



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:50 PM EDT

PDB ID : 2I47
Title : Crystal structure of catalytic domain of TACE with inhibitor
Authors : Xu, W.; Condon, J.S.; Lovering, F.E.
Deposited on : 2006-08-21
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

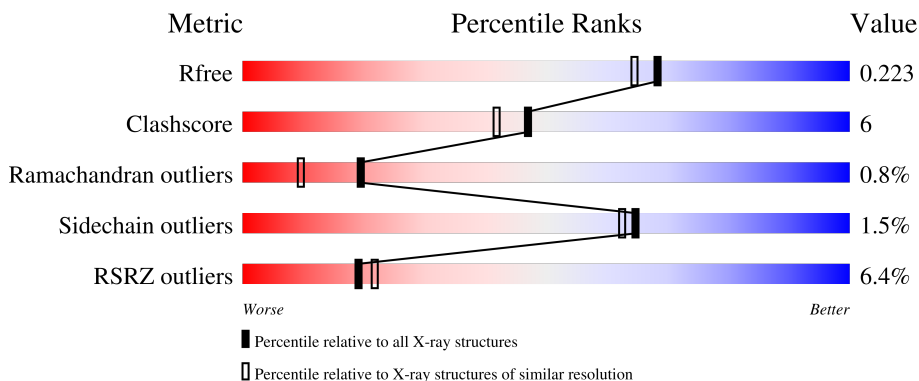
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	288	 6% 74% 14% • 11%
1	B	288	 3% 76% 11% • 12%
1	C	288	 7% 72% 14% • 12%
1	D	288	 6% 75% 12% • 11%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8926 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 ADAM 17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	255	2023	1273	342	395	13	0	0	0
1	B	254	2016	1268	341	394	13	0	0	0
1	C	254	2016	1268	341	394	13	0	0	0
1	D	255	2023	1273	342	395	13	0	0	0

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	266	ALA	SER	engineered mutation	UNP P78536
A	452	GLN	ASN	engineered mutation	UNP P78536
A	493	SER	-	cloning artifact	UNP P78536
A	494	HIS	-	expression tag	UNP P78536
A	495	HIS	-	expression tag	UNP P78536
A	496	HIS	-	expression tag	UNP P78536
A	497	HIS	-	expression tag	UNP P78536
A	498	HIS	-	expression tag	UNP P78536
A	499	HIS	-	expression tag	UNP P78536
B	266	ALA	SER	engineered mutation	UNP P78536
B	452	GLN	ASN	engineered mutation	UNP P78536
B	493	SER	-	cloning artifact	UNP P78536
B	494	HIS	-	expression tag	UNP P78536
B	495	HIS	-	expression tag	UNP P78536
B	496	HIS	-	expression tag	UNP P78536
B	497	HIS	-	expression tag	UNP P78536
B	498	HIS	-	expression tag	UNP P78536
B	499	HIS	-	expression tag	UNP P78536
C	266	ALA	SER	engineered mutation	UNP P78536
C	452	GLN	ASN	engineered mutation	UNP P78536
C	493	SER	-	cloning artifact	UNP P78536

Continued on next page...

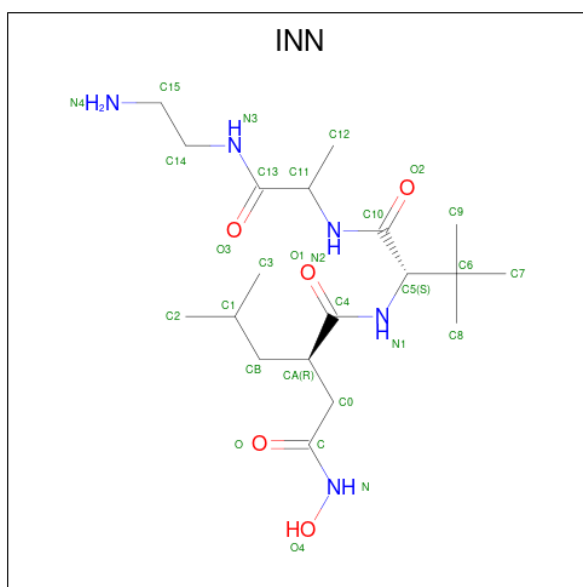
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	494	HIS	-	expression tag	UNP P78536
C	495	HIS	-	expression tag	UNP P78536
C	496	HIS	-	expression tag	UNP P78536
C	497	HIS	-	expression tag	UNP P78536
C	498	HIS	-	expression tag	UNP P78536
C	499	HIS	-	expression tag	UNP P78536
D	266	ALA	SER	engineered mutation	UNP P78536
D	452	GLN	ASN	engineered mutation	UNP P78536
D	493	SER	-	cloning artifact	UNP P78536
D	494	HIS	-	expression tag	UNP P78536
D	495	HIS	-	expression tag	UNP P78536
D	496	HIS	-	expression tag	UNP P78536
D	497	HIS	-	expression tag	UNP P78536
D	498	HIS	-	expression tag	UNP P78536
D	499	HIS	-	expression tag	UNP P78536

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

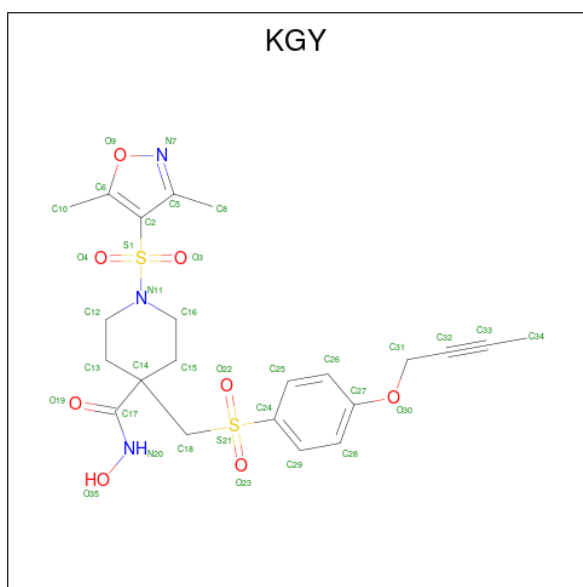
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is N-{(2R)-2-[2-(hydroxyamino)-2-oxoethyl]-4-methylpentanoyl}-3-methyl-L-valyl-N-(2-aminoethyl)-L-alaninamide (three-letter code: INN) (formula: C₁₉H₃₇N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	19	5	5	0	0
3	B	1	29	19	5	5	0	0

