54	0.71
2:D:428:GLU:HG3	2:D:429:THR:HG23	1.73	0.71
1:C:51:GLU:O	1:C:55:LEU:HB2	1.90	0.70
1:C:64:VAL:HG22	1:C:143:LEU:O	1.91	0.70
1:C:214:ARG:HG2	1:C:217:ARG:NH1	2.06	0.70
1:C:217:ARG:HD2	4:C:2065:HOH:O	1.90	0.70
1:C:105:LYS:HE2	1:C:285:PHE:CE1	2.27	0.70
1:A:5:GLN:HG2	1:A:22:ARG:NH1	2.07	0.70
1:C:232:SER:HB2	4:C:2066:HOH:O	1.91	0.69
1:A:250:LYS:HD2	4:A:2103:HOH:O	1.90	0.69
1:A:15:TYR:O	1:A:36:ARG:HG3	1.93	0.69
1:A:121:HIS:O	1:A:122:ARG:HG3	1.91	0.69
1:C:39:THR:HG22	1:C:40:GLU:N	2.07	0.69
1:C:252:VAL:CG1	1:C:255:LEU:HB2	2.23	0.68
1:C:252:VAL:HG12	1:C:255:LEU:HB2	1.75	0.68
2:D:199:TYR:HB2	4:D:2029:HOH:O	1.94	0.68
2:D:332:LEU:HD23	2:D:363:ALA:HA	1.75	0.68
2:D:401:ALA:HB3	2:D:402:PRO:HD3	1.76	0.68
1:A:16:GLY:HA3	1:A:34:LYS:O	1.94	0.67
1:C:223:ASP:OD2	1:C:225:VAL:HG23	1.94	0.67
1:C:273:LYS:HE3	1:C:273:LYS:HA	1.76	0.67
2:D:190:GLU:HG3	2:D:352:PRO:HD2	1.74	0.67
1:A:247:ASP:OD2	1:A:247:ASP:C	2.38	0.67
1:C:214:ARG:HG2	1:C:217:ARG:CZ	2.24	0.67
1:A:293:VAL:CG2	1:A:294:PRO:HD2	2.21	0.67
1:A:85:GLN:HG3	1:A:86:ASP:H	1.60	0.67
2:D:373:PRO:O	2:D:377:ILE:HG13	1.94	0.67
1:C:197:VAL:HG11	1:C:252:VAL:CG1	2.24	0.66
1:C:162:GLU:H	1:C:162:GLU:CD	2.04	0.66
1:A:270:ASP:HB3	1:A:273:LYS:HG2	1.77	0.65
1:C:178:LYS:HD2	1:C:179:TYR:CE2	2.30	0.65
2:B:388:LYS:O	2:B:392:MET:HG2	1.95	0.65
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.64	0.65
1:C:85:GLN:HA	1:C:85:GLN:HE21	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:THR:HG22	1:C:291:LYS:H	1.61	0.65
2:D:296:HIS:HD2	2:D:300:LYS:NZ	1.95	0.65
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.12	0.64
2:B:396:GLN:HE21	2:B:400:LYS:NZ	1.96	0.64
1:C:61:PRO:O	1:C:142:LYS:HE2	1.98	0.64
2:D:322:GLN:CD	2:D:326:ASN:H	2.05	0.64
1:C:236:TYR:HD2	1:C:240:PHE:CE2	2.15	0.64
1:A:100:PRO:HG2	1:A:295:HIS:CE1	2.33	0.63
1:A:129:LYS:HG3	1:A:131:GLN:HG2	1.79	0.63
1:A:154:VAL:O	2:B:316:THR:CG2	2.46	0.63
1:A:290:THR:C	1:A:292:PRO:HD3	2.23	0.63
1:C:217:ARG:HA	1:C:243:TRP:CD1	2.34	0.63
2:D:336:LEU:HD22	2:D:362:LEU:HD23	1.79	0.63
2:D:384:LEU:H	2:D:384:LEU:HD23	1.63	0.63
2:B:215:VAL:O	2:B:219:VAL:HG23	1.98	0.63
2:D:388:LYS:HA	2:D:391:LEU:HB2	1.81	0.62
1:C:230:VAL:HA	1:C:233:MET:HG2	1.81	0.62
1:A:64:VAL:HG22	1:A:143:LEU:O	1.99	0.62
1:A:121:HIS:C	1:A:122:ARG:HG3	2.23	0.62
1:A:230:VAL:HG12	1:A:233:MET:CE	2.29	0.62
1:C:177:CYS:HB2	1:C:233:MET:SD	2.39	0.62
2:D:384:LEU:HD23	2:D:384:LEU:N	2.15	0.62
1:A:296:LEU:C	1:A:296:LEU:HD23	2.24	0.62
1:C:222:PRO:HA	1:C:226:VAL:CG1	2.30	0.62
2:D:404:HIS:HE1	2:D:406:GLN:HG2	1.62	0.62
2:B:229:ASN:HD22	2:B:334:MET:CE	2.13	0.61
2:B:346:PRO:O	2:B:349:LYS:HG2	2.00	0.61
1:C:72:THR:HG22	1:C:73:GLU:N	2.15	0.61
2:D:201:LYS:NZ	2:D:202:LYS:HE3	2.15	0.61
2:D:395:HIS:HB2	2:D:430:LEU:HD11	1.82	0.61
2:D:346:PRO:O	2:D:349:LYS:HG3	2.00	0.61
1:A:52:ILE:O	1:A:56:LYS:HG3	2.01	0.61
1:C:57:GLU:OE2	2:D:307:ALA:HB3	2.01	0.61
1:A:181:SER:HB3	4:A:2077:HOH:O	2.00	0.61
1:A:51:GLU:O	1:A:55:LEU:HB2	2.00	0.60
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.82	0.60
1:C:230:VAL:HB	4:C:2067:HOH:O	2.00	0.60
1:A:230:VAL:N	4:A:2094:HOH:O	1.89	0.60
2:D:346:PRO:HB2	2:D:349:LYS:HZ2	1.67	0.60
2:D:233:HIS:HE1	4:D:2049:HOH:O	1.83	0.60
1:A:95:ALA:HA	1:A:199:ARG:CD	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:296:HIS:CD2	2:B:300:LYS:HZ1	2.19	0.60
