



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:03 AM UTC

PDB ID : 1OIY / pdb_00001oiy
Title : Structure of human Thr160-phospho CDK2/cyclin A complexed with a 6-cyclohexylmethoxy-2-anilino-purine inhibitor
Authors : Pratt, D.J.; Endicott, J.A.; Noble, M.E.M.
Deposited on : 2003-06-26
Resolution : 2.40 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:

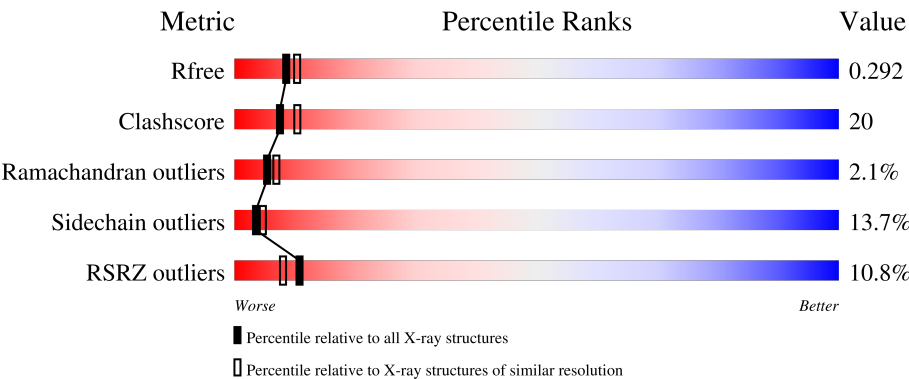
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	302	3% 64% 28% 5% ..
1	C	302	16% 44% 44% 9% ..
2	B	260	% 64% 31% ..
2	D	260	23% 51% 38% 10% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 9273 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.

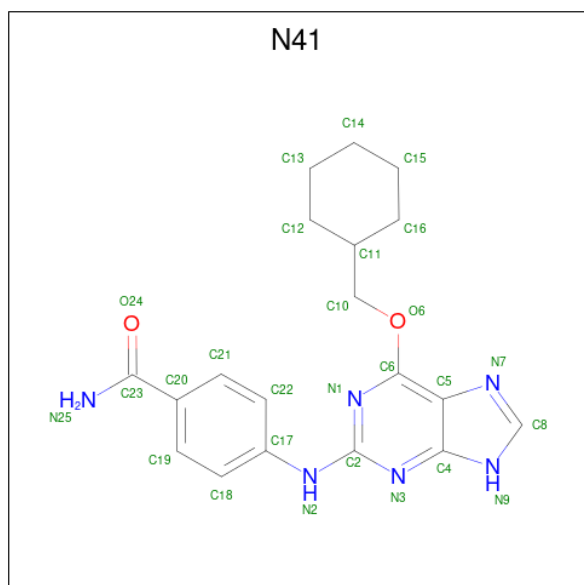
- Molecule 1 is a protein called CELL DIVISION PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	P	S	0	1	0
			2366	1538	401	418	1	8			
1	C	297	Total	C	N	O	P	S	0	1	0
			2391	1552	404	426	1	8			

- Molecule 2 is a protein called CYCLIN A2.

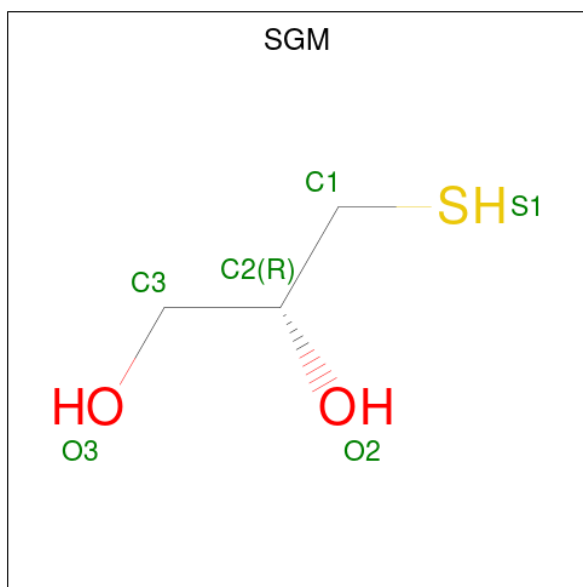
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	258	Total	C	N	O	S	0	1	0
			2088	1354	340	383	11			
2	D	258	Total	C	N	O	S	0	0	0
			2083	1350	339	383	11			

- Molecule 3 is 4-(6-CYCLOHEXYLMETHOXY-9H-PURIN-2-YLAMINO)--BENZAMIDE (CCD ID: N41) (formula: C₁₉H₂₂N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			27	19	6	2		
3	C	1	Total	C	N	O	0	0
			27	19	6	2		

- Molecule 4 is MONOTHIOGLYCEROL (CCD ID: SGM) (formula: $C_3H_8O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	S	0	0
			6	3	2	1		
4	D	1	Total	C	O	S	0	0
			6	3	2	1		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	119	Total	O	0	0
			119	119		
6	B	107	Total	O	0	0
			107	107		

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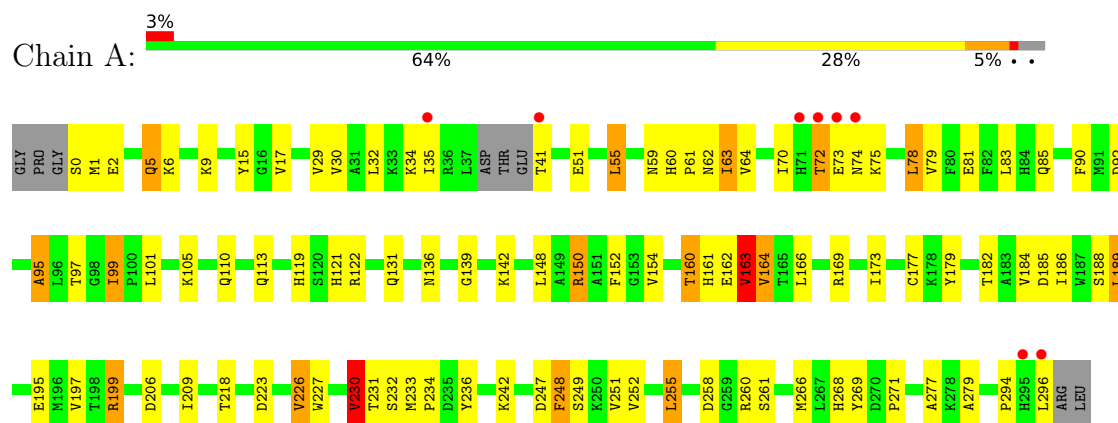
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	35	Total	O	0	0
			35	35		
6	D	17	Total	O	0	0
			17	17		

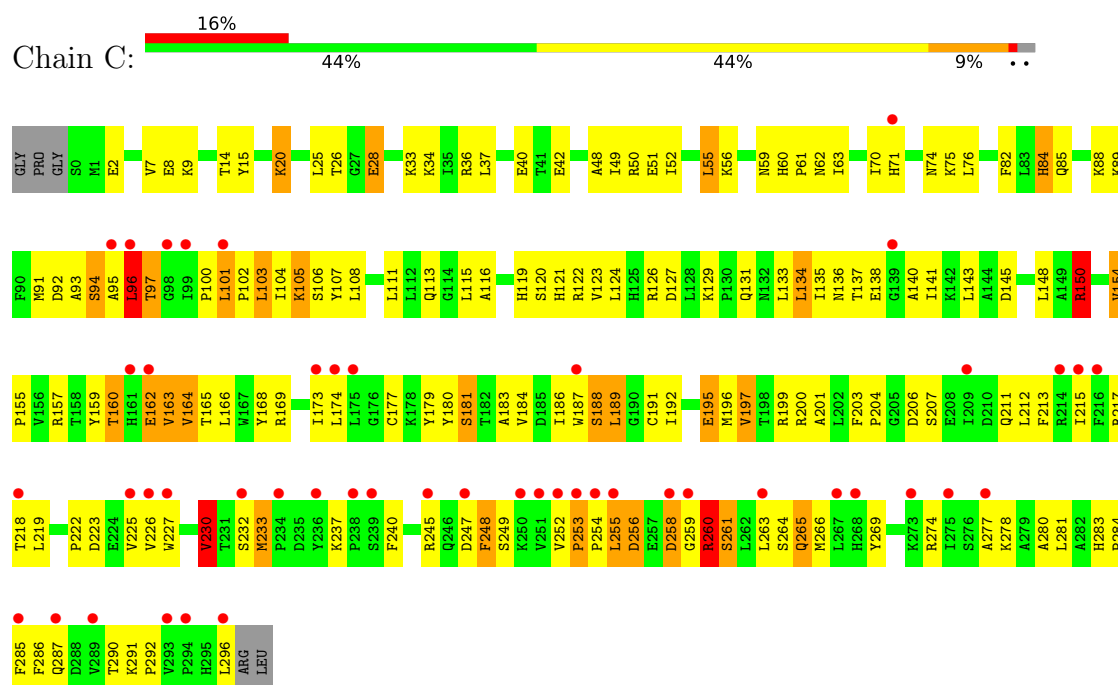
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: CELL DIVISION PROTEIN KINASE 2

