



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:07 PM UTC

PDB ID : 4TW9 / pdb_00004tw9
Title : Difluoro-dioxolo-benzoimidazol-benzamides as potent inhibitors of CK1delta and epsilon with nanomolar inhibitory activity on cancer cell proliferation
Authors : Richter, J.; Bischof, J.; Zaja, M.; Kohlhof, H.; Othersen, O.; Vitt, D.; Alscher, V.; Pospiech, I.; Garcia-Reyes, B.; Berg, S.; Leban, J.; Knippschild, U.
Deposited on : 2014-06-30
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

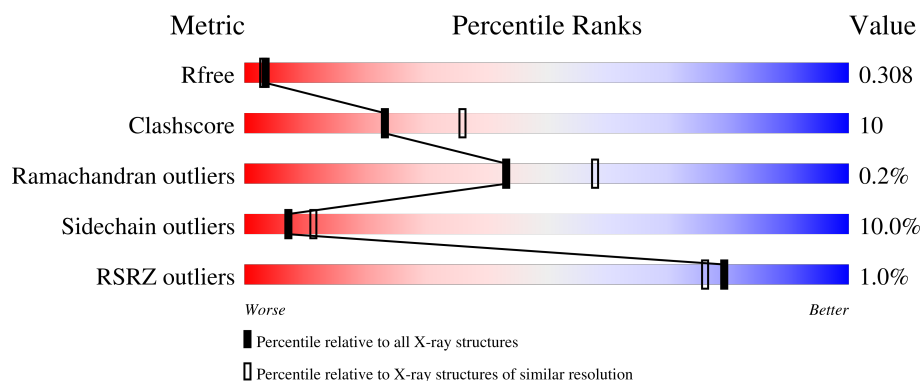
1 Overall quality at a glance

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	295	
1	B	295	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HSJ	A	1005	X	-	-	-
3	HSJ	A	1011	X	-	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5149 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.

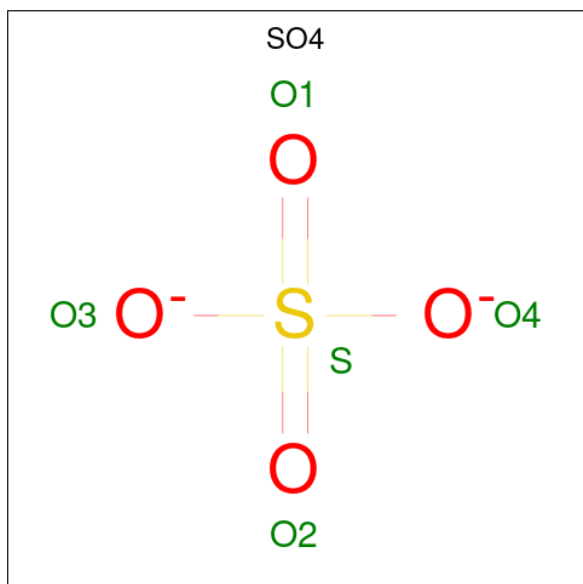
- Molecule 1 is a protein called Casein kinase I isoform delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total	C	N	O	S	0	3	0
			2390	1539	413	424	14			
1	B	289	Total	C	N	O	S	0	0	0
			2366	1521	409	421	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASN	ARG	engineered mutation	UNP P48730
B	13	ASN	ARG	engineered mutation	UNP P48730

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



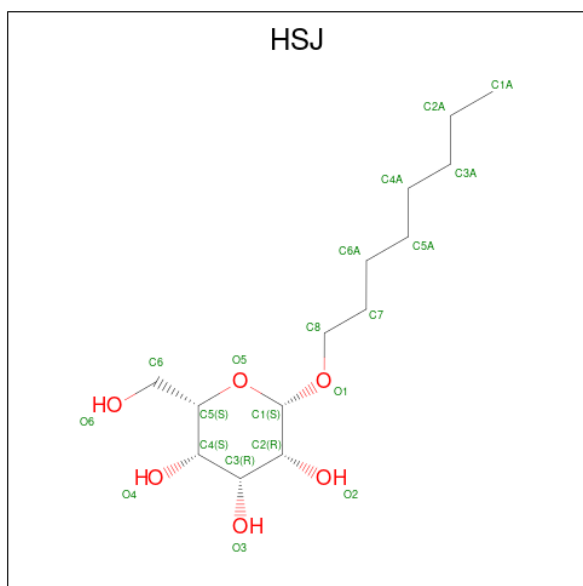
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is octyl beta-L-talopyranoside (CCD ID: HSJ) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			20	14	6		
3	A	1	Total	C	O	0	0
			20	14	6		

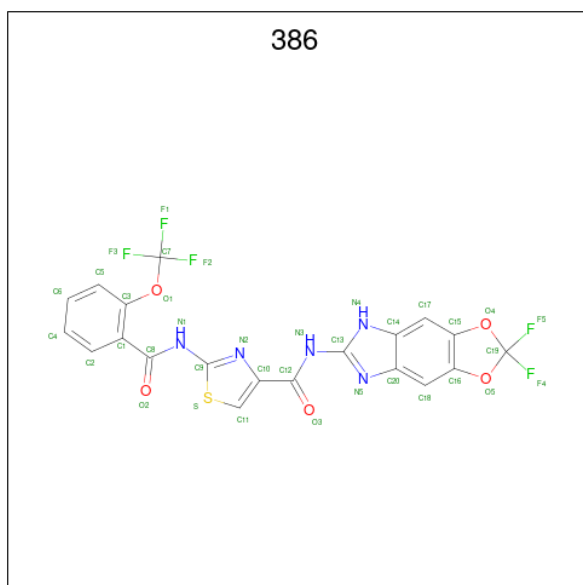
- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Na 2 2	0	0
5	B	2	Total Na 2 2	0	0

