



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:07 PM EDT

PDB ID : 5LL5 / pdb_00005ll5
Title : Crystal structure of human carbonic anhydrase isozyme XII with 4-(1H-benzimidazol-1-ylacetyl)benzenesulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2016-07-26
Resolution : 1.42 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

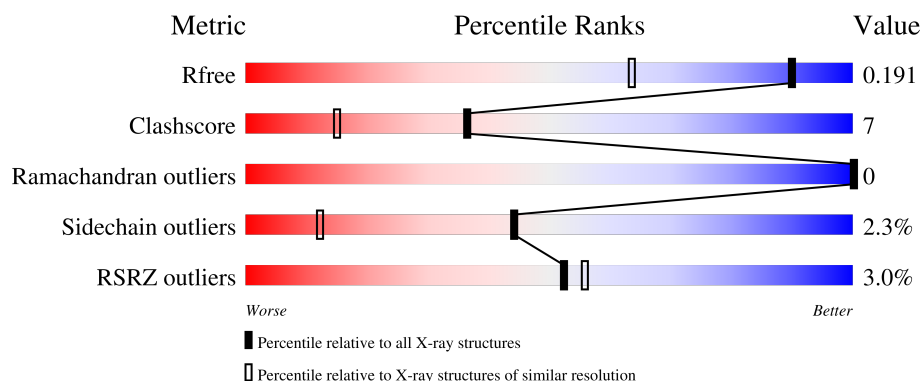
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	263	% 76% 20% ..
1	B	263	4% 81% 16% ..
1	C	263	6% 79% 17% ...
1	D	263	% 87% 11% ..

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
4	EDO	B	305	-	-	X	-
4	EDO	D	305[B]	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9991 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 Carbonic anhydrase 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	11	0
			2188	1389	375	416	8			
1	B	261	Total	C	N	O	S	0	7	0
			2146	1360	364	415	7			
1	C	261	Total	C	N	O	S	0	7	0
			2123	1350	357	408	8			
1	D	261	Total	C	N	O	S	0	9	0
			2172	1376	371	418	7			

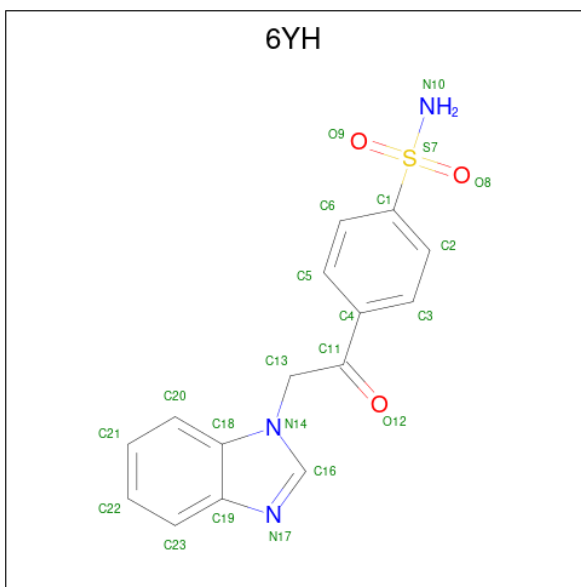
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP O43570
B	1	MET	-	initiating methionine	UNP O43570
C	1	MET	-	initiating methionine	UNP O43570
D	1	MET	-	initiating methionine	UNP O43570

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is 4-[2-(benzimidazol-1-yl)ethanoyl]benzenesulfonamide (CCD ID: 6YH) (formula: C₁₅H₁₃N₃O₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
3	B	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
3	C	1	Total	C	N	O	S	0	0
			22	15	3	3	1		
3	D	1	Total	C	N	O	S	0	1
			44	30	6	6	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	D	1	Total C O 8 4 4	0	1