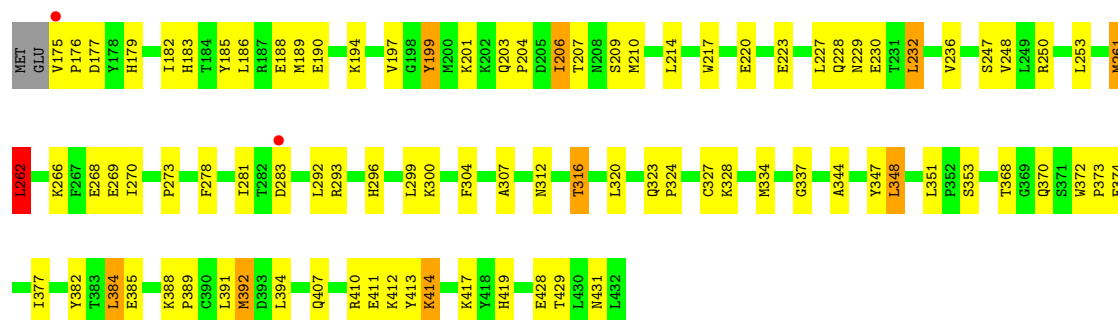


• Molecule 1: CELL DIVISION PROTEIN KINASE 2

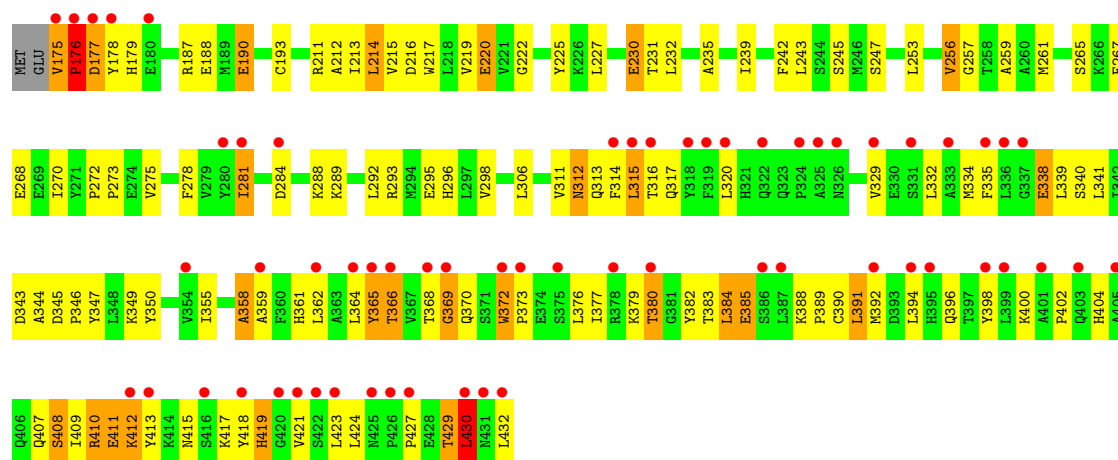


• Molecule 2: CYCLIN A2





• Molecule 2: CYCLIN A2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.00Å 134.87Å 147.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.40 99.65 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.6 (100.00-2.40) 91.6 (99.65-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.244 , 0.309 0.232 , 0.292	Depositor DCC
R_{free} test set	2717 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9273	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SGM, MG, TPO, N41

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	1.05	1/2419 (0.0%)	1.20	7/3280 (0.2%)
1	C	0.81	0/2445	1.10	4/3318 (0.1%)
2	B	1.03	2/2142 (0.1%)	1.19	7/2908 (0.2%)
2	D	0.78	1/2133 (0.0%)	1.11	5/2897 (0.2%)
All	All	0.93	4/9139 (0.0%)	1.15	23/12403 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	307	ALA	CA-CB	-7.88	1.43	1.52
2	B	261	MET	SD-CE	5.44	1.93	1.79
1	A	279	ALA	CA-CB	5.26	1.61	1.53
2	D	256	VAL	CA-CB	5.21	1.60	1.54

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	GLY	N-CA-C	-8.70	102.30	112.73
1	A	230	VAL	CB-CA-C	-8.51	100.65	112.14
1	A	163	VAL	N-CA-C	6.88	118.63	108.45
2	B	199	TYR	N-CA-C	6.72	119.62	111.82
1	A	230	VAL	N-CA-C	6.66	117.42	110.62
2	B	414	LYS	N-CA-C	-6.40	105.51	113.38
2	B	182	ILE	N-CA-C	6.40	117.08	110.36
2	D	430	LEU	N-CA-C	-5.84	104.85	113.61
2	D	176	PRO	N-CA-C	5.78	124.38	112.47
2	B	188	GLU	N-CA-C	-5.65	105.03	111.14
1	C	105	LYS	N-CA-C	-5.65	104.13	111.02
1	C	84	HIS	N-CA-C	5.57	118.08	111.33
1	C	150	ARG	N-CA-C	5.50	117.45	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	412	LYS	N-CA-C	-5.40	106.82	113.41
2	D	188	GLU	N-CA-C	-5.34	105.14	110.97
1	A	166	LEU	N-CA-C	5.33	117.78	111.33
1	C	97	THR	N-CA-C	5.29	117.79	111.71
1	A	218	THR	N-CA-C	-5.27	106.53	113.12
2	D	312	ASN	N-CA-C	5.24	116.99	111.28
2	B	186	LEU	N-CA-C	-5.20	105.79	111.82
1	A	188	SER	N-CA-C	-5.12	105.59	111.07
2	B	262	LEU	N-CA-C	-5.05	105.86	112.23
1	A	248	PHE	N-CA-C	5.05	118.22	111.75

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	2366	0	2413	77	0
1	C	2391	0	2433	136	0
2	B	2088	0	2115	65	0
2	D	2083	0	2107	108	0
3	A	27	0	22	4	0
3	C	27	0	22	2	0
4	B	6	0	7	0	0
4	D	6	0	8	1	0
5	B	1	0	0	0	0
6	A	119	0	0	5	0
6	B	107	0	0	7	0
6	C	35	0	0	8	0
6	D	17	0	0	2	0
All	All	9273	0	9127	368	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 20.