- Molecule 6 is N-(2,2-difluoro-5H-[1,3]dioxolo[4,5-f]benzimidazol-6-yl)-2-{[2-(trifluoromethoxy)benzoyl]amino}-1,3-thiazole-4-carboxamide (CCD ID: 386) (formula: C₂₀H₁₀F₅N₅O₅S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C F N O S 36 20 5 5 5 1	0	0
6	B	1	Total C F N O S 36 20 5 5 5 1	0	0

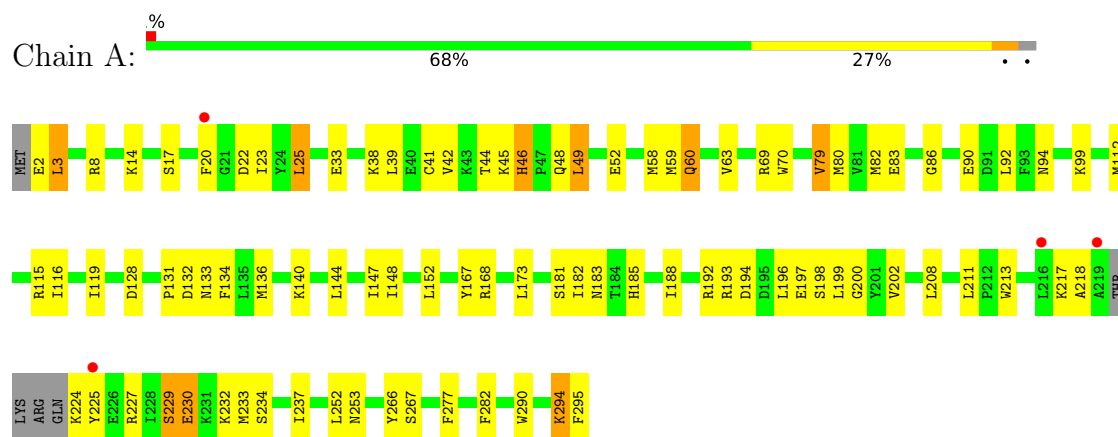
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	104	Total O 104 104	0	0
7	B	131	Total O 131 131	0	0

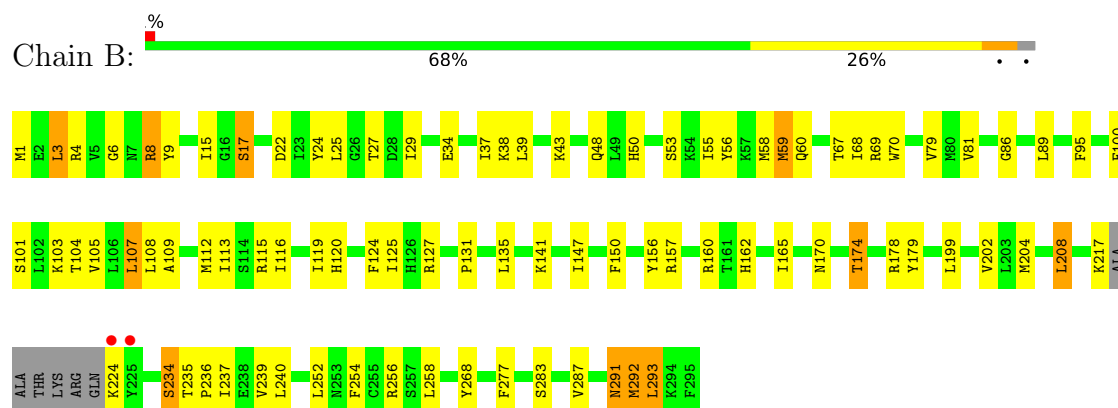
3 Residue-property plots

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: Casein kinase I isoform delta



- Molecule 1: Casein kinase I isoform delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	52.05Å 135.71Å 57.18Å 90.00° 99.42° 90.00°	Depositor
Resolution (Å)	19.86 – 2.40 19.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.2 (19.86-2.40) 86.0 (19.86-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.205 , 0.298 0.223 , 0.308	Depositor DCC
R_{free} test set	1282 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	31.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5149	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NA, CL, 386, HSJ, SO4

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	0.81	1/2452 (0.0%)	0.94	2/3294 (0.1%)
1	B	0.80	0/2421	0.97	3/3252 (0.1%)
All	All	0.81	1/4873 (0.0%)	0.96	5/6546 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	ILE	CA-CB	5.03	1.61	1.54

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	HIS	CA-C-N	7.01	127.04	119.89
1	A	46	HIS	C-N-CA	7.01	127.04	119.89
1	B	6	GLY	N-CA-C	-6.21	100.79	111.47
1	B	234	SER	N-CA-C	-5.46	106.29	113.12
1	B	68	ILE	CB-CA-C	-5.22	104.97	111.08

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	2390	0	2388	50	0
1	B	2366	0	2363	50	0
2	A	20	0	0	0	0
2	B	20	0	0	0	0
3	A	40	0	17	0	0
4	A	2	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	36	0	10	1	0
6	B	36	0	10	2	0
7	A	104	0	0	6	0
7	B	131	0	0	2	0
All	All	5149	0	4788	100	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 10.