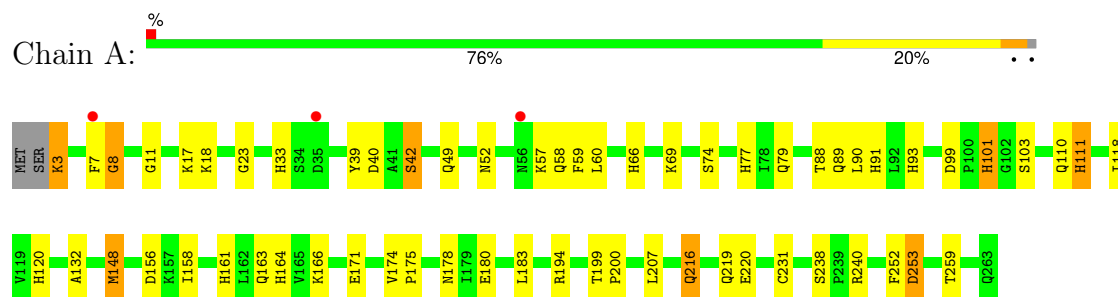
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	273	Total O 273 273	0	0
5	B	324	Total O 324 324	0	0
5	C	276	Total O 276 276	0	0
5	D	327	Total O 327 327	0	0

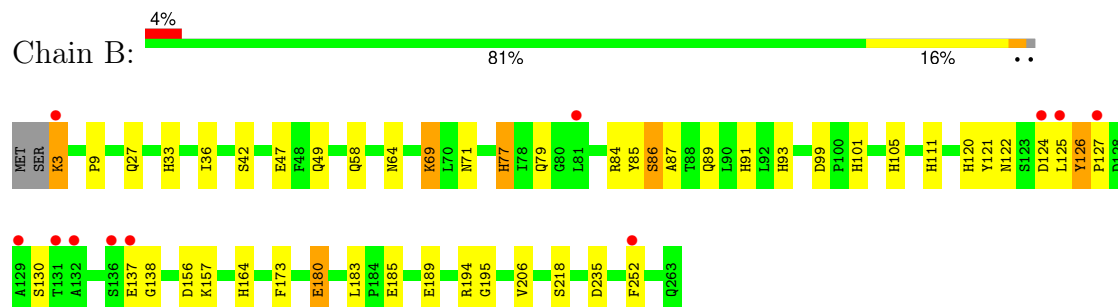
3 Residue-property plots [i](#)

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.