1:C:99:ILE:HB	1:C:104:ILE:HD11	1.84	0.60
1:A:138:GLU:HB3	4:A:2122:HOH:O	2.01	0.60
1:C:126:ARG:HD2	1:C:163:VAL:HG21	1.84	0.60
1:C:220:GLY:HA3	1:C:245:ARG:HB2	1.82	0.60
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.29	0.60
1:C:286:PHE:O	1:C:289:VAL:HG12	2.01	0.60
1:C:37:LEU:HD22	1:C:44:VAL:HG22	1.84	0.59
1:A:57:GLU:HG3	2:B:185:TYR:OH	2.02	0.59
1:C:40:GLU:OE1	1:C:41:THR:N	2.35	0.59
2:D:364:LEU:HD23	2:D:365:TYR:N	2.17	0.59
2:D:361:HIS:O	2:D:364:LEU:HD23	2.01	0.59
2:D:326:ASN:ND2	2:D:328:LYS:H	2.01	0.59
2:B:392:MET:HE2	2:B:392:MET:HA	1.82	0.59
2:D:372:TRP:HB3	2:D:384:LEU:CD2	2.32	0.59
2:D:235:ALA:O	2:D:239:ILE:HG13	2.03	0.59
1:C:121:HIS:O	1:C:122:ARG:HG3	2.03	0.58
1:C:222:PRO:O	1:C:223:ASP:HB3	2.03	0.58
1:A:100:PRO:HG2	1:A:295:HIS:HE1	1.66	0.58
2:D:210:MET:HE1	2:D:250:ARG:CB	2.30	0.58
1:C:222:PRO:HA	1:C:226:VAL:HG11	1.85	0.58
1:C:273:LYS:HD2	1:C:273:LYS:N	2.18	0.58
1:C:217:ARG:HG2	1:C:243:TRP:CE2	2.39	0.58
1:A:154:VAL:O	2:B:316:THR:HG23	2.02	0.58
1:C:38:ASP:HB3	4:C:2015:HOH:O	2.04	0.58
1:C:199:ARG:HG3	1:C:199:ARG:NH2	2.19	0.58
1:A:227:TRP:CH2	1:A:233:MET:HE1	2.39	0.57
1:A:11:GLY:O	1:A:17:VAL:HG12	2.04	0.57
1:A:230:VAL:HG22	4:A:2094:HOH:O	2.03	0.57
2:D:327:CYS:HB2	2:D:419:HIS:NE2	2.19	0.57
1:C:10:ILE:HG23	1:C:10:ILE:O	2.03	0.57
2:D:327:CYS:HB2	2:D:419:HIS:HE2	1.69	0.57
1:A:261:SER:O	1:A:265:GLN:HG3	2.05	0.57
1:A:41:THR:CG2	1:A:42:GLU:N	2.59	0.57
2:D:387:LEU:O	2:D:391:LEU:HB2	2.05	0.57
2:B:210:MET:HE1	2:B:250:ARG:CB	2.35	0.57
2:D:322:GLN:HB3	2:D:325:ALA:HA	1.86	0.57
2:D:296:HIS:CD2	2:D:300:LYS:NZ	2.73	0.56
1:A:37:LEU:O	1:A:38:ASP:HB2	2.05	0.56
2:B:201:LYS:HD3	2:B:202:LYS:HG2	1.85	0.56
2:B:289:LYS:HG3	2:B:293:ARG:HE	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HB2	1:A:243:TRP:CZ3	2.41	0.56
1:A:85:GLN:OE1	1:A:89:LYS:CB	2.49	0.56
1:C:56:LYS:HE3	2:D:305:ASP:OD1	2.05	0.56
1:A:262:LEU:CG	1:A:266:MET:HE2	2.28	0.56
1:C:181:SER:O	1:C:184:VAL:HG22	2.04	0.56
2:D:210:MET:HE1	2:D:250:ARG:CD	2.35	0.56
1:C:233:MET:HA	1:C:233:MET:HE2	1.87	0.55
2:D:180:GLU:OE2	2:D:379:LYS:NZ	2.39	0.55
2:D:201:LYS:HZ2	2:D:202:LYS:CE	2.14	0.55
2:D:402:PRO:HG3	2:D:410:ARG:HH11	1.72	0.55
1:C:47:THR:HG23	4:C:2020:HOH:O	2.06	0.55
1:C:122:ARG:HA	1:C:152:PHE:CE1	2.40	0.55
1:C:227:TRP:HB3	1:C:230:VAL:HG22	1.89	0.55
1:C:253:PRO:HB2	1:C:254:PRO:CD	2.33	0.55
1:A:129:LYS:CD	1:A:131:GLN:HG2	2.36	0.55
2:B:323:GLN:HB3	4:B:2069:HOH:O	2.05	0.55
2:B:396:GLN:NE2	2:B:400:LYS:NZ	2.55	0.55
1:C:197:VAL:HG11	1:C:252:VAL:HG13	1.88	0.55
1:C:198:THR:O	1:C:199:ARG:HB2	2.07	0.55
2:D:211:ARG:HG2	2:D:211:ARG:HH11	1.71	0.55
1:C:121:HIS:C	1:C:122:ARG:HG3	2.32	0.55
1:A:42:GLU:OE1	2:B:275:VAL:HG23	2.06	0.55
1:C:217:ARG:CD	4:C:2065:HOH:O	2.50	0.55
2:D:296:HIS:HD2	2:D:300:LYS:HZ3	1.53	0.55
2:D:332:LEU:O	2:D:335:PHE:HB3	2.07	0.55
1:C:249:SER:HA	1:C:260:ARG:HD3	1.88	0.54
1:A:252:VAL:N	4:A:2105:HOH:O	2.34	0.54
1:A:262:LEU:HG	1:A:266:MET:CE	2.30	0.54
2:B:183:HIS:HB2	2:B:317:GLN:HE22	1.73	0.54
2:B:398:TYR:CE2	2:B:426:PRO:HB3	2.42	0.54
1:C:241:PRO:HB3	1:C:243:TRP:CE3	2.43	0.54
2:B:289:LYS:HE2	2:B:293:ARG:CZ	2.37	0.54
2:D:368:THR:CB	2:D:370:GLN:HE21	2.20	0.54
2:B:296:HIS:HD2	2:B:300:LYS:NZ	2.04	0.54
1:A:10:ILE:CD1	1:A:20:LYS:HB2	2.37	0.54
1:C:56:LYS:HE2	2:D:303:THR:O	2.07	0.54