- Molecule 4 is 4-({[4-(BUT-2-YN-1-YLOXY)PHENYL]SULFONYL}METHYL)-1-[(3,5-DIMETHYLISOXAZOL-4-YL)SULFONYL]-N-HYDROXYPIPERIDINE-4-CARBOXAMIDE (three-letter code: KGY) (formula: C₂₂H₂₇N₃O₈S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	C	1	35	22	3	8	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	S	0	0
			35	22	3	8	2		

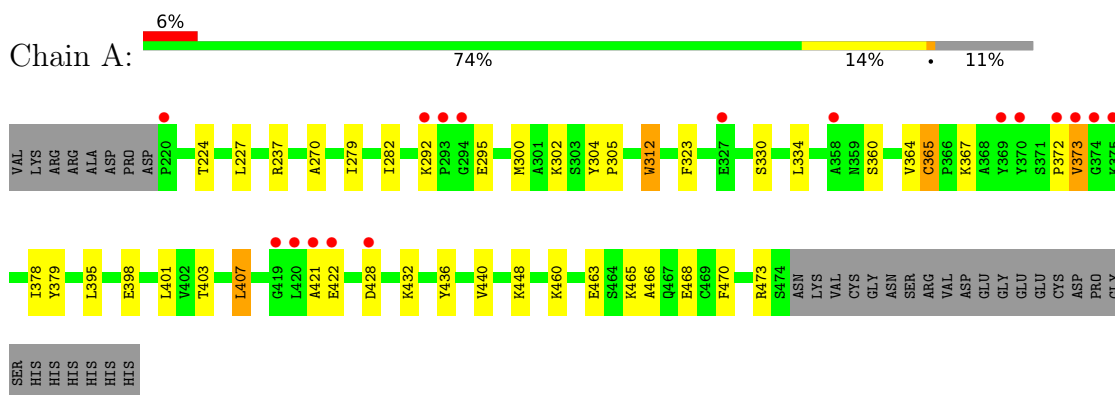
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	213	Total	O	0	0
			213	213		
5	B	165	Total	O	0	0
			165	165		
5	C	169	Total	O	0	0
			169	169		
5	D	169	Total	O	0	0
			169	169		

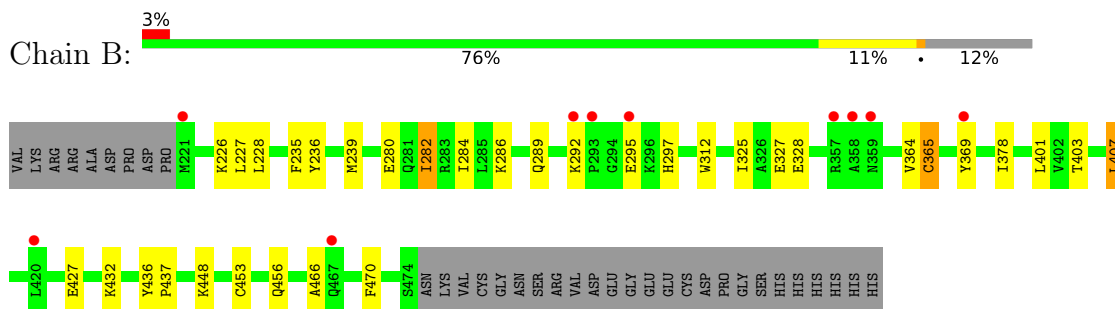
3 Residue-property plots [i](#)

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 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.

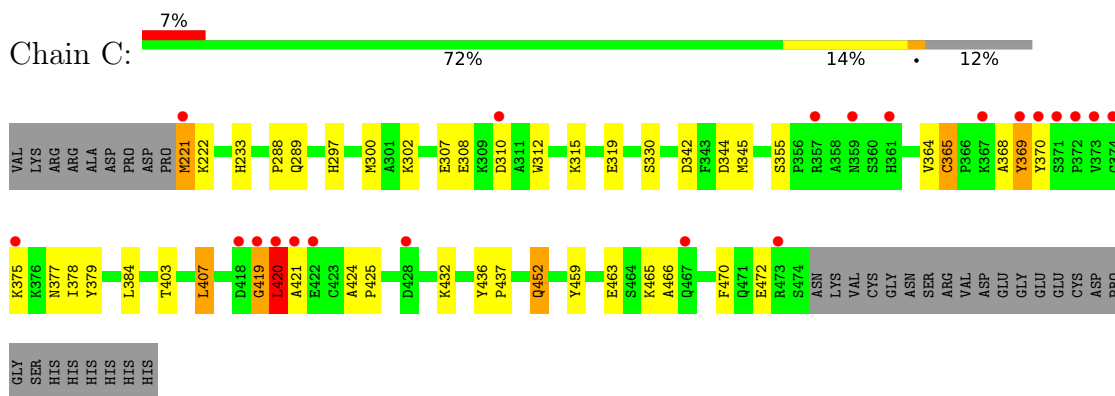
- Molecule 1: ADAM 17



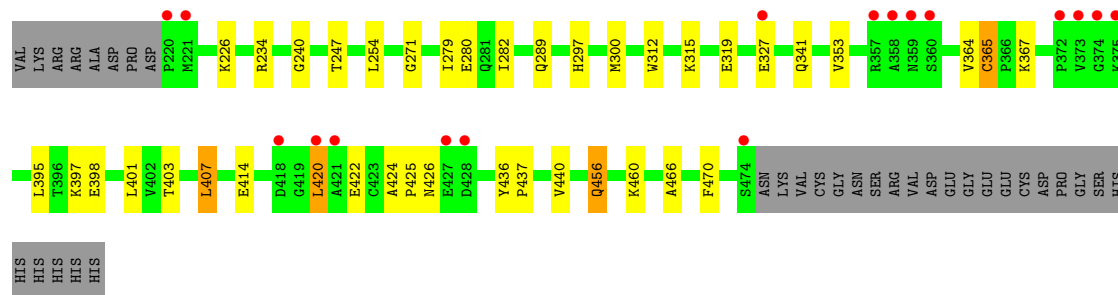
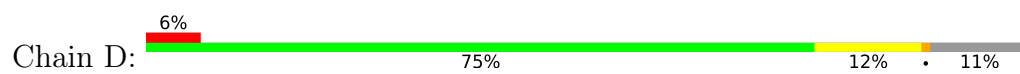
- Molecule 1: ADAM 17