All (100) 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:46:HIS:NE2	7:A:1198:HOH:O	2.04	0.91
1:B:69:ARG:HB2	1:B:81:VAL:HG12	1.69	0.75
1:A:112:MET:HE2	1:A:199:LEU:CD1	2.17	0.75
1:A:46:HIS:CE1	7:A:1198:HOH:O	2.43	0.71
1:A:295:PHE:C	7:A:1141:HOH:O	2.35	0.68
1:B:131:PRO:HG3	1:B:202:VAL:HG13	1.76	0.68
1:A:197:GLU:OE1	7:A:1165:HOH:O	2.14	0.66
1:B:39:LEU:CD2	1:B:79:VAL:HG23	2.27	0.64
1:A:25:LEU:HD13	1:B:292:MET:HB3	1.80	0.63
1:B:237:ILE:HD11	1:B:256:ARG:HD3	1.80	0.63
1:A:59:MET:HE1	1:A:119:ILE:HG23	1.81	0.62
1:B:58:MET:HE1	1:B:124:PHE:CE1	2.34	0.61
1:B:3:LEU:C	1:B:3:LEU:HD12	2.26	0.60
1:B:101:SER:O	1:B:105:VAL:HG23	2.03	0.59
1:A:185:HIS:HB3	1:A:229:SER:OG	2.03	0.58
1:A:200:GLY:HA3	1:A:252:LEU:HD21	1.85	0.58
1:A:80:MET:HE3	1:A:82:MET:SD	2.44	0.57
1:B:86:GLY:O	1:B:135:LEU:HD23	2.06	0.56
1:B:39:LEU:HD23	1:B:79:VAL:HG23	1.87	0.56
1:A:112:MET:HE2	1:A:199:LEU:HD13	1.88	0.56
1:A:196:LEU:HD11	1:A:266:TYR:CE1	2.40	0.55
1:B:237:ILE:HD11	1:B:256:ARG:CD	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ARG:NE	1:B:174:THR:HG21	2.21	0.55
1:A:20[B]:PHE:CE2	1:A:48:GLN:HG3	2.41	0.55
1:A:23:ILE:HD13	6:A:1010:386:H9	1.89	0.54
1:A:33:GLU:OE2	1:A:69:ARG:NH2	2.40	0.54
1:B:37:ILE:HG12	1:B:81:VAL:HG22	1.88	0.54
1:A:49:LEU:HD11	1:A:80:MET:HB2	1.88	0.54
1:B:287:VAL:HG13	1:B:291:ASN:ND2	2.24	0.53
1:B:17:SER:OG	1:B:22:ASP:OD1	2.24	0.52
1:B:254:PHE:CE2	1:B:258:LEU:HD21	2.43	0.52
1:A:70:TRP:HZ3	1:A:79:VAL:HG22	1.73	0.52
1:A:92:LEU:HD22	1:A:290:TRP:CG	2.45	0.52
1:B:204:MET:CE	1:B:208:LEU:HD13	2.40	0.51
1:B:38:LYS:O	1:B:39:LEU:HD23	2.11	0.51
1:B:58:MET:HE1	1:B:124:PHE:HE1	1.74	0.51
1:A:277:PHE:CE2	1:A:282:PHE:HB2	2.45	0.51
1:A:63:VAL:HG12	1:A:115:ARG:CZ	2.42	0.50
1:A:237:ILE:HD12	1:A:253:ASN:OD1	2.11	0.50
1:A:41:CYS:O	1:A:44:THR:HG23	2.13	0.49
1:A:218:ALA:HB2	1:A:227:ARG:HD2	1.95	0.49
1:A:2:GLU:C	1:A:3:LEU:HD12	2.37	0.49
1:A:116:ILE:HD12	1:A:199:LEU:HD22	1.94	0.49
1:B:119:ILE:HG22	1:B:124:PHE:O	2.14	0.48
1:B:234:SER:O	1:B:236:PRO:HD3	2.14	0.47
1:A:182:ILE:HG23	1:A:233:MET:HG2	1.96	0.47
1:A:90:GLU:O	1:A:94:ASN:ND2	2.47	0.47
1:B:95:PHE:CZ	1:B:293:LEU:HD21	2.49	0.47
1:B:103:LYS:O	1:B:107:LEU:HB2	2.15	0.47
1:A:200:GLY:HA3	1:A:252:LEU:CD2	2.45	0.47
1:A:211:LEU:HD13	1:A:213:TRP:CZ2	2.50	0.47
1:A:38:LYS:NZ	1:A:52:GLU:OE1	2.39	0.47
1:A:213:TRP:CE3	1:A:232:LYS:HA	2.50	0.46
1:B:293:LEU:HD23	1:B:293:LEU:N	2.30	0.46
1:A:128:ASP:O	1:A:133:ASN:ND2	2.48	0.46
1:B:157:ARG:NH1	1:B:162:HIS:CE1	2.83	0.46
1:B:59:MET:CE	1:B:150:PHE:CE1	2.99	0.46
1:B:252:LEU:HD23	1:B:252:LEU:HA	1.82	0.46
1:A:230:GLU:HA	1:A:233:MET:HE3	1.98	0.45
1:A:182:ILE:HD12	1:A:233:MET:HG2	1.98	0.45
1:B:70:TRP:HZ3	1:B:79:VAL:HG11	1.81	0.45
1:B:109:ALA:O	1:B:113:ILE:HG13	2.17	0.45
1:A:60:GLN:HE21	1:A:60:GLN:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ARG:HD2	1:B:179:TYR:CZ	2.51	0.45
6:B:1007:386:C5	6:B:1007:386:F1	2.54	0.45
1:B:56:TYR:O	1:B:60:GLN:HG2	2.17	0.45
1:A:198:SER:O	1:A:202:VAL:HG23	2.18	0.44
1:B:3:LEU:HD12	1:B:4:ARG:N	2.32	0.44
1:A:134:PHE:CE1	1:A:147:ILE:HD12	2.53	0.43
1:B:55:ILE:O	1:B:59:MET:CG	2.65	0.43
1:A:86:GLY:N	1:A:136:MET:O	2.51	0.43
1:B:116:ILE:CG2	1:B:120:HIS:CE1	3.02	0.43
1:B:119:ILE:HD11	1:B:147:ILE:HD13	2.00	0.43
1:A:39:LEU:HD23	1:A:79:VAL:HB	2.00	0.43
1:A:42:VAL:HG12	1:A:42:VAL:O	2.19	0.43
1:A:152:LEU:HD12	7:A:1170:HOH:O	2.18	0.43
1:A:294[A]:LYS:HZ2	1:B:34:GLU:CD	2.27	0.43
1:A:14:LYS:HE2	1:A:22:ASP:OD1	2.19	0.42
1:B:60:GLN:OE1	1:B:67:THR:HA	2.19	0.42
1:B:107:LEU:HD13	1:B:277:PHE:CE1	2.54	0.42
1:A:90:GLU:HB2	1:A:131:PRO:HB2	2.01	0.42
1:B:9:TYR:CE1	1:B:81:VAL:HG11	2.54	0.42
6:B:1007:386:F1	6:B:1007:386:H6	2.10	0.42
1:A:192:ARG:O	1:A:193:ARG:C	2.62	0.42
1:B:89:LEU:HD11	1:B:108:LEU:HD22	2.01	0.42
1:B:156:TYR:HA	1:B:165:ILE:HD13	2.02	0.42
1:B:204:MET:HE3	1:B:208:LEU:HD13	2.01	0.42
1:A:116:ILE:CD1	1:A:199:LEU:HD22	2.49	0.41
1:B:112:MET:HE2	1:B:199:LEU:CD1	2.50	0.41
1:A:181:SER:OG	1:A:194:ASP:OD1	2.32	0.41
1:B:8:ARG:HB3	7:B:1151:HOH:O	2.20	0.41
1:A:167:TYR:OH	1:A:188:ILE:HD12	2.20	0.41
1:A:48:GLN:O	1:A:49:LEU:C	2.64	0.41
1:A:183:ASN:ND2	7:A:1148:HOH:O	2.54	0.41
1:B:50:HIS:O	1:B:53:SER:OG	2.37	0.41
1:B:239:VAL:O	1:B:240:LEU:C	2.64	0.41
1:B:24:TYR:CD1	1:B:24:TYR:N	2.88	0.41
1:B:70:TRP:HZ3	1:B:79:VAL:CG1	2.34	0.40
1:B:268:TYR:OH	7:B:1231:HOH:O	2.21	0.40
1:B:4:ARG:NH2	1:B:29:ILE:HD13	2.37	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	289/295 (98%)	268 (93%)	21 (7%)	0	100	100
1	B	285/295 (97%)	272 (95%)	12 (4%)	1 (0%)	30	43
All	All	574/590 (97%)	540 (94%)	33 (6%)	1 (0%)	43	58