All (368) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:HIS:HD2	1:C:62:ASN:H	1.09	0.99
1:C:162:GLU:OE1	1:C:162:GLU:HA	1.65	0.93
1:A:15:TYR:HE2	1:A:35:ILE:CD1	1.82	0.92
1:C:177:CYS:HB2	1:C:233:MET:HE3	1.53	0.91
1:A:197:VAL:HG11	1:A:252:VAL:CG1	2.00	0.91
2:B:210:MET:HE1	2:B:250:ARG:HB2	1.51	0.90
1:A:15:TYR:HE2	1:A:35:ILE:HD11	1.40	0.86
2:D:332:LEU:HD11	2:D:398:TYR:OH	1.76	0.86
2:D:412:LYS:HE2	2:D:418:TYR:HE2	1.39	0.85
1:A:163:VAL:HG13	1:A:164:VAL:HG23	1.58	0.83
2:B:229:ASN:HD22	2:B:334:MET:HE3	1.42	0.83
1:C:203:PHE:CE1	1:C:215:ILE:HA	2.15	0.81
1:C:187:TRP:CD1	1:C:191:CYS:HG	1.99	0.81
1:C:60:HIS:CD2	1:C:62:ASN:H	1.98	0.80
1:A:177:CYS:HB2	1:A:233:MET:CE	2.11	0.80
1:C:259:GLY:O	1:C:261:SER:N	2.13	0.80
1:C:183:ALA:HB1	1:C:274:ARG:NH1	1.97	0.80
1:C:201:ALA:HB3	1:C:204:PRO:HG3	1.64	0.78
2:B:229:ASN:HD22	2:B:334:MET:CE	1.96	0.78
1:C:154:VAL:HG12	2:D:317:GLN:HG2	1.63	0.78
1:A:60:HIS:CD2	1:A:62:ASN:H	2.02	0.77
1:C:115:LEU:HD11	1:C:119:HIS:CE1	2.18	0.77
2:D:362:LEU:HB2	2:D:391:LEU:HD11	1.66	0.77
2:B:374:GLU:HA	2:B:377:ILE:HD12	1.66	0.76
1:A:154:VAL:O	2:B:316:THR:CG2	2.33	0.76
1:A:227:TRP:O	1:A:230:VAL:HG22	1.87	0.74
2:B:353:SER:HG	2:B:382:TYR:HH	1.30	0.74
1:C:223:ASP:O	1:C:226:VAL:HG12	1.87	0.74
2:B:388:LYS:HB3	2:B:389:PRO:HD3	1.70	0.74
2:D:214:LEU:HD21	2:D:239:ILE:HD13	1.68	0.74
2:D:230:GLU:HB3	2:D:268:GLU:HG2	1.69	0.74
1:C:163:VAL:CG1	1:C:164:VAL:HG23	2.19	0.73
1:C:136:ASN:HD21	1:C:140:ALA:HB3	1.54	0.73
2:B:392:MET:HE2	2:B:392:MET:HA	1.70	0.72
1:A:197:VAL:HG11	1:A:252:VAL:HG12	1.72	0.71
1:A:161:HIS:O	6:A:2063:HOH:O	2.08	0.71
1:C:258:ASP:HB3	1:C:285:PHE:HD1	1.55	0.71
2:B:175:VAL:N	2:B:179:HIS:CE1	2.59	0.71
1:A:154:VAL:O	2:B:316:THR:HG23	1.90	0.70
1:A:15:TYR:CE2	1:A:35:ILE:HD11	2.25	0.70
1:C:115:LEU:HD22	1:C:189:LEU:HD12	1.74	0.70
2:D:372:TRP:HZ2	2:D:382:TYR:HB2	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:222:GLY:HA2	2:D:227:LEU:HD12	1.73	0.70
2:B:223:GLU:CD	2:B:412:LYS:HG3	2.17	0.69
2:B:392:MET:HA	2:B:392:MET:CE	2.22	0.69
1:C:258:ASP:HB3	1:C:285:PHE:CD1	2.27	0.69
1:A:197:VAL:CG1	1:A:252:VAL:CG1	2.70	0.69
2:B:177:ASP:HB3	6:B:2015:HOH:O	1.91	0.69
1:C:136:ASN:ND2	1:C:140:ALA:HB3	2.08	0.69
2:D:372:TRP:NE1	2:D:382:TYR:O	2.26	0.69
1:C:133:LEU:C	1:C:134:LEU:HD23	2.17	0.69
2:B:175:VAL:N	2:B:179:HIS:HE1	1.92	0.68
1:A:227:TRP:O	1:A:230:VAL:CG2	2.41	0.68
2:D:361:HIS:HD2	2:D:391:LEU:HD21	1.58	0.68
2:D:215:VAL:O	2:D:219:VAL:HG23	1.94	0.67
2:B:407:GLN:OE1	2:B:410:ARG:HD3	1.95	0.67
1:A:60:HIS:HD2	1:A:62:ASN:H	1.38	0.67
1:C:183:ALA:HB1	1:C:274:ARG:HH11	1.57	0.67
1:A:92:ASP:O	1:A:95:ALA:HB2	1.94	0.67
1:A:177:CYS:SG	1:A:179:TYR:O	2.52	0.67
1:C:60:HIS:HD2	1:C:62:ASN:N	1.90	0.67
1:A:195:GLU:O	1:A:199:ARG:HA	1.94	0.67
1:A:197:VAL:HG11	1:A:252:VAL:HG11	1.75	0.67
1:C:155:PRO:HD2	2:D:316:THR:HG22	1.77	0.66
1:C:71:HIS:CD2	1:C:76:LEU:HD13	2.31	0.66
2:B:210:MET:HE1	2:B:250:ARG:CB	2.26	0.66
1:C:154:VAL:CG1	2:D:317:GLN:HG2	2.25	0.66
2:B:347:TYR:OH	2:B:394:LEU:HA	1.96	0.65
2:D:346:PRO:O	2:D:349:LYS:HG2	1.96	0.65
1:C:71:HIS:NE2	2:D:296:HIS:NE2	2.44	0.65
1:C:163:VAL:HG12	1:C:164:VAL:HG23	1.79	0.65
1:C:255:LEU:HG	1:C:259:GLY:HA3	1.78	0.65
2:D:335:PHE:CZ	2:D:339:LEU:HD11	2.32	0.65
1:A:15:TYR:CE2	1:A:35:ILE:CD1	2.74	0.64
1:A:60:HIS:CG	1:A:61:PRO:HD2	2.32	0.64
1:C:188:SER:O	1:C:192:ILE:HG13	1.98	0.64
2:B:229:ASN:ND2	2:B:334:MET:CE	2.61	0.64
2:B:207:THR:OG1	2:B:210:MET:HG3	1.98	0.64
2:D:214:LEU:HD22	2:D:253:LEU:HD11	1.79	0.64
1:C:258:ASP:O	1:C:261:SER:OG	2.16	0.63
2:D:396:GLN:HB3	2:D:400:LYS:NZ	2.12	0.63
1:C:195:GLU:HG3	1:C:201:ALA:HA	1.80	0.63
1:A:9:LYS:HE3	1:A:17:VAL:HG13	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:O	1:C:215:ILE:HB	1.99	0.62
2:D:412:LYS:HE2	2:D:418:TYR:CE2	2.29	0.62
1:C:115:LEU:CD2	1:C:189:LEU:HD12	2.30	0.62
1:A:15:TYR:HE2	1:A:35:ILE:HD13	1.65	0.62
2:D:407:GLN:O	2:D:411:GLU:HG2	1.99	0.62
1:C:261:SER:O	1:C:265:GLN:HG3	2.01	0.61
2:B:262:LEU:HD11	2:B:266:LYS:HE3	1.82	0.61
1:C:71:HIS:CE1	2:D:296:HIS:CD2	2.88	0.61
1:C:82:PHE:CE1	3:C:1298:N41:H18	2.36	0.61
1:C:107:TYR:O	1:C:111:LEU:HD12	2.02	0.60
1:C:129:LYS:HB3	6:C:2028:HOH:O	2.01	0.60
1:C:196:MET:O	6:C:2034:HOH:O	2.15	0.60
2:D:346:PRO:HD2	2:D:347:TYR:CE2	2.36	0.60
1:A:90:PHE:CE2	1:A:99:ILE:HD13	2.37	0.60
2:D:329:VAL:HG21	2:D:364:LEU:HD12	1.83	0.60
1:C:50:ARG:NE	2:D:267:PHE:O	2.34	0.59
1:C:237:LYS:HB2	1:C:240:PHE:CE1	2.37	0.59
1:A:131:GLN:HG2	3:A:1298:N41:H141	1.83	0.59
2:B:232:LEU:O	2:B:236:VAL:HG23	2.01	0.59
1:C:71:HIS:CD2	2:D:296:HIS:NE2	2.71	0.59
1:A:160:TPO:HG23	1:A:162:GLU:H	1.67	0.59
2:D:368:THR:O	2:D:370:GLN:N	2.35	0.58
1:C:60:HIS:HB3	1:C:63:ILE:HG13	1.85	0.58
1:C:280:ALA:O	1:C:286:PHE:HE2	1.86	0.58
2:B:175:VAL:O	2:B:177:ASP:N	2.37	0.58
1:C:163:VAL:HG13	1:C:164:VAL:HG23	1.84	0.58
1:C:169:ARG:HD2	1:C:174:LEU:HD23	1.86	0.58
1:A:177:CYS:HB2	1:A:233:MET:HE3	1.82	0.58
1:C:100:PRO:O	1:C:104:ILE:HG13	2.04	0.57
3:A:1298:N41:N1	3:A:1298:N41:H22	2.19	0.57
1:A:90:PHE:HE2	1:A:99:ILE:HD13	1.69	0.57
2:B:411:GLU:HA	2:B:414:LYS:HD2	1.87	0.57
1:A:249:SER:HA	1:A:260:ARG:HD3	1.87	0.57
1:C:223:ASP:H	1:C:226:VAL:HG12	1.69	0.57
2:D:372:TRP:HE1	2:D:383:THR:HA	1.70	0.57
1:C:40:GLU:O	2:D:288:LYS:HE3	2.05	0.56
2:D:366:THR:OG1	2:D:427:PRO:HD3	2.05	0.56
1:A:60:HIS:HB3	1:A:63:ILE:HG13	1.87	0.56
2:D:335:PHE:HB2	2:D:413:TYR:CD2	2.40	0.56
1:C:168:TYR:OH	1:C:195:GLU:OE1	2.16	0.56
2:D:230:GLU:HA	2:D:230:GLU:OE1	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:O	1:A:55:LEU:HB2	2.05	0.56
2:D:187:ARG:HD2	2:D:190:GLU:OE2	2.06	0.56
2:D:346:PRO:HB2	2:D:349:LYS:HE2	1.87	0.56
1:A:177:CYS:HB2	1:A:233:MET:HE1	1.87	0.55
2:D:404:HIS:CE1	6:D:2015:HOH:O	2.59	0.55
1:A:62:ASN:HA	1:A:142:LYS:HG2	1.88	0.55
1:A:154:VAL:O	2:B:316:THR:HG22	2.05	0.55
2:D:213:ILE:O	2:D:216:ASP:HB3	2.07	0.55
2:D:273:PRO:HG2	2:D:278:PHE:CZ	2.42	0.55
1:C:256:ASP:OD2	1:C:256:ASP:N	2.38	0.55
2:B:190:GLU:HG3	2:B:351:LEU:HD22	1.88	0.54
1:A:72:THR:HB	1:A:75:LYS:O	2.07	0.54
2:B:296:HIS:C	2:B:296:HIS:CD2	2.86	0.54
1:C:197:VAL:HG11	1:C:255:LEU:HD13	1.88	0.54
1:A:95:ALA:HA	6:A:2081:HOH:O	2.06	0.54
1:C:111:LEU:HD11	1:C:141:ILE:HD13	1.88	0.54
1:C:253:PRO:HB2	1:C:254:PRO:HD3	1.88	0.54
2:D:358:ALA:O	2:D:359:ALA:C	2.50	0.54
1:C:263:LEU:O	1:C:266:MET:N	2.41	0.54
1:C:111:LEU:HD23	1:C:143:LEU:HD23	1.90	0.54
2:D:239:ILE:HG22	2:D:243:LEU:CD1	2.38	0.54
2:D:383:THR:O	2:D:385:GLU:N	2.41	0.54
2:B:428:GLU:HG2	6:B:2105:HOH:O	2.07	0.53
1:A:85:GLN:HE21	1:A:90:PHE:HB2	1.73	0.53
2:D:211:ARG:O	2:D:215:VAL:HG23	2.08	0.53
2:B:299:LEU:HD13	2:B:304:PHE:CE1	2.43	0.53
1:C:278:LYS:HA	1:C:281:LEU:HD12	1.90	0.53
2:B:273:PRO:HB2	2:B:278:PHE:CE2	2.44	0.53
1:A:72:THR:HG22	1:A:75:LYS:H	1.74	0.53
1:C:71:HIS:CE1	2:D:296:HIS:NE2	2.77	0.53
3:A:1298:N41:N1	3:A:1298:N41:C22	2.71	0.53
1:C:183:ALA:O	1:C:186:ILE:HB	2.10	0.52
2:D:346:PRO:HD2	2:D:347:TYR:CD2	2.44	0.52
2:D:365:TYR:O	2:D:366:THR:C	2.51	0.52
1:C:187:TRP:NE1	1:C:191:CYS:SG	2.82	0.52
1:A:121:HIS:HD2	2:B:185:TYR:CE1	2.27	0.52
1:C:292:PRO:HD2	6:C:2026:HOH:O	2.08	0.52
1:A:51:GLU:HG3	1:A:55:LEU:HD22	1.91	0.52
1:C:165:THR:HB	6:C:2028:HOH:O	2.08	0.52
1:C:95:ALA:O	1:C:96:LEU:O	2.28	0.52
1:C:173:ILE:HD11	1:C:184:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:LYS:HD3	2:B:413:TYR:CE1	2.46	0.51
1:A:136:ASN:C	1:A:136:ASN:OD1	2.54	0.51
2:D:388:LYS:HG2	2:D:392:MET:HG2	1.92	0.51
2:D:421:VAL:HA	2:D:424:LEU:HG	1.92	0.51
2:D:239:ILE:HG22	2:D:243:LEU:HD11	1.93	0.51
1:A:223:ASP:OD1	1:A:226:VAL:HG12	2.11	0.51
2:D:314:PHE:O	2:D:315:LEU:C	2.53	0.51
1:A:64:VAL:HG13	1:A:64:VAL:O	2.10	0.51
1:C:160:TPO:OG1	2:D:270:ILE:HG23	2.11	0.51
2:D:313:GLN:O	2:D:317:GLN:HG3	2.10	0.51
1:C:255:LEU:CG	1:C:259:GLY:HA3	2.41	0.50
2:D:175:VAL:O	2:D:177:ASP:N	2.45	0.50
1:C:219:LEU:HB3	1:C:269:TYR:HE2	1.75	0.50
1:C:283:HIS:CG	1:C:284:PRO:HD2	2.47	0.50
1:C:183:ALA:CB	1:C:274:ARG:NH1	2.71	0.50
2:D:372:TRP:CZ2	2:D:382:TYR:HB2	2.42	0.50
2:D:216:ASP:O	2:D:219:VAL:N	2.45	0.50
2:D:176:PRO:HA	2:D:179:HIS:CG	2.47	0.49
2:B:175:VAL:C	2:B:177:ASP:H	2.18	0.49
1:A:64:VAL:O	1:A:64:VAL:CG1	2.60	0.49
1:A:251:VAL:HG12	1:A:252:VAL:HG23	1.93	0.49
2:B:270:ILE:HG13	6:B:2048:HOH:O	2.12	0.49
2:D:235:ALA:O	2:D:239:ILE:HG13	2.10	0.49
2:B:388:LYS:HB3	2:B:389:PRO:CD	2.42	0.49
1:C:92:ASP:O	1:C:94:SER:N	2.46	0.49
2:D:350:TYR:CE1	2:D:390:CYS:HB2	2.48	0.49
1:A:5:GLN:HA	1:A:5:GLN:HE21	1.78	0.49
2:D:376:LEU:O	2:D:380:THR:HG23	2.13	0.49