- Molecule 1: ADAM 17



- Molecule 1: ADAM 17



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.77Å 126.19Å 81.22Å 90.00° 107.41° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 43.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.90) 93.5 (43.07-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.81Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.198 , 0.227 0.195 , 0.223	Depositor DCC
R_{free} test set	5164 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtrriage
Anisotropy	0.290	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8926	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: KGY, ZN, INN

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	0.51	0/2069	0.65	0/2791
1	B	0.50	0/2061	0.64	0/2780
1	C	0.47	0/2061	0.63	0/2780
1	D	0.49	0/2069	0.63	0/2791
All	All	0.49	0/8260	0.64	0/11142

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
1	C	0	2
1	D	0	1
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	TRP	Peptide
1	B	227	LEU	Peptide
1	B	312	TRP	Peptide
1	C	312	TRP	Peptide
1	C	419	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	D	312	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2023	0	1940	28	0
1	B	2016	0	1932	18	0
1	C	2016	0	1932	30	0
1	D	2023	0	1940	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	29	0	36	0	0
3	B	29	0	36	0	0
4	C	35	0	26	0	0
4	D	35	0	26	0	0
5	A	213	0	0	3	0
5	B	165	0	0	0	0
5	C	169	0	0	1	0
5	D	169	0	0	3	0
All	All	8926	0	7868	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 6.

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:372:PRO:O	1:A:373:VAL:HG23	1.64	0.97
1:B:282:ILE:HD11	1:B:284:ILE:HD11	1.62	0.79
1:A:372:PRO:O	1:A:373:VAL:CG2	2.32	0.78
1:B:466:ALA:O	1:B:470:PHE:HB2	1.97	0.65
1:A:372:PRO:O	1:A:373:VAL:CB	2.47	0.61
1:A:323:PHE:HA	1:A:378:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:TYR:CD1	1:D:437:PRO:HD2	2.40	0.57
1:A:330:SER:HB3	1:A:379:TYR:CE1	2.41	0.56
1:C:369:TYR:CE1	1:C:378:ILE:HD11	2.41	0.56
1:A:421:ALA:O	1:A:422:GLU:HB2	2.06	0.56
1:D:353:VAL:HG11	1:D:414:GLU:OE2	2.06	0.54
1:C:419:GLY:O	1:C:420:LEU:C	2.47	0.53
1:D:367:LYS:HE2	5:D:1060:HOH:O	2.09	0.53
1:C:355:SER:O	1:C:465:LYS:HE3	2.09	0.53
1:D:315:LYS:HE2	1:D:319:GLU:OE2	2.08	0.53
1:A:432:LYS:HD3	1:A:436:TYR:CD2	2.44	0.53
1:B:401:LEU:HD21	1:B:448:LYS:HG2	1.91	0.52
1:D:289:GLN:HG2	1:D:297:HIS:CG	2.44	0.52
1:D:456:GLN:HE22	1:D:460:LYS:HE3	1.74	0.52
1:C:459:TYR:O	1:C:463:GLU:HG3	2.10	0.52
1:D:401:LEU:HD13	1:D:440:VAL:HG23	1.91	0.51
1:C:289:GLN:HG2	1:C:297:HIS:CG	2.45	0.51
1:C:436:TYR:CD1	1:C:437:PRO:HD2	2.45	0.51
1:C:432:LYS:HD3	1:C:436:TYR:CD2	2.46	0.50
1:C:368:ALA:HB1	1:C:377:ASN:HB3	1.94	0.50
1:A:279:ILE:HG21	1:A:282:ILE:HG13	1.94	0.50
1:A:465:LYS:O	1:A:468:GLU:HB3	2.11	0.50
1:A:279:ILE:HG21	1:A:282:ILE:CG1	2.42	0.50
1:A:292:LYS:O	1:A:295:GLU:HB3	2.12	0.50
1:A:403:THR:HG22	1:A:407:LEU:HD22	1.94	0.49
1:A:237:ARG:HD3	5:A:1088:HOH:O	2.11	0.49
1:D:327:GLU:HG3	5:D:1030:HOH:O	2.12	0.49
1:B:453:CYS:O	1:B:456:GLN:HG2	2.12	0.49
1:C:344:ASP:OD2	1:C:345:MET:HG3	2.12	0.49
1:D:364:VAL:O	1:D:365:CYS:HB2	2.12	0.49
1:C:466:ALA:O	1:C:470:PHE:HB2	2.13	0.49
1:C:420:LEU:O	1:C:421:ALA:HB2	2.13	0.48