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	235	THR

5.3.2 Protein sidechains [i](#)

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	257/259 (99%)	231 (90%)	26 (10%)	7	11
1	B	255/259 (98%)	229 (90%)	26 (10%)	7	11
All	All	512/518 (99%)	460 (90%)	52 (10%)	7	11

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	8	ARG
1	A	17	SER
1	A	25	LEU
1	A	45	LYS

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Mol	Chain	Res	Type
1	A	49	LEU
1	A	58	MET
1	A	60	GLN
1	A	79	VAL
1	A	83	GLU
1	A	99	LYS
1	A	132	ASP
1	A	140	LYS
1	A	144	LEU
1	A	168	ARG
1	A	173	LEU
1	A	208	LEU
1	A	217	LYS
1	A	224	LYS
1	A	225	TYR
1	A	229	SER
1	A	230	GLU
1	A	234	SER
1	A	267	SER
1	A	294[A]	LYS
1	A	294[B]	LYS
1	B	1	MET
1	B	3	LEU
1	B	8	ARG
1	B	15	ILE
1	B	17	SER
1	B	25	LEU
1	B	27	THR
1	B	43	LYS
1	B	48	GLN
1	B	59	MET
1	B	100	PHE
1	B	104	THR
1	B	107	LEU
1	B	115	ARG
1	B	125	ILE
1	B	141	LYS
1	B	160	ARG
1	B	170	ASN
1	B	174	THR
1	B	208	LEU
1	B	217	LYS