2:D:365:TYR:O	2:D:369:GLY:N	2.46	0.49
2:B:190:GLU:OE2	2:B:353:SER:HB3	2.12	0.49
1:C:84:HIS:CD2	1:C:85:GLN:HG2	2.49	0.48
1:C:187:TRP:NE1	1:C:191:CYS:HG	2.12	0.48
2:B:227:LEU:HD12	2:B:261:MET:HE3	1.95	0.48
2:D:344:ALA:O	2:D:347:TYR:N	2.47	0.48
1:C:223:ASP:N	1:C:226:VAL:HG12	2.29	0.48
1:C:124:LEU:HB3	1:C:126:ARG:HG3	1.94	0.48
2:D:259:ALA:HB1	2:D:295:GLU:HA	1.95	0.48
1:A:169:ARG:HD3	1:A:173:ILE:CG2	2.43	0.48
2:D:396:GLN:HB3	2:D:400:LYS:HZ2	1.78	0.47
2:D:419:HIS:ND1	2:D:419:HIS:N	2.62	0.47
1:C:20:LYS:HD2	1:C:82:PHE:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:PRO:HA	1:C:226:VAL:HG11	1.96	0.47
2:D:193:CYS:SG	4:D:1193:SGM:S1	2.40	0.47
2:D:338:GLU:HB3	2:D:409:ILE:HG21	1.96	0.47
2:D:362:LEU:HD13	2:D:430:LEU:HD22	1.96	0.47
1:A:78:LEU:HD23	1:A:78:LEU:N	2.28	0.47
1:A:162:GLU:HA	6:A:2063:HOH:O	2.15	0.47
1:A:231:THR:HA	1:A:236:TYR:CD1	2.50	0.47
2:B:327:CYS:HB3	2:B:419:HIS:CE1	2.49	0.47
2:B:407:GLN:O	2:B:411:GLU:HG2	2.15	0.47
1:C:51:GLU:O	1:C:55:LEU:HB2	2.15	0.47
2:D:338:GLU:O	2:D:340:SER:N	2.47	0.47
1:C:105:LYS:O	1:C:106:SER:C	2.58	0.47
1:C:71:HIS:HD2	1:C:76:LEU:HD13	1.76	0.47
1:C:7:VAL:HB	1:C:20:LYS:HB3	1.97	0.46
1:A:269:TYR:O	1:A:271:PRO:HD3	2.15	0.46
2:D:343:ASP:HA	6:D:2014:HOH:O	2.15	0.46
1:A:186:ILE:HD11	1:A:277:ALA:N	2.29	0.46
2:B:214:LEU:HD22	2:B:253:LEU:HG	1.97	0.46
1:C:49:ILE:HG23	2:D:306:LEU:CD1	2.46	0.46
1:C:121:HIS:O	1:C:123:VAL:HG23	2.15	0.46
1:C:108:LEU:HD11	1:C:266:MET:HE1	1.96	0.46
1:C:134:LEU:HD23	1:C:134:LEU:N	2.30	0.46
2:D:388:LYS:O	2:D:389:PRO:C	2.58	0.46
1:C:92:ASP:C	1:C:94:SER:N	2.73	0.46
2:B:183:HIS:HE1	6:B:2064:HOH:O	1.98	0.46
1:C:121:HIS:C	1:C:122:ARG:HG3	2.40	0.46
1:A:161:HIS:O	1:A:161:HIS:CD2	2.68	0.46
2:B:175:VAL:C	2:B:177:ASP:N	2.73	0.46
2:D:175:VAL:C	2:D:179:HIS:CE1	2.94	0.46
2:D:256:VAL:O	2:D:257:GLY:C	2.57	0.46
1:A:150:ARG:NH1	2:B:268:GLU:O	2.47	0.45
1:C:201:ALA:CB	1:C:204:PRO:HG3	2.41	0.45
2:D:253:LEU:HD12	2:D:253:LEU:O	2.16	0.45
2:D:329:VAL:HG11	2:D:364:LEU:CD1	2.46	0.45
2:D:365:TYR:HB3	2:D:366:THR:H	1.66	0.45
2:D:427:PRO:HB2	2:D:429:THR:O	2.15	0.45
1:A:32:LEU:CD2	1:A:79:VAL:HG22	2.46	0.45
1:C:253:PRO:CB	1:C:254:PRO:HD3	2.47	0.45
1:A:1:MET:SD	1:A:70:ILE:HD13	2.57	0.45
1:C:55:LEU:HD12	1:C:55:LEU:HA	1.59	0.45
2:D:242:PHE:CD1	2:D:298:VAL:HG22	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:ASN:ND2	6:C:2017:HOH:O	2.49	0.45
2:D:176:PRO:HA	2:D:179:HIS:ND1	2.32	0.45
2:D:212:ALA:O	2:D:216:ASP:HB2	2.16	0.45
2:D:345:ASP:HA	2:D:346:PRO:HA	1.63	0.45
2:D:361:HIS:CD2	2:D:391:LEU:HD21	2.46	0.45
1:A:119:HIS:HD2	6:B:2016:HOH:O	2.00	0.45
1:C:52:ILE:O	1:C:56:LYS:HG3	2.16	0.45
3:C:1298:N41:H141	6:C:2029:HOH:O	2.17	0.45
1:C:115:LEU:HD11	1:C:119:HIS:NE2	2.32	0.45
2:D:372:TRP:NE1	2:D:383:THR:HA	2.32	0.45
2:B:223:GLU:OE2	2:B:412:LYS:HE3	2.16	0.44
2:B:372:TRP:HA	2:B:373:PRO:HD2	1.88	0.44
2:B:411:GLU:O	2:B:412:LYS:C	2.59	0.44
2:B:388:LYS:O	2:B:389:PRO:C	2.59	0.44
1:C:121:HIS:O	1:C:122:ARG:HG3	2.17	0.44
1:C:154:VAL:HA	1:C:155:PRO:HA	1.66	0.44
2:D:225:TYR:HE1	2:D:281:ILE:HG21	1.82	0.44
1:C:37:LEU:HB2	1:C:74:ASN:O	2.17	0.44
1:C:92:ASP:C	1:C:94:SER:H	2.26	0.44
2:D:281:ILE:H	2:D:281:ILE:HG13	1.49	0.44
1:C:256:ASP:C	1:C:258:ASP:N	2.75	0.44
2:D:219:VAL:O	2:D:220:GLU:C	2.60	0.44
2:D:390:CYS:O	2:D:394:LEU:N	2.42	0.44
1:C:261:SER:O	1:C:265:GLN:CG	2.65	0.44
2:D:315:LEU:O	2:D:316:THR:C	2.60	0.44
2:D:317:GLN:O	2:D:320:LEU:HD12	2.18	0.44
2:D:373:PRO:HD2	2:D:376:LEU:HD12	1.98	0.44
2:D:430:LEU:H	2:D:430:LEU:HG	1.54	0.44
1:C:89:LYS:NZ	6:C:2025:HOH:O	2.50	0.44
2:D:329:VAL:HG11	2:D:364:LEU:HD13	1.98	0.44
1:C:15:TYR:CZ	1:C:33:LYS:HE2	2.53	0.43
1:C:207:SER:O	1:C:211:GLN:N	2.41	0.43
1:A:110:GLN:O	1:A:113:GLN:HB2	2.17	0.43
2:B:206:ILE:HD12	2:B:253:LEU:HD13	1.99	0.43
2:D:217:TRP:HA	2:D:220:GLU:HG3	2.00	0.43
2:D:362:LEU:CD1	2:D:430:LEU:HD22	2.48	0.43
2:B:247:SER:OG	1:C:28:GLU:HG3	2.18	0.43
1:C:25:LEU:HD23	1:C:25:LEU:HA	1.90	0.43
2:B:344:ALA:HB1	2:B:348:LEU:HD22	1.99	0.43
2:D:338:GLU:O	2:D:341:LEU:N	2.52	0.43
1:A:55:LEU:HD12	1:A:55:LEU:HA	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:316:THR:HG21	6:B:2009:HOH:O	2.19	0.43
1:C:159:TYR:HB2	1:C:180:TYR:CZ	2.53	0.43
1:C:249:SER:HA	1:C:260:ARG:HD3	1.99	0.43
2:D:396:GLN:HB3	2:D:400:LYS:CE	2.48	0.43
1:A:169:ARG:HD3	1:A:173:ILE:HG22	2.01	0.43
1:C:113:GLN:HG2	1:C:281:LEU:HD21	2.01	0.43
2:D:214:LEU:HD22	2:D:253:LEU:CD1	2.49	0.43
2:D:392:MET:HE1	2:D:430:LEU:HD11	2.00	0.43
2:B:190:GLU:CD	2:B:353:SER:HB3	2.44	0.43
2:B:194:LYS:NZ	6:B:2024:HOH:O	2.51	0.43
2:B:199:TYR:CE2	2:B:348:LEU:HD21	2.54	0.43
2:D:231:THR:HG22	2:D:261:MET:HE3	2.00	0.43
1:A:15:TYR:CE2	1:A:35:ILE:HD13	2.50	0.43
2:D:273:PRO:HG2	2:D:278:PHE:CE2	2.54	0.43
2:B:248:VAL:HG22	1:C:26:THR:HB	1.99	0.42
1:C:213:PHE:O	1:C:217:ARG:N	2.51	0.42
1:C:255:LEU:HD12	1:C:255:LEU:HA	1.86	0.42
1:A:122:ARG:HA	1:A:152:PHE:CE1	2.55	0.42
1:C:248:PHE:CZ	1:C:263:LEU:HD23	2.54	0.42
2:D:402:PRO:HD3	2:D:410:ARG:HH11	1.83	0.42
1:A:139:GLY:HA2	1:A:294:PRO:HD3	2.01	0.42
2:B:203:GLN:HA	2:B:204:PRO:HD2	1.85	0.42
2:B:384:LEU:HD12	2:B:384:LEU:HA	1.82	0.42
1:C:227:TRP:O	1:C:230:VAL:HG22	2.20	0.42
2:D:265:SER:HB3	2:D:272:PRO:HB3	2.02	0.42
1:A:268:HIS:CD2	6:A:2091:HOH:O	2.72	0.42
2:B:217:TRP:O	2:B:220:GLU:HB2	2.19	0.42
1:C:104:ILE:HD13	1:C:196:MET:HB3	2.01	0.42
1:C:126:ARG:CZ	1:C:150:ARG:HB3	2.49	0.42
1:C:136:ASN:HD21	1:C:140:ALA:CB	2.26	0.42
2:D:362:LEU:HB2	2:D:391:LEU:CD1	2.41	0.42
1:A:233:MET:O	1:A:234:PRO:C	2.63	0.42
1:C:227:TRP:O	1:C:230:VAL:CG2	2.68	0.42
1:C:277:ALA:HB3	2:D:178:TYR:OH	2.20	0.42
2:D:312:ASN:O	2:D:316:THR:OG1	2.33	0.42
2:B:320:LEU:HD23	2:B:320:LEU:HA	1.81	0.42
2:B:293:ARG:CZ	1:C:2:GLU:CD	2.93	0.42
2:D:407:GLN:OE1	2:D:410:ARG:HD3	2.19	0.41
1:A:197:VAL:CG1	1:A:252:VAL:HG11	2.45	0.41
2:B:228:GLN:N	2:B:269:GLU:OE2	2.48	0.41
2:B:230:GLU:OE1	2:B:312:ASN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:323:GLN:HA	2:B:324:PRO:HA	1.84	0.41
1:C:101:LEU:N	1:C:102:PRO:CD	2.83	0.41
1:C:259:GLY:C	1:C:261:SER:N	2.78	0.41
1:C:280:ALA:O	1:C:286:PHE:CE2	2.70	0.41
1:A:83:LEU:O	3:A:1298:N41:N2	2.46	0.41
1:C:88:LYS:HB2	1:C:131:GLN:HE21	1.86	0.41
1:C:255:LEU:CD2	1:C:259:GLY:HA3	2.50	0.41
1:C:253:PRO:HD2	1:C:254:PRO:HD3	2.03	0.41
2:D:216:ASP:CG	2:D:408:SER:OG	2.63	0.41
1:A:258:ASP:O	1:A:261:SER:HB3	2.20	0.41
2:B:368:THR:CB	2:B:370:GLN:HE21	2.34	0.41
1:C:60:HIS:CG	1:C:61:PRO:HD2	2.56	0.41
1:C:116:ALA:O	1:C:120:SER:OG	2.34	0.41
2:D:278:PHE:HA	2:D:281:ILE:HD11	2.01	0.41
2:D:289:LYS:HG3	2:D:293:ARG:HD2	2.01	0.41
2:D:409:ILE:O	2:D:413:TYR:HD1	2.03	0.41
1:C:101:LEU:HD22	1:C:101:LEU:HA	1.91	0.41
1:A:119:HIS:CD2	1:A:182:THR:HB	2.56	0.41
1:A:195:GLU:O	1:A:199:ARG:CA	2.66	0.41
1:A:199:ARG:HD2	6:A:2081:HOH:O	2.21	0.41
1:C:137:THR:O	1:C:138:GLU:HG3	2.20	0.41
1:C:219:LEU:HB3	1:C:269:TYR:CE2	2.53	0.41
1:C:263:LEU:O	1:C:265:GLN:N	2.54	0.41
1:A:9:LYS:HE3	1:A:17:VAL:CG1	2.48	0.41
1:A:119:HIS:HE1	1:A:185:ASP:OD2	2.04	0.41
1:A:209:ILE:HD12	1:A:209:ILE:HA	1.94	0.41
1:A:105:LYS:HB2	1:A:105:LYS:HE3	1.72	0.40
1:C:42:GLU:HA	2:D:275:VAL:CG2	2.51	0.40
1:C:177:CYS:C	1:C:179:TYR:H	2.28	0.40
1:A:189:LEU:HB3	1:A:266:MET:HE1	2.04	0.40
2:B:388:LYS:O	2:B:392:MET:HG2	2.21	0.40
1:C:103:LEU:HD11	1:C:107:TYR:CZ	2.56	0.40
1:C:169:ARG:HD2	1:C:174:LEU:CD2	2.49	0.40
1:A:255:LEU:O	1:A:260:ARG:NH1	2.54	0.40
1:C:15:TYR:OH	1:C:48:ALA:HA	2.22	0.40
1:C:181:SER:C	1:C:183:ALA:H	2.28	0.40
1:C:181:SER:N	6:C:2033:HOH:O	2.52	0.40
2:B:429:THR:OG1	2:B:431:ASN:ND2	2.54	0.40
1:C:105:LYS:HE3	1:C:105:LYS:HB2	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	290/302 (96%)	272 (94%)	16 (6%)	2 (1%)	18	28
1	C	295/302 (98%)	250 (85%)	33 (11%)	12 (4%)	2	2
2	B	257/260 (99%)	248 (96%)	8 (3%)	1 (0%)	30	43
2	D	256/260 (98%)	217 (85%)	31 (12%)	8 (3%)	3	3
All	All	1098/1124 (98%)	987 (90%)	88 (8%)	23 (2%)	5	7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	96	LEU
1	C	260	ARG
2	D	176	PRO
2	D	365	TYR
2	D	369	GLY
1	A	95	ALA
1	A	164	VAL
1	C	93	ALA
1	C	166	LEU
1	C	264	SER
2	D	311	VAL
2	B	176	PRO
1	C	127	ASP
1	C	145	ASP
1	C	164	VAL
1	C	261	SER
2	D	384	LEU
1	C	258	ASP
2	D	315	LEU
2	D	358	ALA
2	D	372	TRP
1	C	253	PRO
1	C	230	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	259/264 (98%)	225 (87%)	34 (13%)	4	5
1	C	262/264 (99%)	213 (81%)	49 (19%)	1	2
2	B	233/234 (100%)	214 (92%)	19 (8%)	10	18
2	D	232/234 (99%)	199 (86%)	33 (14%)	3	4
All	All	986/996 (99%)	851 (86%)	135 (14%)	3	5