1:C:108:LEU:HD21	1:C:266:MET:HE1	1.88	0.54
1:C:155:PRO:HD2	2:D:316:THR:CG2	2.33	0.54
2:D:299:LEU:HD22	2:D:304:PHE:CE1	2.43	0.54
2:D:384:LEU:N	2:D:384:LEU:CD2	2.70	0.54
1:A:86:ASP:OD2	1:A:89:LYS:HD2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LYS:HE3	3:A:1298:INR:HC4	1.89	0.53
1:C:216:PHE:HA	1:C:269:TYR:OH	2.09	0.53
1:C:284:PRO:HA	1:C:287:GLN:OE1	2.07	0.53
1:A:71:HIS:NE2	2:B:296:HIS:CE1	2.77	0.53
1:C:236:TYR:HD2	1:C:240:PHE:HE2	1.53	0.53
1:C:40:GLU:OE2	2:D:288:LYS:HD3	2.08	0.53
1:C:126:ARG:HB3	1:C:163:VAL:HG22	1.90	0.53
2:D:326:ASN:HD22	2:D:327:CYS:N	2.07	0.53
2:D:341:LEU:HD23	4:D:2050:HOH:O	2.09	0.53
1:A:227:TRP:CZ2	1:A:233:MET:HE1	2.44	0.53
1:C:177:CYS:CB	1:C:233:MET:SD	2.98	0.52
1:C:198:THR:O	1:C:199:ARG:CB	2.57	0.52
1:C:246:GLN:HE21	1:C:246:GLN:HA	1.73	0.52
2:B:300:LYS:HE2	4:B:2060:HOH:O	2.09	0.52
2:D:347:TYR:OH	2:D:394:LEU:HA	2.09	0.52
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.89	0.52
1:C:84:HIS:CD2	1:C:137:THR:HG23	2.45	0.52
1:A:88:LYS:HE3	1:A:131:GLN:HE22	1.74	0.52
2:D:430:LEU:HB3	2:D:432:LEU:CD1	2.40	0.52
2:B:371:SER:O	2:B:372:TRP:C	2.51	0.52
2:D:210:MET:CE	2:D:250:ARG:HD3	2.38	0.52
1:A:49:ILE:HG23	2:B:306:LEU:HD12	1.92	0.52
1:C:17:VAL:HG12	1:C:18:VAL:N	2.25	0.52
1:C:134:LEU:O	1:C:141:ILE:HA	2.10	0.52
1:C:238:PRO:C	1:C:240:PHE:H	2.16	0.52
1:A:255:LEU:HG	1:A:259:GLY:HA3	1.92	0.51
1:A:88:LYS:CD	1:A:131:GLN:HE22	2.22	0.51
2:B:233:HIS:HD2	4:B:2065:HOH:O	1.93	0.51
1:A:70:ILE:HB	1:A:77:TYR:HB2	1.92	0.51
1:A:71:HIS:CD2	1:A:76:LEU:HD12	2.46	0.51
2:B:273:PRO:HG2	2:B:278:PHE:CE2	2.45	0.51
1:C:71:HIS:ND1	2:D:300:LYS:HG2	2.26	0.51
2:B:407:GLN:O	2:B:411:GLU:HG2	2.10	0.51
1:A:67:LEU:HB3	4:A:2011:HOH:O	2.10	0.51
1:A:293:VAL:HG13	1:A:294:PRO:O	2.11	0.51
1:C:34:LYS:HE2	1:C:75:LYS:HD2	1.91	0.51
1:C:72:THR:HG22	1:C:73:GLU:H	1.76	0.51
1:C:83:LEU:HD22	1:C:134:LEU:HB2	1.93	0.51
2:D:319:PHE:CD2	2:D:330:GLU:HG2	2.46	0.50
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.93	0.50
1:C:233:MET:O	1:C:236:TYR:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:388:LYS:HD2	2:D:432:LEU:HB3	1.93	0.50
1:C:236:TYR:CD2	1:C:240:PHE:CE2	2.99	0.50
1:A:129:LYS:HD2	1:A:131:GLN:CG	2.39	0.50
1:A:129:LYS:CG	1:A:131:GLN:HG2	2.41	0.50
2:D:289:LYS:O	2:D:293:ARG:HG3	2.12	0.50
2:D:418:TYR:O	2:D:421:VAL:HG13	2.11	0.50
2:D:407:GLN:O	2:D:411:GLU:HG2	2.12	0.50
1:A:99:ILE:HG22	1:A:104:ILE:HG13	1.93	0.49
1:C:156:VAL:HB	1:C:159:TYR:CE2	2.46	0.49
2:D:326:ASN:CG	2:D:329:VAL:H	2.20	0.49
1:A:155:PRO:HD2	2:B:316:THR:HG23	1.93	0.49
2:D:231:THR:OG1	2:D:269:GLU:OE2	2.30	0.49
2:B:392:MET:HE3	2:B:432:LEU:HD12	1.93	0.49
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.94	0.49
1:A:88:LYS:CE	1:A:131:GLN:HE22	2.26	0.49
1:A:98:GLY:N	1:A:199:ARG:NH1	2.56	0.49
2:B:430:LEU:O	2:B:431:ASN:HB2	2.11	0.49
2:D:326:ASN:HB3	2:D:329:VAL:HB	1.93	0.49
1:A:230:VAL:O	1:A:232:SER:N	2.45	0.49
2:B:185:TYR:O	2:B:189:MET:HG2	2.13	0.49
1:A:17:VAL:HG23	1:A:34:LYS:HE3	1.94	0.49
2:B:401:ALA:HB3	2:B:402:PRO:HD3	1.95	0.49
1:C:34:LYS:NZ	1:C:36:ARG:HG3	2.28	0.49
1:C:249:SER:HA	1:C:260:ARG:CD	2.43	0.49
1:C:268:HIS:CE1	1:C:273:LYS:HB3	2.47	0.48
2:D:343:ASP:HB3	2:D:345:ASP:O	2.13	0.48
1:A:169:ARG:HD2	1:A:174:LEU:CD2	2.44	0.48
2:B:190:GLU:OE1	2:B:352:PRO:HG2	2.13	0.48