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Mol	Chain	Res	Type
1	B	224	LYS
1	B	283	SER
1	B	291	ASN
1	B	292	MET
1	B	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	78	ASN
1	A	94	ASN
1	A	143	ASN
1	A	183	ASN
1	A	190	GLN
1	A	214	GLN
1	B	46	HIS
1	B	50	HIS
1	B	190	GLN
1	B	291	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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
2	SO4	B	1001	-	4,4,4	0.24	0	6,6,6	0.20	0
2	SO4	A	1003	-	4,4,4	0.20	0	6,6,6	0.52	0
2	SO4	B	1004	-	4,4,4	0.22	0	6,6,6	0.31	0
3	HSJ	A	1005	-	20,20,20	0.75	1 (5%)	25,25,25	1.20	3 (12%)
2	SO4	A	1004	-	4,4,4	0.28	0	6,6,6	0.10	0
2	SO4	A	1001	-	4,4,4	0.28	0	6,6,6	0.64	0
6	386	A	1010	-	40,40,40	2.14	12 (30%)	60,61,61	2.62	18 (30%)
6	386	B	1007	-	40,40,40	2.37	11 (27%)	60,61,61	2.15	14 (23%)
3	HSJ	A	1011	-	20,20,20	0.72	1 (5%)	25,25,25	1.07	1 (4%)
2	SO4	B	1003	-	4,4,4	0.28	0	6,6,6	0.24	0
2	SO4	B	1002	-	4,4,4	0.27	0	6,6,6	0.22	0
2	SO4	A	1002	-	4,4,4	0.23	0	6,6,6	0.33	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
6	386	B	1007	-	-	10/21/31/31	0/5/5/5
3	HSJ	A	1005	-	1/1/5/5	6/11/31/31	0/1/1/1
3	HSJ	A	1011	-	1/1/5/5	5/11/31/31	0/1/1/1
6	386	A	1010	-	-	11/21/31/31	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1007	386	C9-S	-9.58	1.61	1.74
6	A	1010	386	C9-S	-7.59	1.63	1.74
6	B	1007	386	C11-S	-4.77	1.60	1.71
6	B	1007	386	O5-C19	4.53	1.44	1.38
6	A	1010	386	O4-C19	4.38	1.44	1.38
6	A	1010	386	C14-N4	-3.63	1.32	1.38
6	A	1010	386	C11-S	-3.60	1.63	1.71
6	B	1007	386	O4-C19	3.51	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1007	386	C14-N4	-3.14	1.33	1.38
6	A	1010	386	C20-N5	-3.07	1.33	1.39
6	A	1010	386	O5-C19	3.04	1.42	1.38
6	B	1007	386	F5-C19	3.04	1.37	1.33
6	B	1007	386	C20-N5	-2.80	1.34	1.39
6	A	1010	386	C11-C10	2.80	1.41	1.36
6	A	1010	386	O5-C16	-2.76	1.33	1.38
6	B	1007	386	F4-C19	2.57	1.36	1.33
6	A	1010	386	C10-N2	-2.40	1.33	1.38
3	A	1011	HSJ	O1-C1	2.39	1.44	1.40
6	A	1010	386	F5-C19	2.38	1.36	1.33
6	B	1007	386	C11-C10	2.25	1.40	1.36
6	B	1007	386	O5-C16	-2.17	1.34	1.38
6	A	1010	386	F4-C19	2.15	1.36	1.33
6	B	1007	386	C10-N2	-2.06	1.34	1.38
6	A	1010	386	O4-C15	-2.04	1.34	1.38
3	A	1005	HSJ	O1-C1	2.03	1.43	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1007	386	C11-S-C9	10.15	96.30	88.40
6	A	1010	386	F4-C19-F5	8.85	112.74	105.85
6	A	1010	386	C11-S-C9	8.19	94.77	88.40
6	A	1010	386	F5-C19-O5	-6.88	105.29	110.10
6	A	1010	386	S-C9-N1	6.80	135.42	123.29
6	B	1007	386	F4-C19-F5	5.42	110.07	105.85
6	A	1010	386	N1-C9-N2	-4.82	112.84	121.18
6	B	1007	386	S-C9-N1	4.74	131.75	123.29
6	B	1007	386	S-C9-N2	-4.20	111.27	115.69
6	B	1007	386	O5-C19-O4	-4.12	107.21	110.46
6	A	1010	386	S-C9-N2	-3.77	111.73	115.69
3	A	1011	HSJ	O1-C1-C2	3.44	113.50	108.27
6	A	1010	386	C11-C10-C12	3.40	129.57	123.92
6	A	1010	386	F4-C19-O5	-3.21	107.86	110.10
6	A	1010	386	C14-C17-C15	-3.12	113.66	119.52
6	A	1010	386	C19-O4-C15	-2.91	103.53	106.09
6	B	1007	386	C20-C14-N4	2.78	109.05	105.71
6	B	1007	386	C3-C1-C8	-2.77	121.24	126.24
6	A	1010	386	C9-N1-C8	2.69	128.13	123.67
6	B	1007	386	C9-N1-C8	2.68	128.10	123.67
6	B	1007	386	F5-C19-O5	2.66	111.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1010	386	O1-C3-C1	2.63	121.91	117.27
3	A	1005	HSJ	C1-O5-C5	2.60	118.80	113.72
6	B	1007	386	C10-C11-S	-2.49	107.36	110.24
6	B	1007	386	N1-C9-N2	-2.47	116.92	121.18
3	A	1005	HSJ	C1-C2-C3	2.33	114.91	110.01
3	A	1005	HSJ	O1-C1-C2	2.26	111.71	108.27
6	A	1010	386	F5-C19-O4	2.26	111.68	110.10
6	A	1010	386	C16-C18-C20	-2.20	113.94	119.00
6	A	1010	386	C12-C10-N2	-2.18	116.55	120.67
6	A	1010	386	C10-C11-S	-2.12	107.79	110.24
6	B	1007	386	O4-C15-C16	2.05	111.21	109.65
6	B	1007	386	C13-N3-C12	-2.03	121.58	125.77
6	B	1007	386	C14-C17-C15	-2.01	115.73	119.52
6	A	1010	386	O5-C19-O4	-2.01	108.88	110.46
6	A	1010	386	C18-C16-C15	2.01	124.55	122.03

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1005	HSJ	C5
3	A	1011	HSJ	C5

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1005	HSJ	C7-C8-O1-C1
3	A	1005	HSJ	O5-C1-O1-C8
3	A	1011	HSJ	O5-C1-O1-C8
6	A	1010	386	C11-C10-C12-N3
6	A	1010	386	C11-C10-C12-O3
6	A	1010	386	C1-C3-O1-C7
6	B	1007	386	C11-C10-C12-N3
6	B	1007	386	C11-C10-C12-O3
3	A	1005	HSJ	O5-C5-C6-O6
3	A	1005	HSJ	C4-C5-C6-O6
6	A	1010	386	N2-C10-C12-N3
6	B	1007	386	N2-C10-C12-N3
6	B	1007	386	F2-C7-O1-C3
3	A	1011	HSJ	C2A-C3A-C4A-C5A
3	A	1011	HSJ	C6A-C7-C8-O1
6	A	1010	386	N2-C10-C12-O3
6	B	1007	386	N2-C10-C12-O3