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	SER
1	A	2	GLU
1	A	5	GLN
1	A	6	LYS
1	A	29	VAL
1	A	30	VAL
1	A	34	LYS
1	A	41	THR
1	A	55	LEU
1	A	59	ASN
1	A	63	ILE
1	A	72	THR
1	A	73	GLU
1	A	74	ASN
1	A	78	LEU
1	A	81	GLU
1	A	97	THR
1	A	99	ILE
1	A	101	LEU
1	A	148	LEU
1	A	150	ARG
1	A	163	VAL
1	A	184	VAL
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	199	ARG
1	A	206	ASP
1	A	226	VAL
1	A	230	VAL
1	A	232	SER
1	A	242	LYS
1	A	247	ASP
1	A	248	PHE
1	A	255	LEU
1	A	296	LEU
2	B	189	MET
2	B	197	VAL
2	B	201	LYS
2	B	206	ILE
2	B	209	SER
2	B	232	LEU
2	B	262	LEU
2	B	281	ILE
2	B	283	ASP
2	B	292	LEU
2	B	300	LYS
2	B	316	THR
2	B	328	LYS
2	B	348	LEU
2	B	384	LEU
2	B	385	GLU
2	B	391	LEU
2	B	392	MET
2	B	417	LYS
1	C	8	GLU
1	C	9	LYS
1	C	14	THR
1	C	20	LYS
1	C	28	GLU
1	C	34	LYS
1	C	36	ARG
1	C	55	LEU
1	C	70	ILE
1	C	75	LYS
1	C	91	MET
1	C	94	SER
1	C	96	LEU