1:C:222:PRO:CG	1:C:230:VAL:HG11	2.43	0.48
1:C:227:TRP:CD2	1:C:230:VAL:HG13	2.48	0.48
1:A:84:HIS:CD2	1:A:137:THR:HG23	2.49	0.48
1:C:34:LYS:HZ1	1:C:36:ARG:NH1	2.12	0.48
1:C:72:THR:HG22	1:C:74:ASN:H	1.77	0.48
1:C:126:ARG:HB3	1:C:163:VAL:CG2	2.43	0.48
1:C:162:GLU:CD	1:C:162:GLU:N	2.71	0.48
2:D:336:LEU:HD13	2:D:362:LEU:HB3	1.94	0.48
1:A:230:VAL:HG23	1:A:231:THR:H	1.78	0.48
2:B:421:VAL:C	2:B:423:LEU:H	2.22	0.48
1:C:217:ARG:HG2	1:C:243:TRP:CD1	2.48	0.48
2:D:328:LYS:HE2	2:D:367:VAL:CG1	2.44	0.48
1:C:177:CYS:SG	1:C:179:TYR:O	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:311:VAL:O	2:D:315:LEU:HG	2.14	0.48
2:B:203:GLN:OE1	2:B:247:SER:HA	2.14	0.48
1:C:177:CYS:HB2	1:C:233:MET:HE1	1.96	0.48
1:C:222:PRO:HD3	1:C:269:TYR:CE1	2.48	0.48
1:C:177:CYS:HA	1:C:234:PRO:HG2	1.96	0.48
2:D:395:HIS:CE1	2:D:427:PRO:O	2.67	0.48
2:D:288:LYS:O	2:D:292:LEU:HD22	2.13	0.47
2:D:326:ASN:ND2	2:D:327:CYS:N	2.62	0.47
1:C:161:HIS:O	1:C:163:VAL:N	2.48	0.47
1:C:240:PHE:O	1:C:240:PHE:CD2	2.68	0.47
2:B:296:HIS:CD2	2:B:300:LYS:NZ	2.81	0.47
1:C:122:ARG:HA	1:C:152:PHE:CZ	2.48	0.47
1:C:290:THR:HG22	1:C:291:LYS:N	2.28	0.47
2:B:193:CYS:O	2:B:241:ARG:HD2	2.15	0.47
1:C:214:ARG:CG	1:C:217:ARG:CZ	2.91	0.47
2:D:346:PRO:CB	2:D:349:LYS:HZ2	2.26	0.47
1:C:34:LYS:NZ	1:C:36:ARG:NH1	2.63	0.47
1:C:97:THR:HG21	1:C:295:HIS:HE1	1.80	0.47
1:C:129:LYS:HA	1:C:192:ILE:HD11	1.96	0.47
1:C:214:ARG:HG3	1:C:217:ARG:NH2	2.30	0.47
1:C:219:LEU:HB2	1:C:269:TYR:CE2	2.50	0.47
2:B:233:HIS:CD2	2:B:341:LEU:HD21	2.50	0.47
2:B:289:LYS:O	2:B:293:ARG:HG3	2.15	0.47
1:C:154:VAL:O	2:D:316:THR:CG2	2.61	0.47
2:D:326:ASN:OD1	2:D:329:VAL:N	2.47	0.47
1:A:230:VAL:C	1:A:232:SER:N	2.73	0.46
1:A:90:PHE:HB2	1:A:135:ILE:HD11	1.97	0.46
1:A:65:LYS:HD2	1:A:67:LEU:HD23	1.97	0.46
2:B:192:LYS:HE2	4:B:2028:HOH:O	2.14	0.46
1:C:240:PHE:O	1:C:240:PHE:HD2	1.99	0.46
2:D:346:PRO:CB	2:D:349:LYS:NZ	2.70	0.46
1:A:296:LEU:HD23	1:A:296:LEU:OXT	2.16	0.46
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.31	0.46
2:D:186:LEU:HD12	2:D:317:GLN:OE1	2.16	0.46
2:D:346:PRO:HB2	2:D:349:LYS:HZ3	1.76	0.46
2:B:332:LEU:HD23	2:B:363:ALA:HA	1.97	0.46
1:C:39:THR:CG2	1:C:40:GLU:H	2.16	0.46
1:C:216:PHE:HD1	1:C:269:TYR:OH	1.99	0.46
2:D:326:ASN:ND2	2:D:326:ASN:C	2.73	0.46
1:C:248:PHE:HA	1:C:251:VAL:HG23	1.98	0.46
1:A:217:ARG:HG2	1:A:243:TRP:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:340:SER:HB2	2:D:347:TYR:CD1	2.51	0.46
1:A:36:ARG:HG2	1:A:36:ARG:HH11	1.80	0.46
1:C:157:ARG:NH2	2:D:228:GLN:HG3	2.31	0.46
1:A:256:ASP:OD2	1:A:258:ASP:N	2.49	0.45
2:D:296:HIS:CD2	2:D:300:LYS:HZ2	2.33	0.45
2:D:430:LEU:HB3	2:D:432:LEU:HD12	1.97	0.45
1:A:82:PHE:C	1:A:83:LEU:HD12	2.41	0.45
2:B:233:HIS:HE1	4:B:2072:HOH:O	2.00	0.45
2:D:388:LYS:O	2:D:389:PRO:C	2.60	0.45
2:D:361:HIS:HA	2:D:364:LEU:HD22	1.98	0.45
1:A:161:HIS:O	1:A:163:VAL:N	2.48	0.45
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.99	0.45
1:C:251:VAL:HG12	1:C:252:VAL:HG23	1.98	0.45
2:D:200:MET:HG2	2:D:208:ASN:OD1	2.16	0.45
2:D:419:HIS:ND1	2:D:419:HIS:N	2.65	0.45
1:A:219:LEU:HB2	1:A:269:TYR:CE2	2.51	0.45
2:D:230:GLU:HA	2:D:230:GLU:OE1	2.16	0.45
1:A:262:LEU:O	1:A:266:MET:HG3	2.17	0.45
2:B:282:THR:O	2:B:283:ASP:C	2.60	0.45
2:B:361:HIS:CE1	2:B:384:LEU:HD11	2.52	0.45
1:C:230:VAL:O	1:C:233:MET:HB2	2.16	0.45