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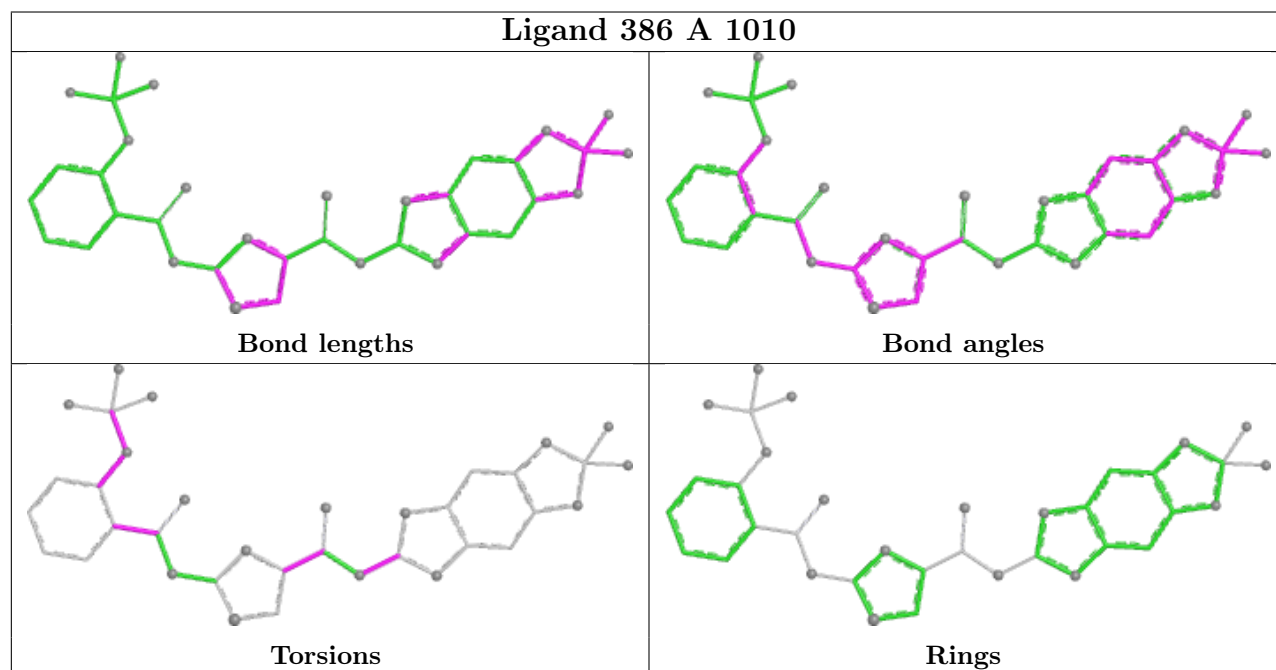
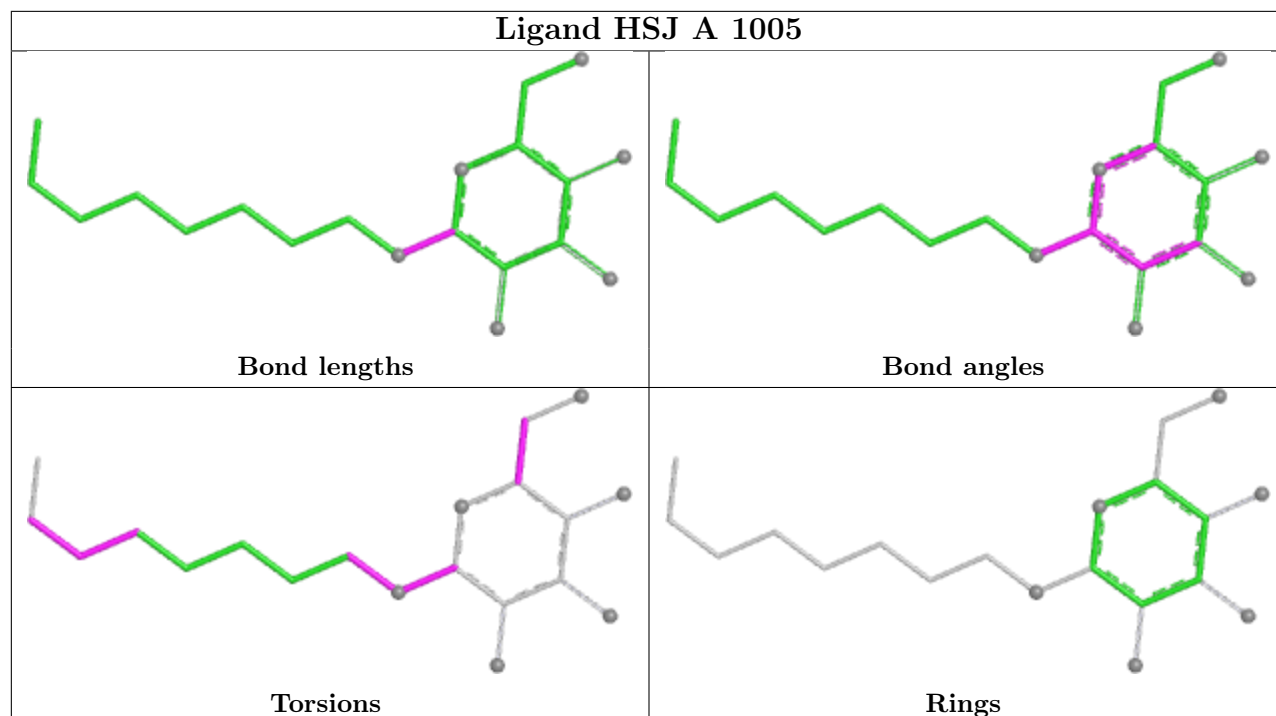
Mol	Chain	Res	Type	Atoms
3	A	1005	HSJ	C1A-C2A-C3A-C4A
3	A	1011	HSJ	C7-C8-O1-C1
6	A	1010	386	F3-C7-O1-C3
6	A	1010	386	C3-C1-C8-O2
6	B	1007	386	C3-C1-C8-N1
6	B	1007	386	C3-C1-C8-O2
6	A	1010	386	C3-C1-C8-N1
6	B	1007	386	F3-C7-O1-C3
6	A	1010	386	C5-C3-O1-C7
6	B	1007	386	F1-C7-O1-C3
3	A	1005	HSJ	C2A-C3A-C4A-C5A
3	A	1011	HSJ	C1A-C2A-C3A-C4A
6	A	1010	386	F2-C7-O1-C3
6	A	1010	386	N5-C13-N3-C12
6	B	1007	386	N5-C13-N3-C12