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Mol	Chain	Res	Type
1	C	97	THR
1	C	101	LEU
1	C	103	LEU
1	C	134	LEU
1	C	135	ILE
1	C	148	LEU
1	C	150	ARG
1	C	154	VAL
1	C	157	ARG
1	C	162	GLU
1	C	163	VAL
1	C	181	SER
1	C	188	SER
1	C	189	LEU
1	C	195	GLU
1	C	197	VAL
1	C	199	ARG
1	C	200	ARG
1	C	206	ASP
1	C	218	THR
1	C	225	VAL
1	C	230	VAL
1	C	232	SER
1	C	233	MET
1	C	245	ARG
1	C	247	ASP
1	C	248	PHE
1	C	252	VAL
1	C	255	LEU
1	C	256	ASP
1	C	260	ARG
1	C	265	GLN
1	C	287	GLN
1	C	290	THR
1	C	291	LYS
1	C	296	LEU
2	D	175	VAL
2	D	176	PRO
2	D	177	ASP
2	D	190	GLU
2	D	214	LEU
2	D	220	GLU

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Mol	Chain	Res	Type
2	D	230	GLU
2	D	232	LEU
2	D	245	SER
2	D	247	SER
2	D	281	ILE
2	D	284	ASP
2	D	292	LEU
2	D	334	MET
2	D	338	GLU
2	D	355	ILE
2	D	366	THR
2	D	377	ILE
2	D	379	LYS
2	D	380	THR
2	D	384	LEU
2	D	385	GLU
2	D	391	LEU
2	D	408	SER
2	D	410	ARG
2	D	411	GLU
2	D	415	ASN
2	D	417	LYS
2	D	419	HIS
2	D	423	LEU
2	D	429	THR
2	D	430	LEU
2	D	432	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	5	GLN
1	A	60	HIS
1	A	119	HIS
1	A	121	HIS
1	A	161	HIS
1	A	265	GLN
1	A	268	HIS
2	B	179	HIS
2	B	183	HIS
2	B	254	GLN
2	B	296	HIS

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Mol	Chain	Res	Type
2	B	317	GLN
2	B	322	GLN
2	B	370	GLN
2	B	425	ASN
2	B	431	ASN
1	C	60	HIS
1	C	62	ASN
1	C	71	HIS
1	C	74	ASN
1	C	85	GLN
1	C	265	GLN
1	C	268	HIS
1	C	295	HIS
2	D	179	HIS
2	D	254	GLN
2	D	322	GLN
2	D	395	HIS

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	1.28	1 (12%)	10,14,16	1.17	1 (10%)
1	TPO	A	160	1	8,10,11	1.60	1 (12%)	10,14,16	1.29	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	-
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	A	160	TPO	P-O1P	3.31	1.60	1.50
1	C	160	TPO	P-O1P	2.59	1.58	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	TPO	P-OG1-CB	-2.57	116.34	123.33

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	160	TPO	CB-OG1-P-O3P
1	A	160	TPO	CB-OG1-P-O1P
1	C	160	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	SGM	D	1193	-	5,5,5	0.28	0	5,5,5	0.69	0
3	N41	A	1298	-	30,30,30	1.55	5 (16%)	40,41,41	2.11	10 (25%)
4	SGM	B	1193	2	5,5,5	0.55	0	5,5,5	0.78	0
3	N41	C	1298	-	30,30,30	1.08	3 (10%)	40,41,41	1.78	8 (20%)

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	SGM	D	1193	-	-	3/4/4/4	-
3	N41	A	1298	-	-	1/13/21/21	0/4/4/4
4	SGM	B	1193	2	-	1/4/4/4	-
3	N41	C	1298	-	-	6/13/21/21	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	N41	C8-N7	3.92	1.40	1.32
3	A	1298	N41	C5-C6	3.36	1.47	1.41
3	A	1298	N41	C5-C4	3.22	1.44	1.39
3	C	1298	N41	C5-C6	3.13	1.47	1.41
3	A	1298	N41	C6-N1	2.74	1.36	1.32
3	C	1298	N41	C8-N7	2.52	1.37	1.32
3	A	1298	N41	O6-C6	2.20	1.38	1.34
3	C	1298	N41	C5-C4	2.00	1.42	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1298	N41	C4-N9-C8	-5.58	101.23	106.43
3	A	1298	N41	C5-C4-N3	-5.37	121.28	126.55
3	A	1298	N41	C5-C6-N1	-4.53	117.44	123.49
3	C	1298	N41	C5-C4-N3	-4.47	122.17	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1298	N41	C2-N1-C6	4.35	122.88	115.38
3	A	1298	N41	C5-C4-N9	4.33	111.46	105.67
3	A	1298	N41	C2-N1-C6	4.14	122.51	115.38
3	A	1298	N41	O6-C6-C5	3.62	121.52	116.73
3	C	1298	N41	C17-N2-C2	-3.53	119.87	129.38
3	C	1298	N41	N3-C2-N1	-3.47	120.58	126.26
3	C	1298	N41	C5-C6-N1	-3.24	119.16	123.49
3	C	1298	N41	C4-N9-C8	-3.21	103.44	106.43
3	A	1298	N41	N3-C2-N1	-2.97	121.40	126.26
3	C	1298	N41	C5-C4-N9	2.48	108.98	105.67
3	C	1298	N41	O6-C6-C5	2.38	119.88	116.73
3	A	1298	N41	C16-C11-C12	2.25	114.80	109.29
3	A	1298	N41	C17-N2-C2	-2.25	123.32	129.38
3	A	1298	N41	C4-C5-N7	-2.21	107.60	110.67