1:A:10:ILE:HD11	1:A:20:LYS:HB2	1.98	0.45
2:B:358:ALA:HB1	2:B:391:LEU:HD13	1.99	0.45
2:D:324:PRO:O	2:D:325:ALA:C	2.60	0.45
2:D:395:HIS:HE1	2:D:427:PRO:O	1.99	0.45
2:D:402:PRO:HG3	2:D:410:ARG:NH1	2.31	0.45
1:A:162:GLU:CD	1:A:162:GLU:H	2.25	0.45
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.51	0.45
1:A:95:ALA:HA	1:A:199:ARG:NE	2.32	0.45
1:A:174:LEU:HB2	1:A:212:LEU:HD21	1.99	0.45
2:B:421:VAL:C	2:B:423:LEU:N	2.76	0.44
1:C:262:LEU:CG	1:C:266:MET:HE3	2.42	0.44
2:D:262:LEU:HD13	2:D:278:PHE:CD2	2.53	0.44
1:A:107:TYR:O	1:A:111:LEU:HG	2.18	0.44
1:A:292:PRO:HB2	1:A:293:VAL:H	1.60	0.44
1:C:270:ASP:HB3	1:C:273:LYS:HG2	1.99	0.44
2:D:340:SER:HB2	2:D:347:TYR:CG	2.52	0.44
1:A:5:GLN:HG2	1:A:22:ARG:HH11	1.82	0.44
1:A:291:LYS:O	1:A:292:PRO:O	2.35	0.44
1:A:268:HIS:CD2	1:A:273:LYS:HB2	2.52	0.44
1:C:186:ILE:HD13	1:C:186:ILE:HA	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:LEU:HD23	1:C:248:PHE:HE1	1.83	0.44
2:D:178:TYR:O	2:D:179:HIS:C	2.61	0.44
2:D:314:PHE:CZ	2:D:353:SER:HB3	2.53	0.44
1:A:57:GLU:OE1	2:B:189:MET:HE2	2.18	0.44
2:B:223:GLU:OE1	2:B:412:LYS:HG3	2.18	0.44
1:C:131:GLN:H	1:C:131:GLN:CD	2.25	0.44
2:D:190:GLU:OE1	2:D:353:SER:N	2.50	0.44
1:C:199:ARG:HA	4:C:2059:HOH:O	2.17	0.44
1:C:238:PRO:C	1:C:240:PHE:N	2.75	0.44
2:D:374:GLU:HA	2:D:377:ILE:HD12	2.00	0.44
1:C:85:GLN:HA	1:C:85:GLN:NE2	2.32	0.44
1:C:92:ASP:C	1:C:94:SER:N	2.75	0.44
1:C:278:LYS:HA	1:C:281:LEU:HD12	1.99	0.44
2:D:211:ARG:HG2	2:D:211:ARG:NH1	2.33	0.44
2:D:413:TYR:HB2	2:D:422:SER:HB3	1.99	0.44
1:A:10:ILE:HD12	1:A:20:LYS:HB2	2.00	0.44
1:A:46:SER:HB2	2:B:266:LYS:O	2.18	0.44
1:A:200:ARG:O	1:A:201:ALA:C	2.60	0.44
1:A:230:VAL:C	1:A:232:SER:H	2.25	0.44
2:B:206:ILE:HG22	2:B:210:MET:HE1	1.99	0.44
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.66	0.44
1:C:72:THR:CG2	1:C:73:GLU:N	2.81	0.44
1:C:231:THR:HA	1:C:236:TYR:CE1	2.53	0.44
1:C:293:VAL:HG13	1:C:294:PRO:HD2	1.99	0.44
2:D:322:GLN:HE22	2:D:326:ASN:H	1.63	0.44
1:A:84:HIS:CD2	1:A:137:THR:H	2.35	0.43
2:B:183:HIS:CE1	4:B:2025:HOH:O	2.71	0.43
2:D:421:VAL:HA	2:D:424:LEU:HG	2.00	0.43
2:B:201:LYS:HD3	2:B:202:LYS:CG	2.47	0.43
2:D:239:ILE:HD11	2:D:257:GLY:HA2	2.01	0.43
2:D:362:LEU:HD11	2:D:430:LEU:HD21	1.99	0.43
1:A:88:LYS:CD	1:A:131:GLN:NE2	2.82	0.43
1:A:210:ASP:O	1:A:214:ARG:HD2	2.18	0.43
2:B:230:GLU:OE1	2:B:312:ASN:HB3	2.18	0.43
2:D:250:ARG:NH1	4:D:2031:HOH:O	2.51	0.43
2:B:425:ASN:HD22	2:B:425:ASN:HA	1.64	0.43
2:D:328:LYS:HE2	2:D:367:VAL:HG11	2.00	0.43
2:D:409:ILE:O	2:D:412:LYS:HB3	2.17	0.43
1:A:42:GLU:CD	2:B:275:VAL:HG23	2.44	0.43
1:A:122:ARG:HD2	1:A:122:ARG:O	2.19	0.43
2:B:215:VAL:HB	2:B:342:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:THR:HG21	1:C:295:HIS:CE1	2.53	0.43
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.84	0.43
2:D:275:VAL:HG21	2:D:292:LEU:HD11	2.00	0.43
2:D:326:ASN:HD21	2:D:328:LYS:HG3	1.82	0.43
2:D:332:LEU:CD2	2:D:363:ALA:HA	2.45	0.43
1:A:39:THR:O	1:A:40:GLU:C	2.62	0.43
2:B:210:MET:HE1	2:B:250:ARG:HB2	2.00	0.43
2:B:407:GLN:OE1	2:B:410:ARG:HD3	2.17	0.43
1:C:34:LYS:NZ	1:C:36:ARG:CZ	2.82	0.43
1:C:236:TYR:CE1	1:C:238:PRO:HD3	2.54	0.43
1:A:188:SER:O	1:A:192:ILE:HG13	2.18	0.43
2:D:362:LEU:HD12	2:D:362:LEU:HA	1.92	0.43
1:A:64:VAL:CG1	1:A:134:LEU:HD12	2.48	0.43
1:A:91:MET:HE1	1:A:195:GLU:HG2	2.01	0.43