1:B:226:LYS:HB3	1:B:280:GLU:HB2	1.94	0.48
1:D:466:ALA:O	1:D:470:PHE:HB2	2.13	0.48
1:C:420:LEU:HB2	1:D:271:GLY:HA3	1.96	0.48
1:D:315:LYS:O	1:D:319:GLU:HG3	2.14	0.48
1:D:254:LEU:C	1:D:254:LEU:HD23	2.34	0.48
1:A:448:LYS:HD3	5:A:1058:HOH:O	2.14	0.47
1:C:452:GLN:HG3	5:C:1160:HOH:O	2.13	0.47
1:C:310:ASP:OD2	1:C:342:ASP:HB2	2.14	0.47
1:C:330:SER:HB3	1:C:379:TYR:CE1	2.49	0.47
1:D:397:LYS:O	1:D:401:LEU:HG	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HB2	1:A:398:GLU:HG3	1.97	0.47
1:D:279:ILE:HG21	1:D:282:ILE:HG13	1.96	0.47
1:A:300:MET:HG3	1:A:302:LYS:O	2.16	0.46
1:C:436:TYR:CG	1:C:437:PRO:HD2	2.49	0.46
1:B:432:LYS:HD3	1:B:436:TYR:CG	2.51	0.46
1:A:460:LYS:HD3	1:A:463:GLU:OE2	2.15	0.46
1:C:315:LYS:O	1:C:319:GLU:HG3	2.16	0.46
1:C:420:LEU:HD23	1:C:420:LEU:HA	1.82	0.45
1:D:436:TYR:CG	1:D:437:PRO:HD2	2.51	0.45
1:C:364:VAL:O	1:C:365:CYS:HB2	2.16	0.45
1:D:240:GLY:HA3	1:D:247:THR:OG1	2.16	0.45
1:D:395:LEU:HB2	1:D:398:GLU:HG3	1.98	0.45
1:A:270:ALA:O	1:B:327:GLU:HG3	2.17	0.45
1:A:372:PRO:O	1:A:373:VAL:HB	2.16	0.44
1:D:426:ASN:HB2	5:D:1046:HOH:O	2.17	0.44
1:A:432:LYS:HD3	1:A:436:TYR:CG	2.52	0.43
1:A:401:LEU:HD13	1:A:440:VAL:HG23	1.99	0.43
1:D:297:HIS:O	1:D:300:MET:HG2	2.18	0.43
1:A:304:TYR:CD1	1:A:305:PRO:HA	2.53	0.43
1:D:420:LEU:C	1:D:420:LEU:HD23	2.39	0.43
1:B:228:LEU:HD22	1:B:328:GLU:HB3	2.00	0.43
1:C:368:ALA:HB2	1:C:379:TYR:CE2	2.52	0.43
1:D:420:LEU:HD23	1:D:420:LEU:O	2.18	0.43
1:B:403:THR:HG22	1:B:407:LEU:HD22	2.01	0.43
1:C:302:LYS:HB3	1:C:307:GLU:HG3	2.00	0.43
1:D:234:ARG:NH1	1:D:341:GLN:HG2	2.33	0.42
1:D:403:THR:HG22	1:D:407:LEU:HD22	2.02	0.42
1:B:369:TYR:HD2	1:B:378:ILE:HD11	1.84	0.42
1:B:289:GLN:HG2	1:B:297:HIS:CG	2.54	0.42
1:C:233:HIS:CD2	1:C:288:PRO:HG3	2.55	0.42
1:B:292:LYS:HB2	1:B:295:GLU:OE1	2.19	0.42
1:C:384:LEU:C	1:C:384:LEU:HD12	2.40	0.42
1:A:360:SER:O	1:A:367:LYS:HG2	2.19	0.41
1:C:221:MET:HB3	1:C:222:LYS:H	1.63	0.41
1:C:424:ALA:N	1:C:425:PRO:HD3	2.35	0.41
1:B:325:ILE:O	1:B:325:ILE:HG13	2.19	0.41
1:B:236:TYR:CD2	1:B:286:LYS:HA	2.55	0.41
1:B:364:VAL:O	1:B:365:CYS:HB2	2.20	0.41
1:A:227:LEU:CD2	1:A:334:LEU:HB2	2.51	0.41
1:B:427:GLU:HG2	1:B:427:GLU:O	2.20	0.41
1:A:466:ALA:O	1:A:470:PHE:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:LYS:HB3	1:D:280:GLU:HB2	2.03	0.41
1:A:224:THR:OG1	1:A:473:ARG:HG2	2.21	0.41
1:A:364:VAL:O	1:A:365:CYS:HB2	2.21	0.41
1:C:221:MET:O	1:C:472:GLU:HA	2.20	0.41
1:C:403:THR:HG22	1:C:407:LEU:HD22	2.03	0.40
1:A:302:LYS:HG2	5:A:997:HOH:O	2.21	0.40
1:B:436:TYR:CG	1:B:437:PRO:HD2	2.57	0.40
1:C:370:TYR:OH	1:C:375:LYS:HD2	2.20	0.40
1:D:424:ALA:N	1:D:425:PRO:HD3	2.35	0.40
1:B:235:PHE:CE1	1:B:239:MET:HG3	2.57	0.40
1:C:297:HIS:O	1:C:300:MET:HG2	2.22	0.40
1:C:300:MET:HE3	1:C:302:LYS:O	2.22	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	253/288 (88%)	239 (94%)	11 (4%)	3 (1%)	13	4
1	B	252/288 (88%)	241 (96%)	10 (4%)	1 (0%)	34	24
1	C	252/288 (88%)	243 (96%)	7 (3%)	2 (1%)	19	9
1	D	253/288 (88%)	243 (96%)	8 (3%)	2 (1%)	19	9
All	All	1010/1152 (88%)	966 (96%)	36 (4%)	8 (1%)	19	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	C	420	LEU
1	A	312	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	365	CYS
1	B	365	CYS
1	C	365	CYS
1	D	365	CYS
1	D	420	LEU