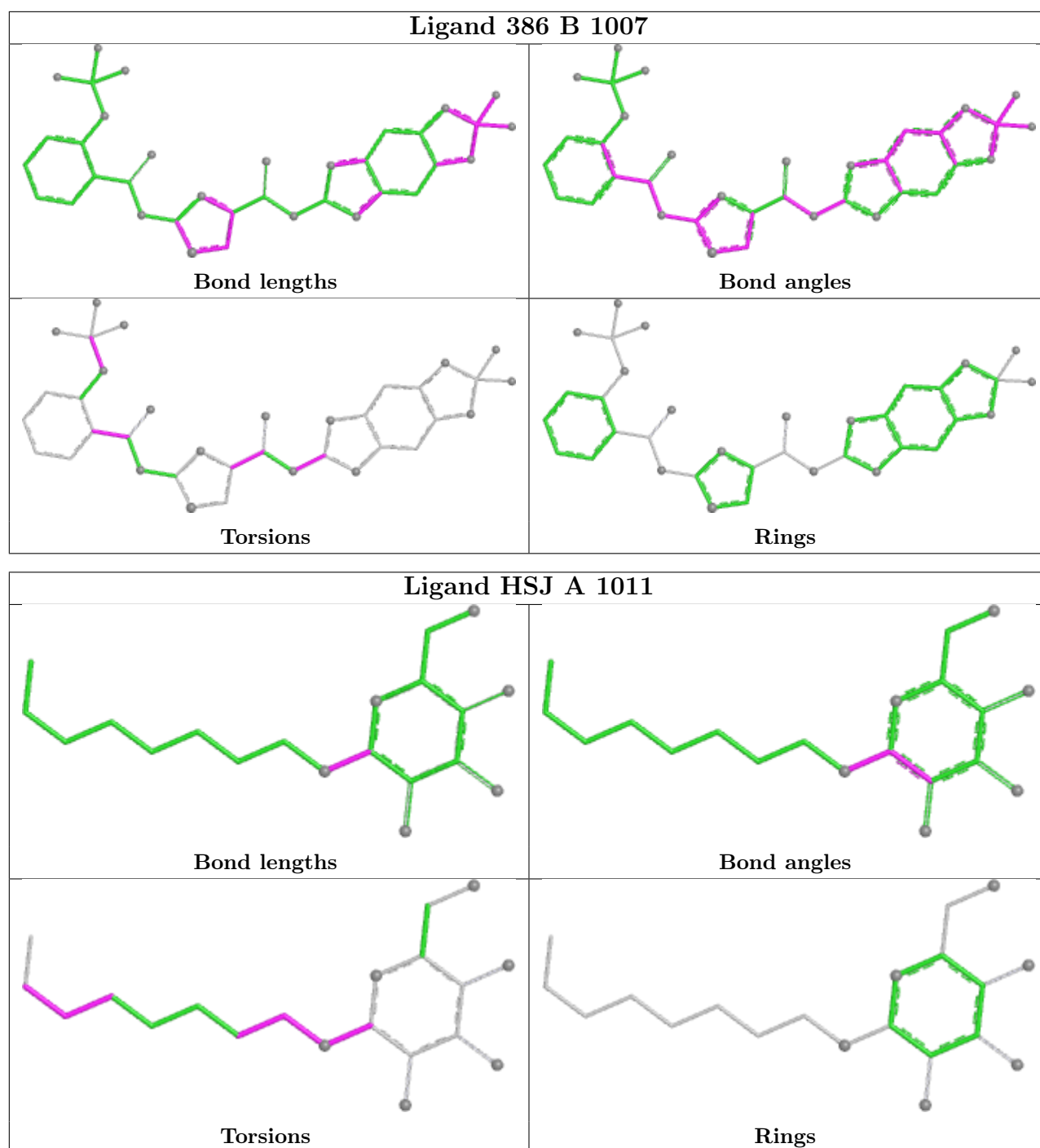
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1010	386	1	0
6	B	1007	386	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	290/295 (98%)	0.17	4 (1%) 73 69	22, 41, 62, 98	3 (1%)
1	B	289/295 (97%)	0.09	2 (0%) 84 81	24, 40, 65, 81	0
All	All	579/590 (98%)	0.13	6 (1%) 79 76	22, 40, 65, 98	3 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20[A]	PHE	3.6
1	A	219	ALA	2.9
1	A	225	TYR	2.7
1	B	225	TYR	2.5
1	A	216	LEU	2.5
1	B	224	LYS	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