1:C:15:TYR:O	1:C:16:GLY:O	2.36	0.43
1:A:134:LEU:O	1:A:141:ILE:HA	2.19	0.42
2:B:199:TYR:CD1	2:B:199:TYR:C	2.97	0.42
2:D:372:TRP:CZ3	2:D:376:LEU:HD13	2.54	0.42
1:A:228:PRO:C	4:A:2094:HOH:O	2.59	0.42
2:B:229:ASN:HD22	2:B:334:MET:HE2	1.80	0.42
1:C:295:HIS:HB3	4:C:2042:HOH:O	2.19	0.42
2:D:415:ASN:OD1	2:D:417:LYS:N	2.45	0.42
1:A:63:ILE:O	1:A:64:VAL:C	2.62	0.42
1:C:9:LYS:HE2	1:C:12:GLU:HG3	2.01	0.42
2:D:185:TYR:O	2:D:188:GLU:HG2	2.20	0.42
1:A:163:VAL:CG1	1:A:164:VAL:HG23	2.38	0.42
1:C:214:ARG:HA	1:C:217:ARG:NE	2.34	0.42
2:D:344:ALA:O	2:D:348:LEU:HB2	2.19	0.42
2:B:335:PHE:CE1	2:B:409:ILE:HG22	2.55	0.42
1:A:18:VAL:HA	1:A:32:LEU:O	2.20	0.42
1:C:227:TRP:O	1:C:230:VAL:HG22	2.20	0.42
1:C:247:ASP:OD2	1:C:247:ASP:C	2.62	0.42
2:B:216:ASP:OD2	2:B:408:SER:HB2	2.20	0.42
1:C:18:VAL:HA	1:C:32:LEU:O	2.20	0.42
1:C:236:TYR:OH	1:C:238:PRO:HA	2.19	0.42
2:D:203:GLN:HB3	2:D:206:ILE:HG12	2.02	0.42
2:B:200:MET:HE3	2:B:208:ASN:HA	2.01	0.42
1:C:219:LEU:HB2	1:C:269:TYR:HE2	1.85	0.42
1:A:88:LYS:HD2	1:A:131:GLN:NE2	2.34	0.42
1:A:230:VAL:HA	1:A:233:MET:CE	2.44	0.42
2:B:392:MET:CE	2:B:432:LEU:HD12	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:PHE:HE2	1:C:263:LEU:HG	1.84	0.42
2:D:283:ASP:O	2:D:284:ASP:C	2.62	0.42
1:A:253:PRO:HG2	1:A:254:PRO:HD3	2.02	0.41
2:B:217:TRP:O	2:B:221:VAL:HG23	2.20	0.41
2:B:254:GLN:HE21	2:B:254:GLN:HB3	1.63	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.54	0.41
2:D:250:ARG:NE	4:D:2031:HOH:O	2.53	0.41
1:A:106:SER:HB2	1:A:290:THR:O	2.20	0.41
1:C:57:GLU:HG3	4:D:2042:HOH:O	2.20	0.41
2:D:201:LYS:O	2:D:201:LYS:HG2	2.19	0.41
2:D:414:LYS:HG3	2:D:422:SER:OG	2.20	0.41
2:B:182:ILE:O	2:B:186:LEU:HG	2.21	0.41
1:C:85:GLN:HG3	1:C:86:ASP:O	2.21	0.41
1:C:227:TRP:HB3	1:C:230:VAL:CG2	2.49	0.41
2:D:199:TYR:CD1	2:D:199:TYR:C	2.98	0.41
2:D:346:PRO:O	2:D:348:LEU:N	2.53	0.41
2:D:361:HIS:CD2	2:D:361:HIS:C	2.98	0.41
2:B:180:GLU:OE1	2:B:180:GLU:HA	2.20	0.41
1:C:72:THR:HB	1:C:75:LYS:O	2.20	0.41
1:C:241:PRO:HG2	1:C:243:TRP:HZ3	1.85	0.41
1:A:17:VAL:HB	1:A:19:TYR:CE1	2.55	0.41
1:A:95:ALA:HA	1:A:199:ARG:HD2	2.02	0.41
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.54	0.41
1:A:241:PRO:HB2	1:A:243:TRP:CH2	2.56	0.41
2:D:237:ASN:OD1	2:D:241:ARG:HD3	2.20	0.41
1:A:194:ALA:HB1	1:A:202:LEU:HD13	2.03	0.41
1:C:110:GLN:O	1:C:113:GLN:HB2	2.20	0.41
1:C:219:LEU:C	1:C:245:ARG:HG3	2.46	0.41
1:C:237:LYS:O	1:C:240:PHE:N	2.53	0.41
1:C:252:VAL:HG11	1:C:255:LEU:HB2	2.00	0.41
1:C:290:THR:CG2	1:C:291:LYS:H	2.22	0.41
2:D:259:ALA:CB	2:D:294:MET:HG3	2.51	0.41
1:A:9:LYS:HE3	1:A:17:VAL:CG1	2.51	0.41
1:A:33:LYS:O	1:A:33:LYS:HG2	2.20	0.41
1:A:101:LEU:N	1:A:102:PRO:CD	2.84	0.41
1:C:40:GLU:OE1	1:C:40:GLU:CA	2.68	0.41
1:C:70:ILE:N	1:C:70:ILE:HD12	2.36	0.41
1:C:129:LYS:HG3	1:C:131:GLN:OE1	2.21	0.41
1:C:197:VAL:CG1	1:C:252:VAL:HG13	2.51	0.41
2:D:194:LYS:HD2	2:D:195:PRO:HD2	2.01	0.41
1:A:80:PHE:CB	3:A:1298:INR:H17	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:LEU:O	1:A:102:PRO:C	2.60	0.41
1:A:167:TRP:CD1	1:A:204:PRO:HA	2.56	0.41
2:B:190:GLU:HG3	2:B:351:LEU:HD22	2.03	0.41
2:B:216:ASP:OD2	2:B:408:SER:CB	2.68	0.41
2:B:229:ASN:ND2	2:B:334:MET:HE2	2.36	0.41
2:D:248:VAL:HG12	2:D:249:LEU:O	2.20	0.41
1:C:64:VAL:CG2	1:C:144:ALA:HA	2.51	0.41
1:C:135:ILE:HA	1:C:140:ALA:O	2.21	0.40