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	218/247 (88%)	216 (99%)	2 (1%)	78	79
1	B	217/247 (88%)	215 (99%)	2 (1%)	78	79
1	C	217/247 (88%)	211 (97%)	6 (3%)	43	36
1	D	218/247 (88%)	215 (99%)	3 (1%)	67	65
All	All	870/988 (88%)	857 (98%)	13 (2%)	65	62

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	407	LEU
1	A	428	ASP
1	B	282	ILE
1	B	407	LEU
1	C	221	MET
1	C	308	GLU
1	C	369	TYR
1	C	407	LEU
1	C	420	LEU
1	C	452	GLN
1	D	407	LEU
1	D	422	GLU
1	D	456	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	281	GLN
1	D	361	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are 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
3	INN	B	902	2	28,28,28	0.74	1 (3%)	36,38,38	1.31	4 (11%)
4	KGY	C	1001	2	35,37,37	1.70	9 (25%)	43,55,55	2.20	14 (32%)
3	INN	A	901	2	28,28,28	0.55	0	36,38,38	1.33	4 (11%)
4	KGY	D	1002	2	35,37,37	1.68	7 (20%)	43,55,55	2.17	12 (27%)

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	INN	B	902	2	-	0/40/40/40	-
4	KGY	C	1001	2	-	6/30/49/49	0/3/3/3
3	INN	A	901	2	-	0/40/40/40	-
4	KGY	D	1002	2	-	6/30/49/49	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	KGY	C2-S1	-4.85	1.71	1.79
4	C	1001	KGY	C2-S1	-4.75	1.71	1.79
4	D	1002	KGY	C28-C27	3.53	1.45	1.38
4	C	1001	KGY	C28-C27	3.34	1.45	1.38
4	C	1001	KGY	C25-C24	3.14	1.43	1.38
4	D	1002	KGY	C25-C24	3.11	1.43	1.38
4	D	1002	KGY	C29-C24	3.07	1.43	1.38
4	C	1001	KGY	C29-C24	2.96	1.43	1.38
4	C	1001	KGY	C26-C27	2.37	1.43	1.38
4	C	1001	KGY	C26-C25	2.35	1.43	1.38
4	D	1002	KGY	C26-C27	2.34	1.43	1.38
4	C	1001	KGY	C2-C6	2.27	1.40	1.38
4	D	1002	KGY	C29-C28	2.27	1.42	1.38
4	D	1002	KGY	C26-C25	2.19	1.42	1.38
4	C	1001	KGY	C29-C28	2.16	1.42	1.38
4	C	1001	KGY	C15-C14	2.09	1.57	1.54
3	B	902	INN	C7-C6	2.03	1.57	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	KGY	C16-N11-C12	7.32	120.27	112.17
4	C	1001	KGY	O3-S1-N11	5.93	112.09	106.69
4	D	1002	KGY	O3-S1-N11	5.64	111.83	106.69
4	C	1001	KGY	C16-N11-C12	5.38	118.12	112.17
3	A	901	INN	C14-N3-C13	-5.03	113.61	122.59
4	C	1001	KGY	C12-C13-C14	4.84	114.87	109.17
4	C	1001	KGY	C16-C15-C14	4.31	114.24	109.17
4	D	1002	KGY	C15-C16-N11	3.82	113.84	109.14
3	B	902	INN	C14-N3-C13	-3.67	116.04	122.59
4	D	1002	KGY	C18-S21-C24	3.58	114.15	105.45
4	C	1001	KGY	C15-C14-C13	3.54	112.80	108.13
3	B	902	INN	C0-CA-C4	-3.51	104.68	109.77
3	B	902	INN	C11-N2-C10	-3.49	113.73	121.29
4	C	1001	KGY	C13-C14-C18	-3.48	102.46	109.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	KGY	C12-C13-C14	3.39	113.16	109.17
4	D	1002	KGY	C16-C15-C14	3.28	113.03	109.17
4	C	1001	KGY	C18-S21-C24	3.25	113.37	105.45
4	D	1002	KGY	O22-S21-C24	-3.17	105.15	108.36
4	C	1001	KGY	O4-S1-O3	-2.92	114.79	119.52
4	D	1002	KGY	O4-S1-O3	-2.71	115.14	119.52
4	C	1001	KGY	O22-S21-C24	-2.60	105.72	108.36
4	D	1002	KGY	C13-C12-N11	2.57	112.30	109.14
4	D	1002	KGY	C15-C14-C18	2.55	115.35	109.89
3	A	901	INN	CA-C0-C	-2.49	107.38	112.10
4	D	1002	KGY	C13-C14-C17	-2.39	106.42	111.08
4	C	1001	KGY	O23-S21-O22	-2.31	115.73	118.44
4	C	1001	KGY	C12-N11-S1	2.27	121.18	117.05
4	D	1002	KGY	O23-S21-O22	-2.18	115.89	118.44
3	A	901	INN	C11-N2-C10	-2.17	116.59	121.29
4	C	1001	KGY	O4-S1-N11	2.15	108.65	106.69
3	B	902	INN	CA-C0-C	-2.11	108.10	112.10
3	A	901	INN	C0-CA-C4	-2.02	106.84	109.77
4	C	1001	KGY	C16-N11-S1	2.01	120.70	117.05
4	C	1001	KGY	C15-C16-N11	2.01	111.61	109.14

There are no chirality outliers.

All (12) torsion outliers are listed below:

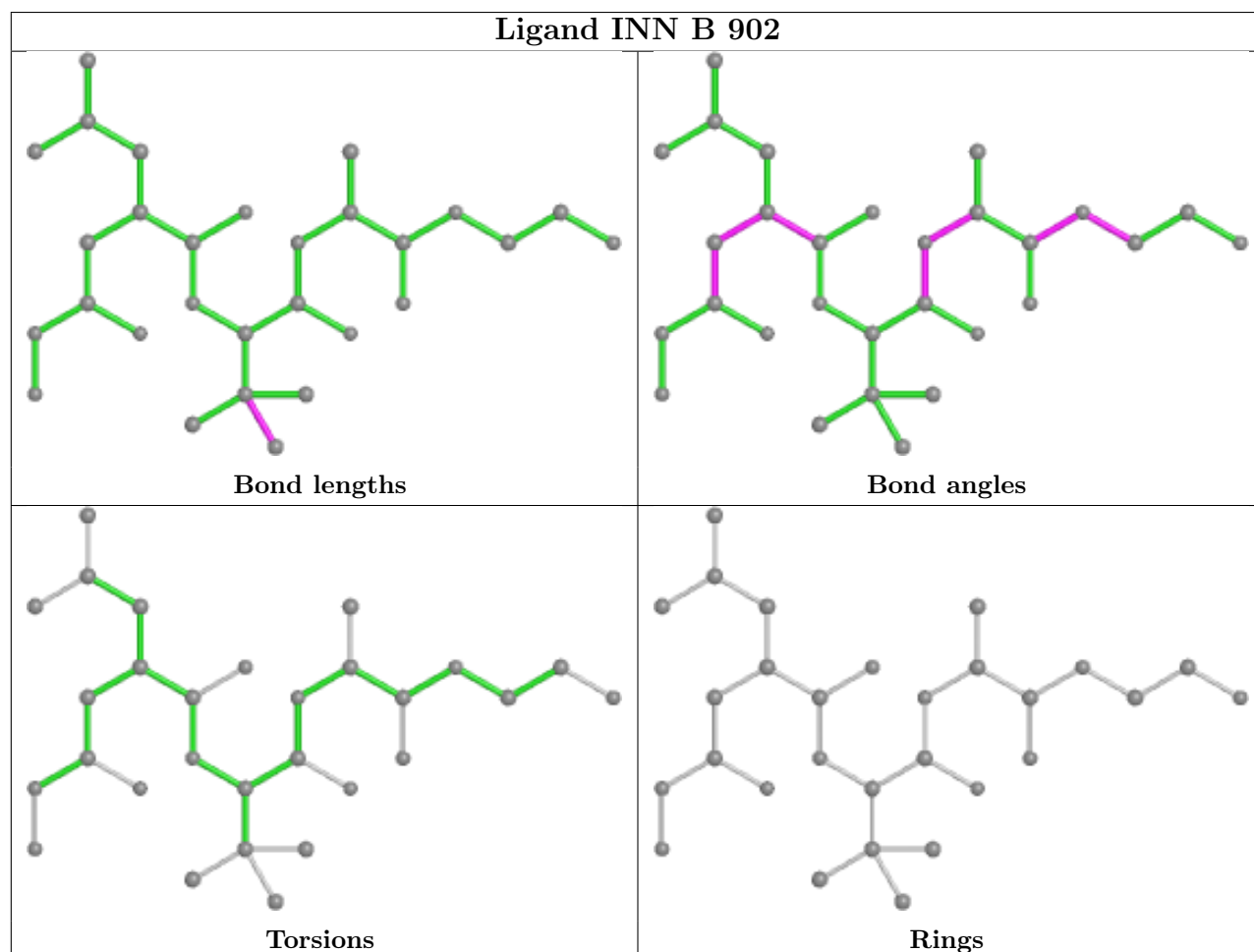
Mol	Chain	Res	Type	Atoms
4	C	1001	KGY	O30-C31-C32-C33
4	C	1001	KGY	C12-N11-S1-O4
4	C	1001	KGY	C12-N11-S1-O3
4	D	1002	KGY	C12-N11-S1-C2
4	D	1002	KGY	C12-N11-S1-O4
4	C	1001	KGY	C12-N11-S1-C2
4	D	1002	KGY	C12-N11-S1-O3
4	D	1002	KGY	C26-C27-O30-C31
4	C	1001	KGY	C26-C27-O30-C31
4	D	1002	KGY	C28-C27-O30-C31
4	C	1001	KGY	C28-C27-O30-C31
4	D	1002	KGY	O30-C31-C32-C33