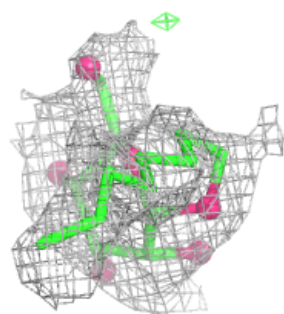
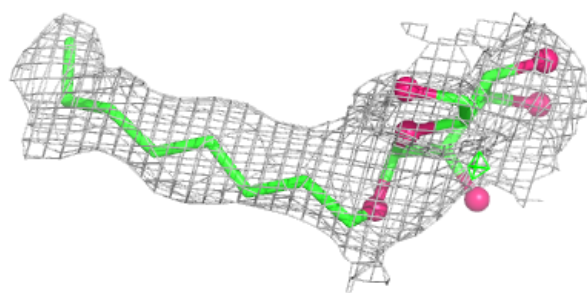
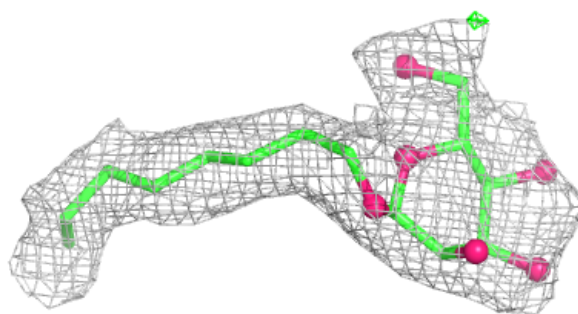
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	1004	5/5	0.77	0.13	118,121,122,124	0
3	HSJ	A	1005	20/20	0.82	0.20	82,93,99,101	0
2	SO4	B	1004	5/5	0.84	0.17	108,109,111,111	0
3	HSJ	A	1011	20/20	0.87	0.16	80,93,100,100	0
2	SO4	B	1002	5/5	0.89	0.13	77,79,84,84	0
2	SO4	A	1003	5/5	0.90	0.13	68,69,74,77	0
2	SO4	A	1001	5/5	0.91	0.10	57,61,65,65	0
6	386	B	1007	36/36	0.93	0.11	43,62,73,74	0
4	CL	A	1006	1/1	0.94	0.24	75,75,75,75	0
6	386	A	1010	36/36	0.94	0.11	39,60,83,86	0
2	SO4	B	1003	5/5	0.94	0.09	64,70,76,76	0
2	SO4	A	1002	5/5	0.95	0.08	57,58,59,64	0
2	SO4	B	1001	5/5	0.95	0.09	69,72,74,78	0
5	NA	B	1006	1/1	0.97	0.24	44,44,44,44	0
5	NA	B	1005	1/1	0.98	0.06	47,47,47,47	0
4	CL	A	1007	1/1	0.98	0.09	75,75,75,75	0
5	NA	A	1008	1/1	0.98	0.05	47,47,47,47	0
5	NA	A	1009	1/1	0.98	0.20	50,50,50,50	0

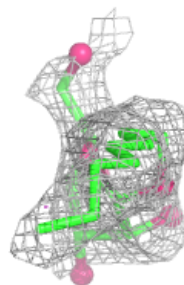
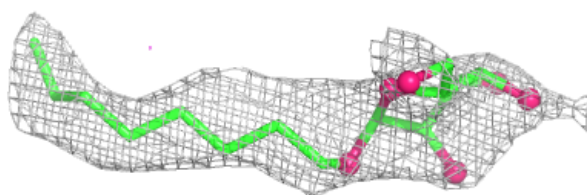
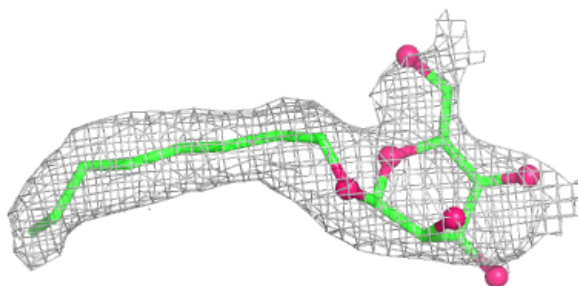
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HSJ A 1005:

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

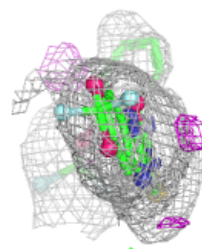
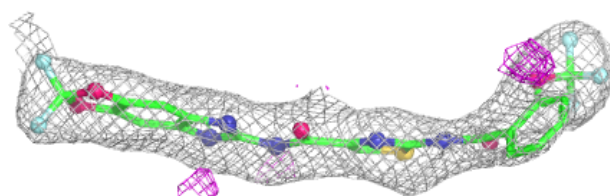
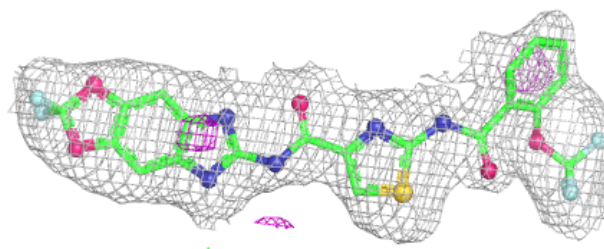
**Electron density around HSJ A 1011:**

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

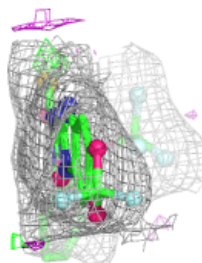
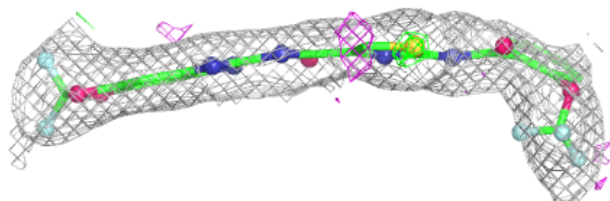
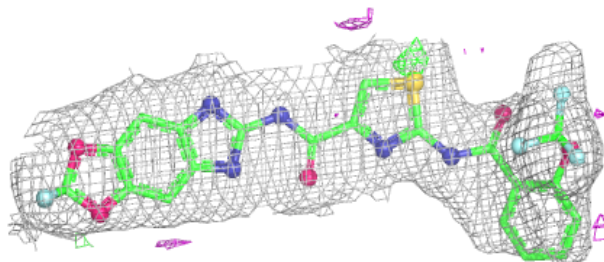


Electron density around 386 B 1007:

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

**Electron density around 386 A 1010:**

$2mF_o-DF_c$ (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.