1:C:233:MET:HA	1:C:233:MET:CE	2.52	0.40
2:D:183:HIS:ND1	2:D:317:GLN:NE2	2.69	0.40
2:D:430:LEU:CB	2:D:432:LEU:HD12	2.51	0.40
1:A:249:SER:HA	1:A:260:ARG:HD3	2.03	0.40
1:C:71:HIS:CD2	1:C:76:LEU:CD1	3.04	0.40
1:C:214:ARG:CG	1:C:217:ARG:NH2	2.84	0.40
1:C:236:TYR:CD2	1:C:240:PHE:HE2	2.35	0.40
2:D:211:ARG:HD3	2:D:344:ALA:HB2	2.02	0.40
2:D:287:THR:HG23	2:D:290:GLN:OE1	2.22	0.40
2:B:345:ASP:HA	2:B:346:PRO:HA	1.91	0.40
1:C:34:LYS:HE3	1:C:36:ARG:NH1	2.37	0.40
1:C:34:LYS:HZ2	1:C:36:ARG:HG3	1.85	0.40
1:C:227:TRP:CE3	1:C:230:VAL:HG13	2.56	0.40
2:D:223:GLU:OE2	2:D:412:LYS:HE3	2.21	0.40
2:B:403:GLN:N	2:B:403:GLN:NE2	2.69	0.40
2:D:426:PRO:O	2:D:427:PRO:C	2.64	0.40
2:B:202:LYS:HE3	2:B:202:LYS:HB3	1.93	0.40
2:D:308:ALA:HA	2:D:309:PRO:HD3	1.90	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	293/297 (99%)	260 (89%)	23 (8%)	10 (3%)	3	4
1	C	294/297 (99%)	245 (83%)	36 (12%)	13 (4%)	2	2
2	B	256/261 (98%)	242 (94%)	12 (5%)	2 (1%)	16	31
2	D	256/261 (98%)	225 (88%)	30 (12%)	1 (0%)	30	49
All	All	1099/1116 (98%)	972 (88%)	101 (9%)	26 (2%)	4	8

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	PRO
1	C	16	GLY
1	C	41	THR
1	C	241	PRO
2	D	347	TYR
1	A	40	GLU
1	A	164	VAL
1	C	39	THR
1	C	164	VAL
1	C	223	ASP
1	C	234	PRO
1	C	251	VAL
1	A	41	THR
1	A	95	ALA
1	A	201	ALA
1	A	231	THR
2	B	176	PRO
1	C	224	GLU
1	C	239	SER
1	C	289	VAL
1	C	145	ASP
1	C	166	LEU
1	A	38	ASP
1	A	39	THR
1	A	17	VAL
2	B	420	GLY

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	260/261 (100%)	237 (91%)	23 (9%)	9	20
1	C	261/261 (100%)	230 (88%)	31 (12%)	5	11
2	B	232/235 (99%)	217 (94%)	15 (6%)	15	32
2	D	232/235 (99%)	211 (91%)	21 (9%)	9	19
All	All	985/992 (99%)	895 (91%)	90 (9%)	9	19

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	10	ILE
1	A	17	VAL
1	A	35	ILE
1	A	64	VAL
1	A	65	LYS
1	A	74	ASN
1	A	75	LYS
1	A	78	LEU
1	A	85	GLN
1	A	96	LEU
1	A	97	THR
1	A	101	LEU
1	A	131	GLN
1	A	143	LEU
1	A	150	ARG
1	A	163	VAL
1	A	199	ARG
1	A	226	VAL
1	A	230	VAL
1	A	247	ASP
1	A	248	PHE
1	A	250	LYS
2	B	201	LYS
2	B	232	LEU
2	B	254	GLN
2	B	274	GLU
2	B	292	LEU
2	B	316	THR
2	B	322	GLN

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Mol	Chain	Res	Type
2	B	327	CYS
2	B	346	PRO
2	B	348	LEU
2	B	391	LEU
2	B	403	GLN
2	B	409	ILE
2	B	417	LYS
2	B	432	LEU
1	C	5	GLN
1	C	10	ILE
1	C	15	TYR
1	C	37	LEU
1	C	55	LEU
1	C	64	VAL
1	C	71	HIS
1	C	74	ASN
1	C	78	LEU
1	C	85	GLN
1	C	101	LEU
1	C	148	LEU
1	C	150	ARG
1	C	156	VAL
1	C	177	CYS
1	C	178	LYS
1	C	186	ILE
1	C	189	LEU
1	C	209	ILE
1	C	225	VAL
1	C	230	VAL
1	C	232	SER
1	C	234	PRO
1	C	240	PHE
1	C	241	PRO
1	C	243	TRP
1	C	247	ASP
1	C	248	PHE
1	C	250	LYS
1	C	273	LYS
1	C	295	HIS
2	D	182	ILE
2	D	190	GLU
2	D	196	LYS

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Mol	Chain	Res	Type
2	D	226	LYS
2	D	232	LEU
2	D	283	ASP
2	D	289	LYS
2	D	292	LEU
2	D	293	ARG
2	D	316	THR
2	D	322	GLN
2	D	328	LYS
2	D	334	MET
2	D	346	PRO
2	D	364	LEU
2	D	384	LEU
2	D	387	LEU
2	D	391	LEU
2	D	392	MET
2	D	417	LYS
2	D	419	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	59	ASN
1	A	60	HIS
1	A	84	HIS
1	A	119	HIS
1	A	131	GLN
1	A	246	GLN
1	A	268	HIS
1	A	295	HIS
2	B	179	HIS
2	B	183	HIS
2	B	233	HIS
2	B	254	GLN
2	B	296	HIS
2	B	317	GLN
2	B	370	GLN
2	B	395	HIS
2	B	396	GLN
2	B	403	GLN
2	B	425	ASN