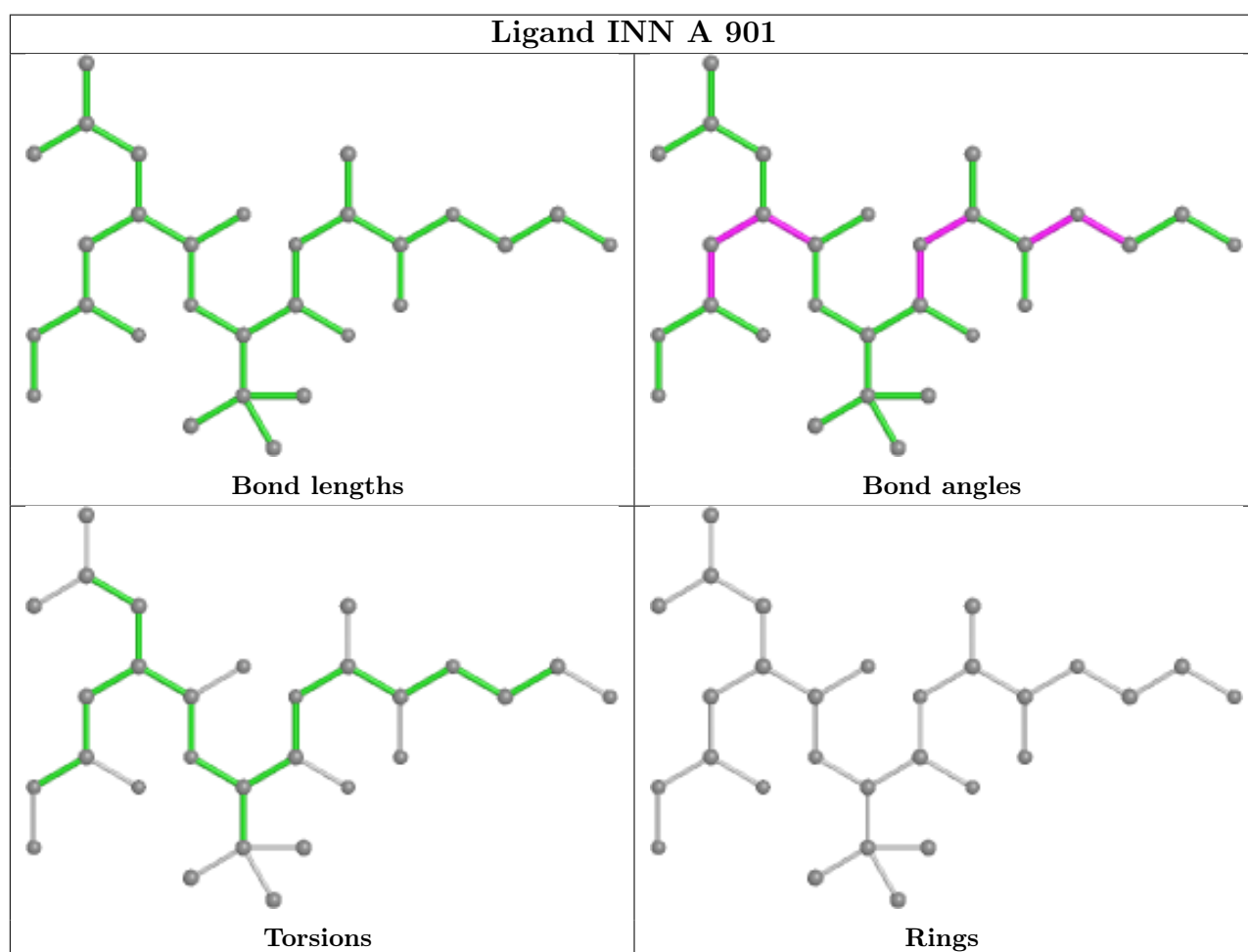
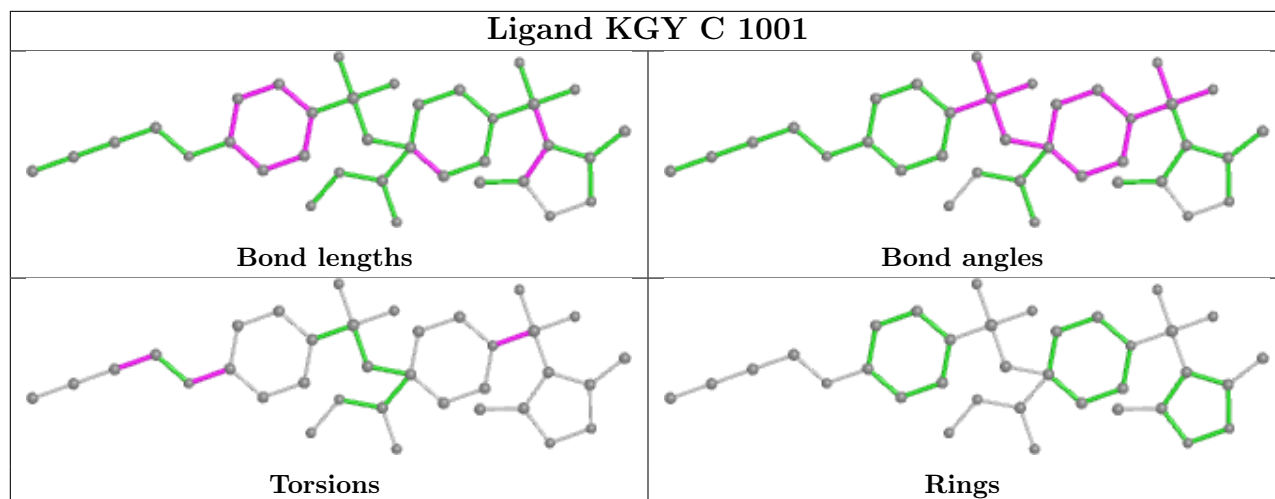
There are no ring outliers.