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1193	SGM	C1-C2-C3-O3
4	D	1193	SGM	O2-C2-C3-O3
3	C	1298	N41	C19-C20-C23-N25
3	C	1298	N41	C19-C20-C23-O24
3	C	1298	N41	C21-C20-C23-N25
3	C	1298	N41	C21-C20-C23-O24
3	C	1298	N41	C18-C17-N2-C2
4	B	1193	SGM	S1-C1-C2-O2
4	D	1193	SGM	S1-C1-C2-O2
3	C	1298	N41	C22-C17-N2-C2
3	A	1298	N41	O6-C10-C11-C12

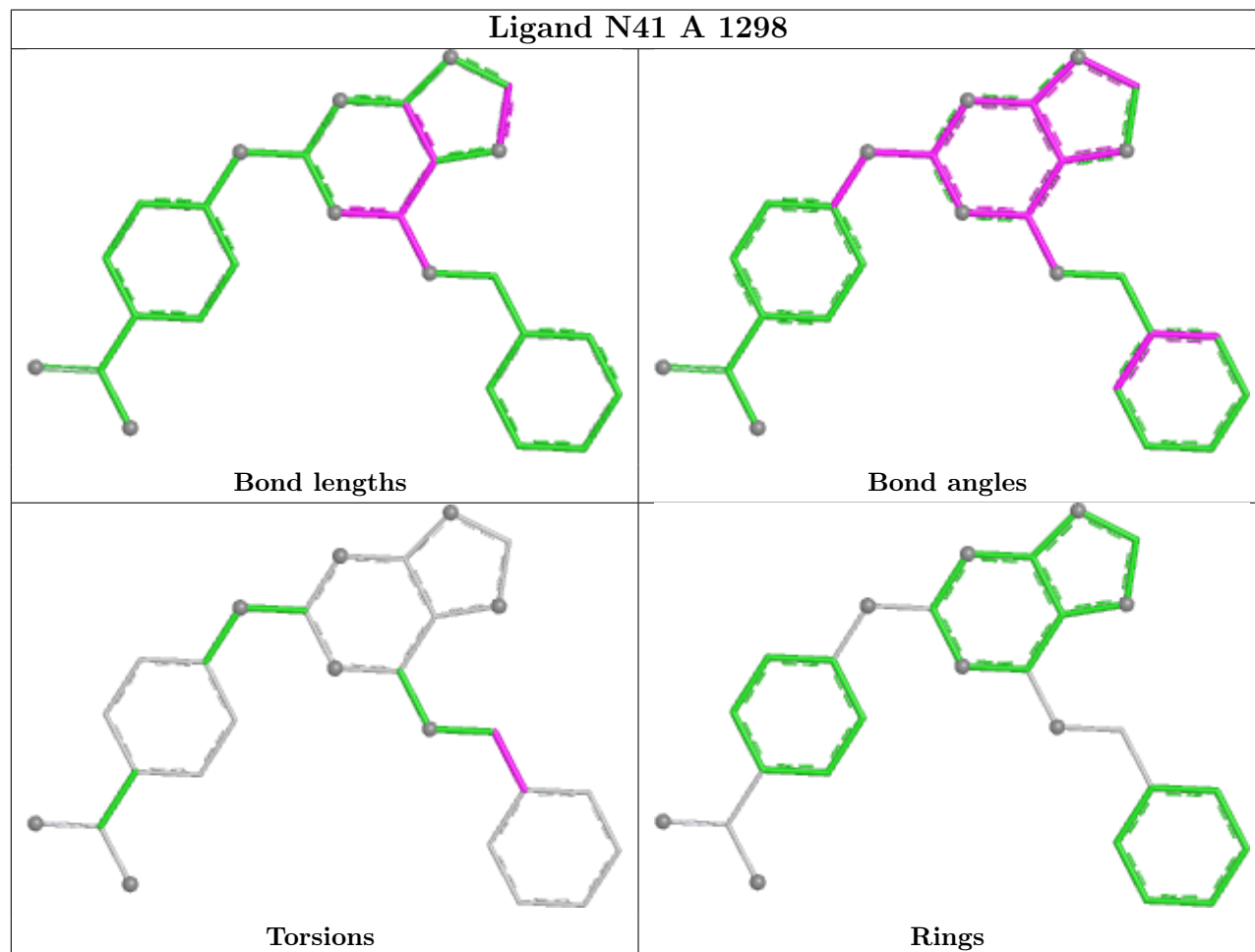
There are no ring outliers.