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Mol	Chain	Res	Type
2	B	431	ASN
1	C	59	ASN
1	C	60	HIS
1	C	84	HIS
1	C	85	GLN
1	C	246	GLN
1	C	295	HIS
2	D	228	GLN
2	D	229	ASN
2	D	233	HIS
2	D	254	GLN
2	D	296	HIS
2	D	317	GLN
2	D	370	GLN
2	D	395	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	A	160	1	8,10,11	1.49	1 (12%)	10,14,16	1.03	0
1	TPO	C	160	1	8,10,11	1.50	2 (25%)	10,14,16	1.04	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	A	160	1	-	0/9/11/13	-
1	TPO	C	160	1	-	1/9/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	TPO	P-OG1	-3.36	1.53	1.59
1	C	160	TPO	P-OG1	-3.13	1.54	1.59
1	C	160	TPO	P-O3P	-2.31	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	INR	C	1298	-	27,27,27	2.10	10 (37%)	39,42,42	2.14	11 (28%)
3	INR	A	1298	-	27,27,27	2.16	12 (44%)	39,42,42	2.17	12 (30%)

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	INR	C	1298	-	-	1/10/34/34	0/4/4/4
3	INR	A	1298	-	-	1/10/34/34	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1298	INR	C12-N14	-5.97	1.29	1.36
3	A	1298	INR	C12-N14	-5.50	1.30	1.36
3	C	1298	INR	C9-N7	-4.68	1.31	1.38
3	A	1298	INR	C9-N7	-4.28	1.32	1.38
3	A	1298	INR	C15-C11	2.94	1.53	1.46
3	C	1298	INR	C16-N14	-2.89	1.33	1.38
3	A	1298	INR	C5-C6	2.68	1.43	1.38
3	A	1298	INR	C16-N14	-2.66	1.34	1.38
3	A	1298	INR	C5-C4	2.65	1.44	1.38
3	A	1298	INR	C20-C19	2.62	1.43	1.39
3	C	1298	INR	C5-C6	2.59	1.43	1.38
3	A	1298	INR	C4-C3	2.49	1.43	1.38
3	A	1298	INR	C1-N7	-2.47	1.34	1.38
3	C	1298	INR	C4-C3	2.46	1.43	1.38
3	C	1298	INR	C5-C4	2.35	1.43	1.38
3	A	1298	INR	C17-C18	2.34	1.42	1.38
3	A	1298	INR	C18-C19	2.31	1.42	1.38
3	C	1298	INR	C18-C19	2.24	1.42	1.38
3	C	1298	INR	C15-C11	2.14	1.51	1.46
3	A	1298	INR	C20-C15	2.01	1.43	1.39
3	C	1298	INR	C1-N7	-2.01	1.35	1.38
3	C	1298	INR	C17-C18	2.00	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	INR	C1-C2-C8	-6.42	103.05	107.35
3	A	1298	INR	C1-C2-C8	-6.36	103.09	107.35
3	A	1298	INR	C1-N7-C9	4.76	114.23	109.00
3	C	1298	INR	C1-N7-C9	4.54	113.99	109.00
3	A	1298	INR	C16-C15-C11	-3.90	103.55	106.63
3	C	1298	INR	O10-C8-C9	3.75	129.73	125.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	INR	C11-C12-N14	3.75	109.55	107.01
3	C	1298	INR	C3-C2-C1	3.46	122.43	118.84
3	A	1298	INR	O10-C8-C9	3.37	129.31	125.63
3	C	1298	INR	C15-C11-C12	-3.27	102.82	105.46
3	A	1298	INR	C15-C11-C12	-3.25	102.83	105.46
3	C	1298	INR	C16-C15-C11	-3.23	104.08	106.63
3	A	1298	INR	C3-C2-C1	3.20	122.16	118.84
3	C	1298	INR	C11-C12-N14	3.17	109.16	107.01
3	A	1298	INR	C15-C16-N14	3.10	111.72	108.23
3	C	1298	INR	C15-C16-N14	3.03	111.64	108.23
3	A	1298	INR	C3-C2-C8	2.60	134.75	129.70
3	C	1298	INR	C2-C1-N7	2.57	111.12	108.23
3	C	1298	INR	C3-C2-C8	2.48	134.52	129.70
3	A	1298	INR	C17-C16-N14	-2.33	126.12	130.83
3	A	1298	INR	C2-C1-N7	2.28	110.79	108.23
3	C	1298	INR	C17-C16-N14	-2.24	126.30	130.83
3	A	1298	INR	O13-C12-C11	-2.22	124.15	128.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1298	INR	C18-C19-S21-O24
3	C	1298	INR	C18-C19-S21-O24

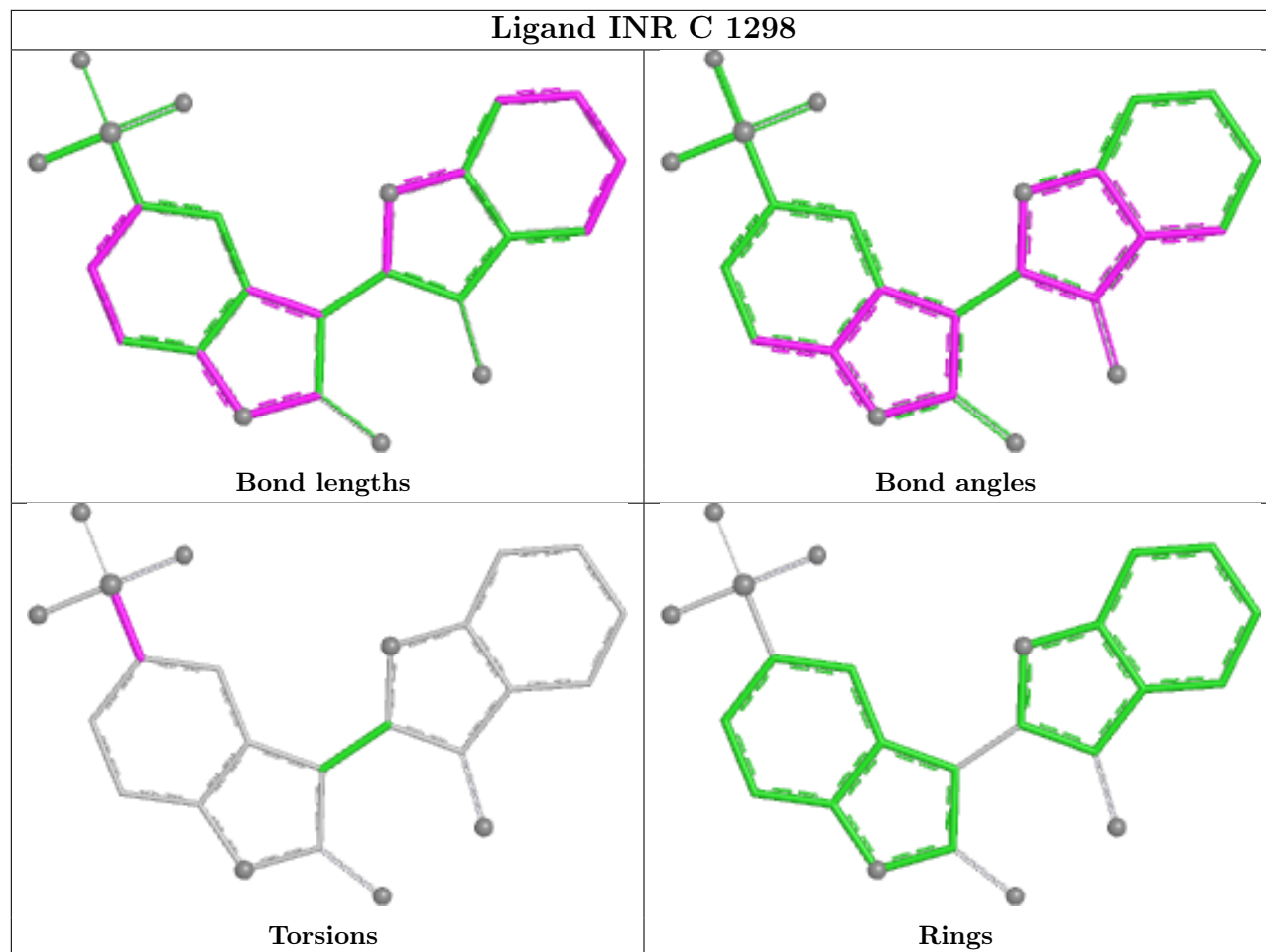
There are no ring outliers.

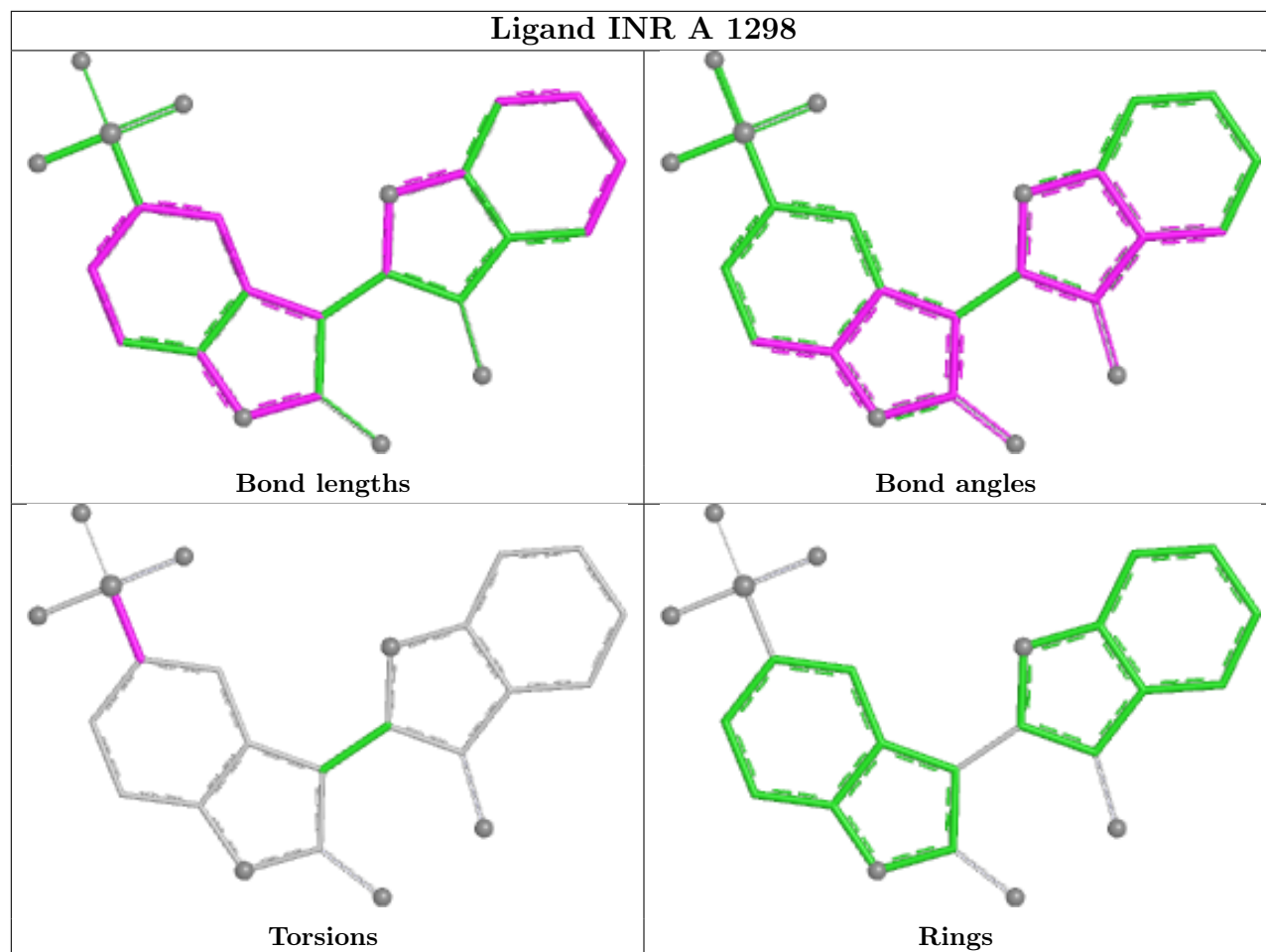
1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1298	INR	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 [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.