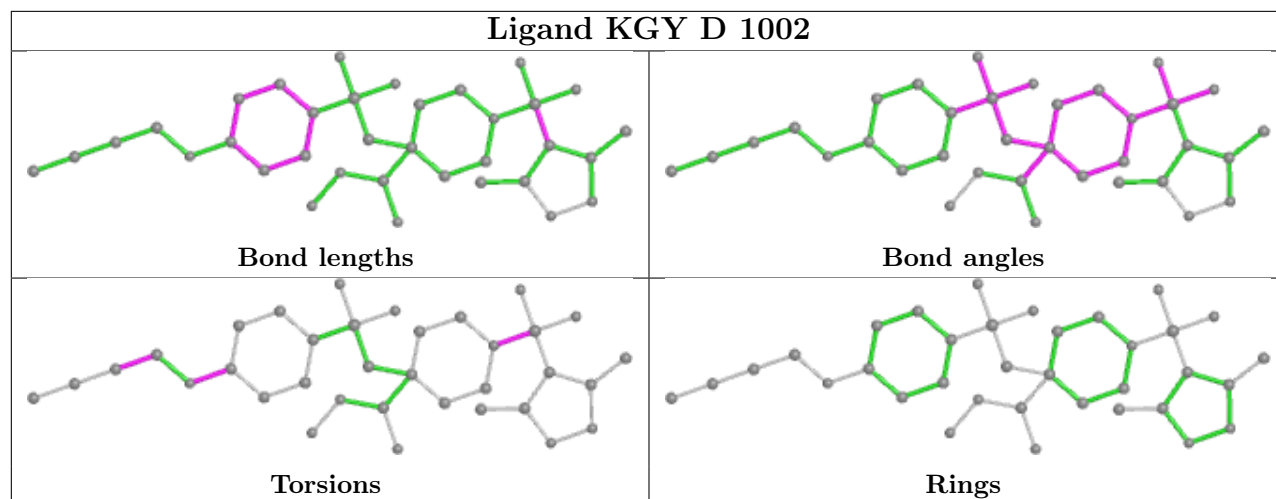
No monomer is involved in short contacts.

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	255/288 (88%)	0.12	17 (6%) 17 20	7, 19, 44, 54	0
1	B	254/288 (88%)	0.01	10 (3%) 39 42	7, 18, 40, 53	0
1	C	254/288 (88%)	0.12	21 (8%) 11 13	7, 20, 48, 54	0
1	D	255/288 (88%)	-0.05	17 (6%) 17 20	7, 18, 47, 55	0
All	All	1018/1152 (88%)	0.05	65 (6%) 19 22	7, 19, 45, 55	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	420	LEU	15.2
1	D	420	LEU	8.7
1	A	220	PRO	7.6
1	A	420	LEU	7.1
1	B	358	ALA	6.9
1	A	421	ALA	6.8
1	C	373	VAL	6.3
1	A	373	VAL	6.2
1	C	419	GLY	5.8
1	C	369	TYR	5.8
1	D	421	ALA	5.7
1	A	369	TYR	5.6
1	C	375	LYS	5.1
1	C	418	ASP	4.9
1	D	220	PRO	4.9
1	B	420	LEU	4.9
1	B	359	ASN	4.7
1	B	369	TYR	4.7
1	D	373	VAL	4.6
1	C	428	ASP	4.5
1	A	293	PRO	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	372	PRO	4.2
1	C	421	ALA	4.0
1	C	372	PRO	4.0
1	C	422	GLU	4.0
1	D	359	ASN	3.9
1	B	293	PRO	3.8
1	D	372	PRO	3.6
1	D	428	ASP	3.6
1	C	374	GLY	3.6
1	A	292	LYS	3.4
1	C	359	ASN	3.4
1	B	467	GLN	3.4
1	A	375	LYS	3.3
1	C	221	MET	3.2
1	D	358	ALA	3.2
1	D	374	GLY	3.2
1	A	358	ALA	3.1
1	C	371	SER	3.1
1	C	370	TYR	3.0
1	D	221	MET	3.0
1	D	474	SER	2.8
1	C	361	HIS	2.8
1	D	360	SER	2.8
1	A	419	GLY	2.8
1	C	367	LYS	2.8
1	D	327	GLU	2.6
1	B	292	LYS	2.6
1	C	467	GLN	2.6
1	A	374	GLY	2.5
1	D	418	ASP	2.4
1	A	370	TYR	2.4
1	C	473	ARG	2.4
1	B	295	GLU	2.4
1	C	357	ARG	2.4
1	D	375	LYS	2.3
1	D	427	GLU	2.3
1	A	422	GLU	2.3
1	B	221	MET	2.1
1	A	327	GLU	2.1
1	C	310	ASP	2.1
1	A	294	GLY	2.1
1	B	357	ARG	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	357	ARG	2.1
1	A	428	ASP	2.0

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 monosaccharides in this entry.

6.4 Ligands [i](#)

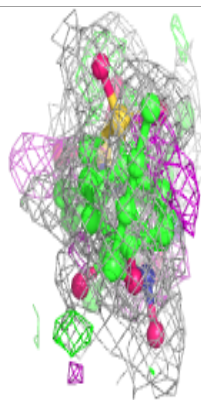
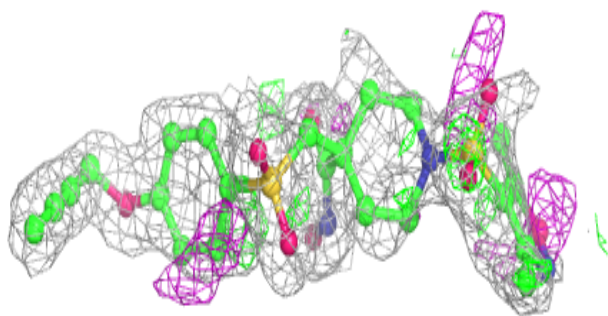
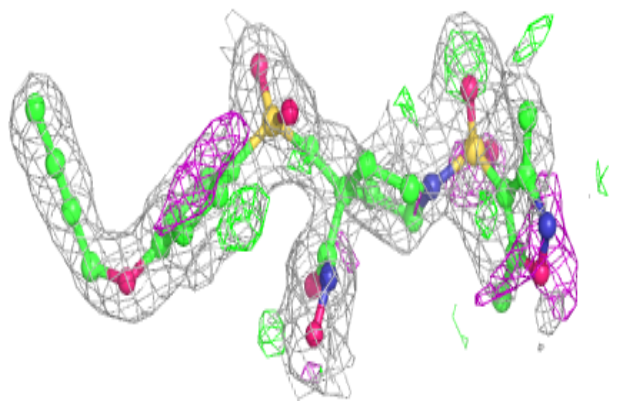
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	KGY	C	1001	35/35	0.87	0.18	17,24,61,62	0
4	KGY	D	1002	35/35	0.93	0.12	13,21,42,43	0
3	INN	A	901	29/29	0.95	0.09	6,11,27,34	0
3	INN	B	902	29/29	0.96	0.11	8,11,26,28	0
2	ZN	C	804	1/1	0.99	0.06	14,14,14,14	0
2	ZN	D	803	1/1	0.99	0.08	14,14,14,14	0
2	ZN	A	802	1/1	1.00	0.07	11,11,11,11	0
2	ZN	B	801	1/1	1.00	0.10	12,12,12,12	0