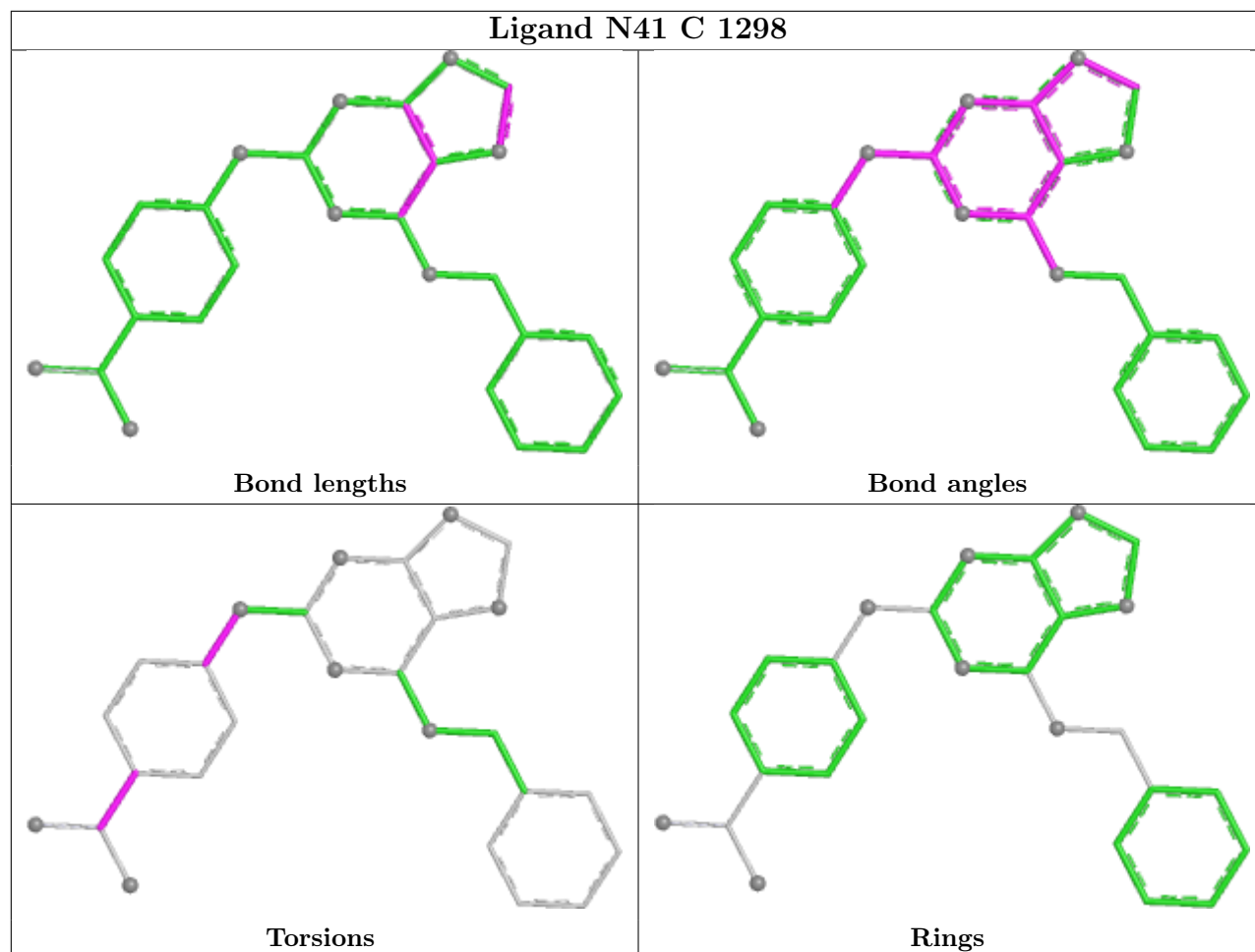
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1193	SGM	1	0
3	A	1298	N41	4	0
3	C	1298	N41	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	293/302 (97%)	-0.17	8 (2%) 56 52	11, 22, 45, 55	1 (0%)
1	C	296/302 (98%)	1.04	48 (16%) 4 4	24, 47, 70, 80	1 (0%)
2	B	258/260 (99%)	-0.19	2 (0%) 82 80	11, 25, 44, 55	1 (0%)
2	D	258/260 (99%)	1.18	61 (23%) 2 1	20, 48, 73, 78	0
All	All	1105/1124 (98%)	0.47	119 (10%) 11 8	11, 35, 69, 80	3 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	175	VAL	5.2
1	C	296	LEU	5.0
2	D	175	VAL	4.8
2	D	176	PRO	4.6
2	D	399	LEU	3.9
2	D	432	LEU	3.8
2	D	386	SER	3.8
1	C	258	ASP	3.7
1	C	215	ILE	3.7
2	D	372	TRP	3.7
2	D	324	PRO	3.6
2	D	373	PRO	3.6
2	D	329	VAL	3.5
2	D	430	LEU	3.5
1	C	238	PRO	3.5
1	C	252	VAL	3.5
2	D	336	LEU	3.4
2	D	368	THR	3.3
2	D	420	GLY	3.3
1	C	96	LEU	3.3
1	C	71	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	293	VAL	3.3
2	D	362	LEU	3.2
1	A	295	HIS	3.2
2	D	365	TYR	3.2
2	D	401	ALA	3.2
2	D	322	GLN	3.2
1	C	251	VAL	3.2
1	A	72	THR	3.2
2	D	366	THR	3.2
2	D	413	TYR	3.1
2	D	315	LEU	3.1
2	D	369	GLY	3.0
1	A	73	GLU	3.0
2	D	423	LEU	2.9
2	D	418	TYR	2.9
1	C	277	ALA	2.9
1	C	245	ARG	2.9
2	D	392	MET	2.9
1	A	296	LEU	2.8
1	C	255	LEU	2.8
2	D	333	ALA	2.8
2	D	378	ARG	2.8
1	C	227	TRP	2.8
1	C	101	LEU	2.8
2	D	359	ALA	2.8
2	D	398	TYR	2.7
2	D	316	THR	2.7
2	D	394	LEU	2.7
1	C	218	THR	2.7
2	D	405	ALA	2.6
1	C	161	HIS	2.6
2	D	281	ILE	2.5
2	D	319	PHE	2.5
2	D	395	HIS	2.5
1	A	74	ASN	2.5
2	D	421	VAL	2.5
2	D	431	ASN	2.5
1	C	253	PRO	2.5
2	D	380	THR	2.5
2	D	318	TYR	2.4
2	D	403	GLN	2.4
2	D	326	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	95	ALA	2.4
1	C	98	GLY	2.4
2	D	364	LEU	2.4
1	A	41	THR	2.4
1	C	254	PRO	2.4
1	C	247	ASP	2.4
1	C	162	GLU	2.4
1	C	294	PRO	2.3
1	C	175	LEU	2.3
2	D	177	ASP	2.3
1	C	99	ILE	2.3
1	C	234	PRO	2.3
1	C	259	GLY	2.3
1	A	71	HIS	2.3
1	C	174	LEU	2.3
1	C	263	LEU	2.3
1	C	225	VAL	2.3
2	D	320	LEU	2.3
1	C	216	PHE	2.3
1	C	285	PHE	2.3
2	D	314	PHE	2.3
2	D	427	PRO	2.3
1	A	35	ILE	2.2
1	C	209	ILE	2.2
2	D	416	SER	2.2
2	D	325	ALA	2.2
2	D	280	TYR	2.2
1	C	250	LYS	2.2
1	C	173	ILE	2.2
1	C	232	SER	2.2
2	D	331	SER	2.2
2	D	284	ASP	2.2
2	D	387	LEU	2.2
1	C	239	SER	2.2
1	C	287	GLN	2.2
1	C	236	TYR	2.2
2	B	283	ASP	2.2
1	C	273	LYS	2.2
2	D	412	LYS	2.2
2	D	354	VAL	2.1
1	C	139	GLY	2.1
1	C	267	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	337	GLY	2.1
2	D	180	GLU	2.1
2	D	375	SER	2.1
1	C	275	ILE	2.1
2	D	422	SER	2.1
2	D	335	PHE	2.1
2	D	178	TYR	2.1
1	C	187	TRP	2.1
2	D	425	ASN	2.1
1	C	226	VAL	2.0
1	C	289	VAL	2.0
2	D	426	PRO	2.0
1	C	214	ARG	2.0
1	C	268	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TPO	C	160	11/12	0.91	0.12	38,46,48,49	0
1	TPO	A	160	11/12	0.98	0.06	12,16,17,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	N41	C	1298	27/27	0.89	0.14	42,45,59,61	0
4	SGM	D	1193	6/6	0.90	0.13	62,63,64,66	0

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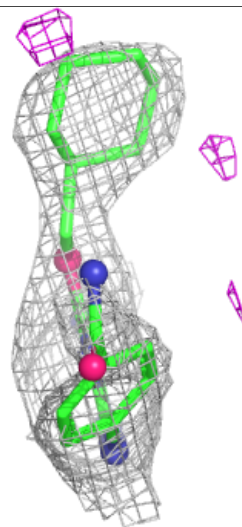
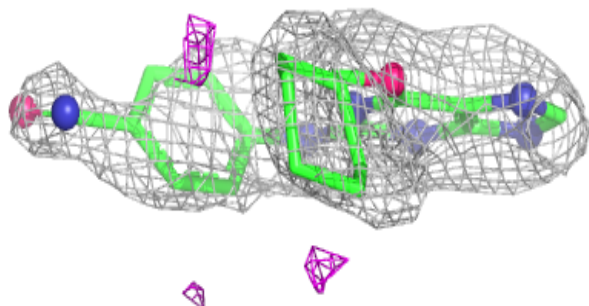
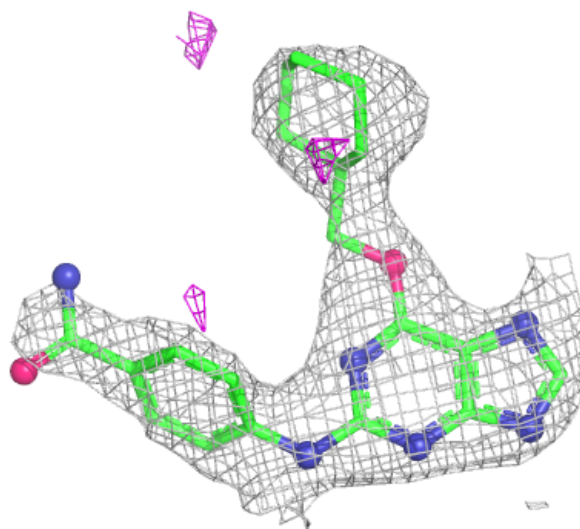
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	N41	A	1298	27/27	0.92	0.09	25,30,34,35	0
4	SGM	B	1193	6/6	0.93	0.11	35,37,39,43	0
5	MG	B	1433	1/1	0.96	0.05	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

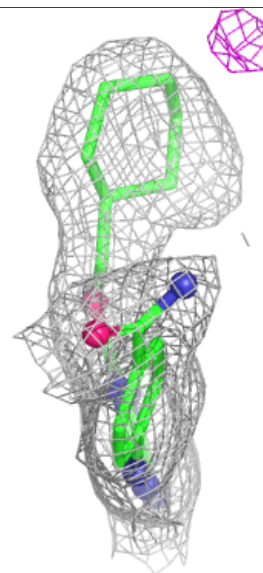
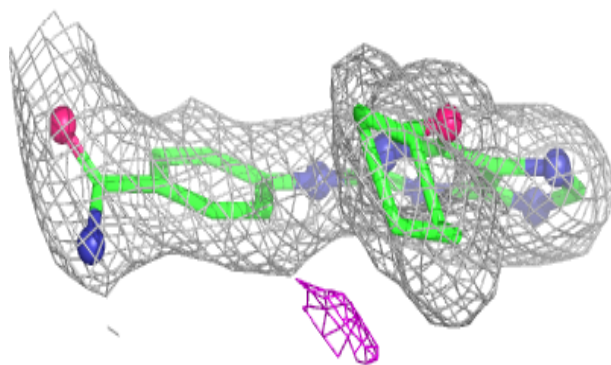
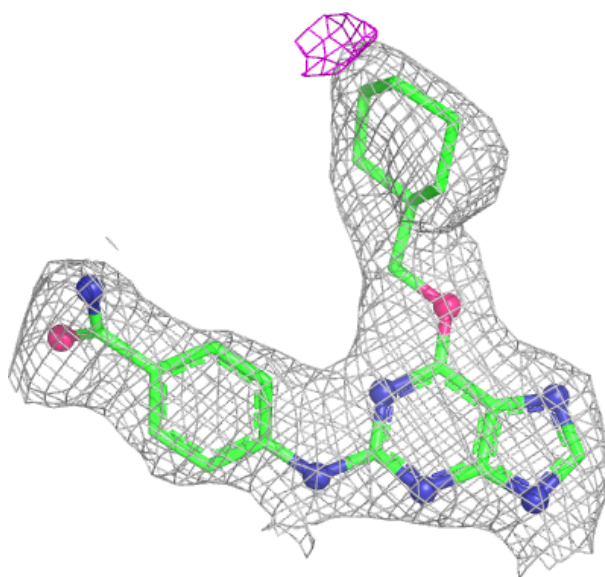
Electron density around N41 C 1298:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around N41 A 1298:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.