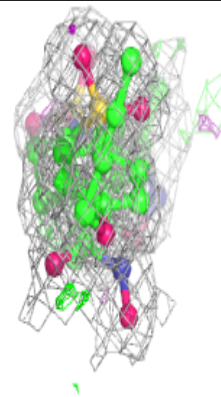
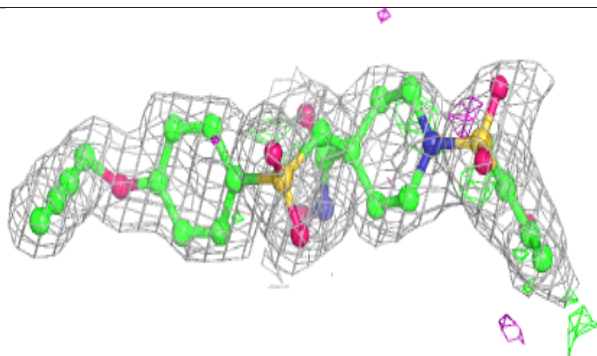
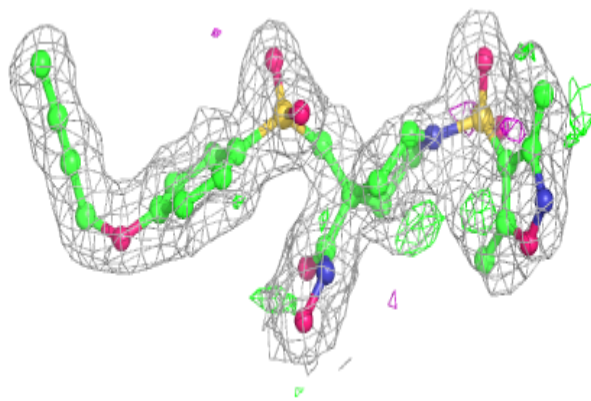
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KGY C 1001:

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

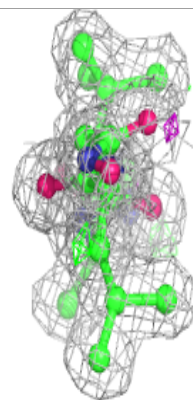
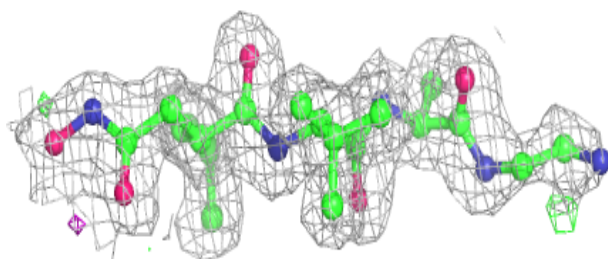
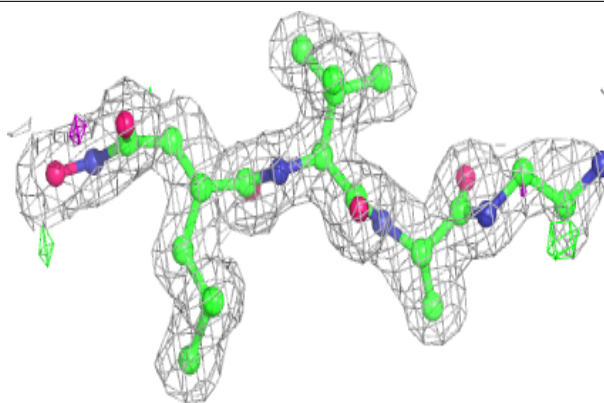
**Electron density around KGY D 1002:**

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

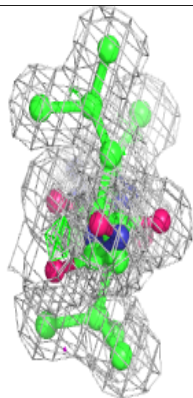
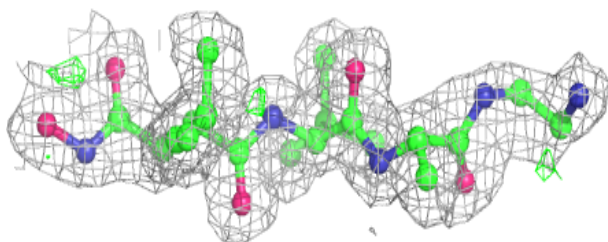
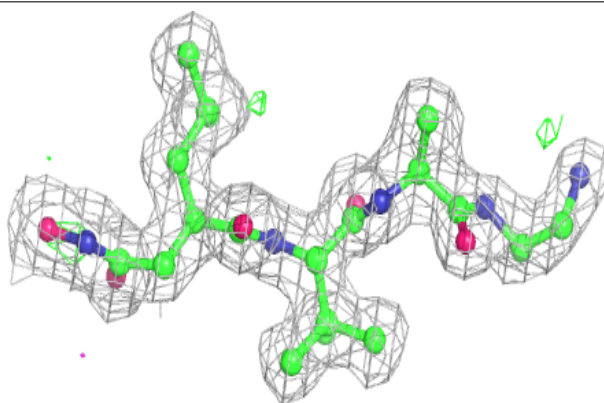


Electron density around INN A 901:

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

**Electron density around INN B 902:**

$2mF_o-DF_c$ (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.