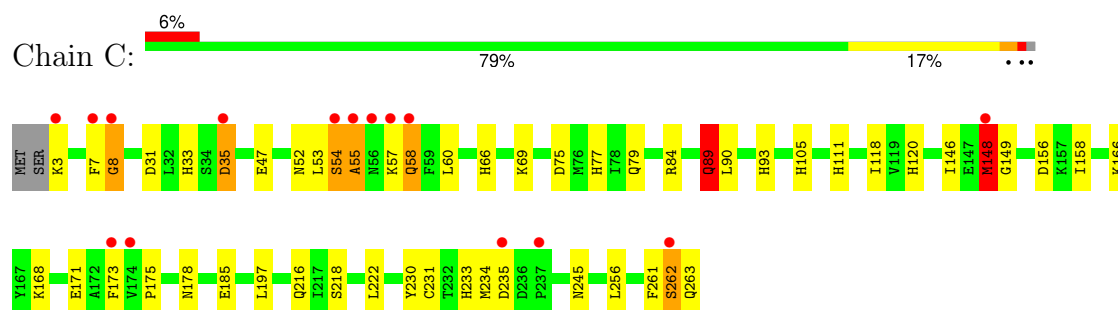
• Molecule 1: Carbonic anhydrase 12



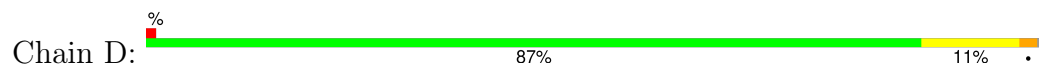
• Molecule 1: Carbonic anhydrase 12

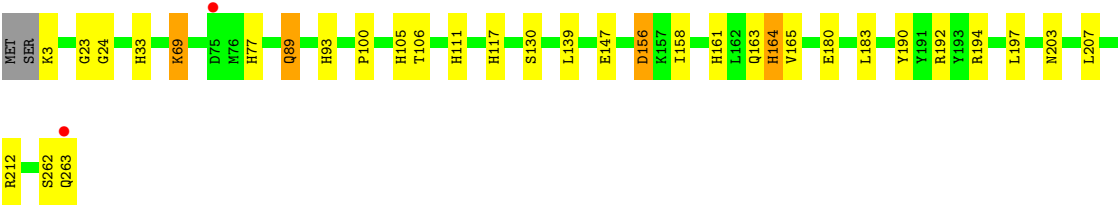


• Molecule 1: Carbonic anhydrase 12



• Molecule 1: Carbonic anhydrase 12





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.42Å 73.96Å 91.33Å 90.00° 108.96° 90.00°	Depositor
Resolution (Å)	67.76 – 1.42 67.76 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.1 (67.76-1.42) 99.1 (67.76-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.164 , 0.193 0.162 , 0.191	Depositor DCC
R_{free} test set	18027 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	13.0	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9991	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.01 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6240e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 6YH, EDO, ZN

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	1.61	24/2253 (1.1%)	1.31	4/3063 (0.1%)
1	B	1.73	25/2210 (1.1%)	1.47	12/3010 (0.4%)
1	C	1.59	24/2187 (1.1%)	1.35	11/2980 (0.4%)
1	D	1.63	20/2236 (0.9%)	1.34	5/3043 (0.2%)
All	All	1.64	93/8886 (1.0%)	1.37	32/12096 (0.3%)

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	120	HIS	CE1-NE2	9.68	1.42	1.32
1	B	91	HIS	CE1-NE2	8.34	1.40	1.32
1	D	105	HIS	ND1-CE1	8.25	1.40	1.32
1	D	77	HIS	ND1-CE1	7.90	1.40	1.32
1	D	24	GLY	N-CA	7.88	1.53	1.45
1	B	71	ASN	N-CA	7.77	1.55	1.46
1	A	216	GLN	CA-C	-7.49	1.43	1.52
1	B	93	HIS	CD2-NE2	7.47	1.46	1.37
1	B	164	HIS	CG-CD2	7.26	1.43	1.35
1	A	120	HIS	N-CA	7.25	1.55	1.45
1	A	33	HIS	ND1-CE1	7.22	1.39	1.32
1	B	86	SER	CA-C	7.21	1.61	1.52
1	D	93	HIS	CD2-NE2	7.19	1.45	1.37
1	C	105	HIS	ND1-CE1	7.06	1.39	1.32
1	A	220	GLU	N-CA	-7.04	1.37	1.46
1	D	161	HIS	CE1-NE2	6.91	1.39	1.32
1	A	120	HIS	ND1-CE1	6.69	1.39	1.32
1	C	118	ILE	C-O	6.67	1.31	1.24
1	A	259	THR	C-O	6.65	1.32	1.24
1	B	33	HIS	ND1-CE1	6.63	1.39	1.32
1	C	93	HIS	CG-CD2	6.63	1.43	1.35
1	A	91	HIS	CE1-NE2	6.61	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	146	ILE	N-CA	6.55	1.53	1.46
1	A	101	HIS	ND1-CE1	6.48	1.39	1.32
1	D	139	LEU	N-CA	6.45	1.54	1.45
1	B	164	HIS	ND1-CE1	6.27	1.38	1.32
1	B	27	GLN	N-CA	6.25	1.54	1.45
1	C	158	ILE	C-O	6.19	1.30	1.23
1	B	105	HIS	CE1-NE2	6.18	1.38	1.32
1	B	121	TYR	CA-C	6.16	1.60	1.52
1	C	185	GLU	C-O	6.08	1.31	1.23
1	B	91	HIS	CG-CD2	6.05	1.42	1.35
1	C	77	HIS	N-CA	6.04	1.53	1.45
1	C	93	HIS	ND1-CE1	5.98	1.38	1.32
1	D	93	HIS	ND1-CE1	5.97	1.38	1.32
1	A	33	HIS	CG-CD2	5.95	1.42	1.35
1	A	17	LYS	N-CA	5.91	1.53	1.46
1	C	120	HIS	N-CA	5.90	1.53	1.45
1	B	77	HIS	CB-CG	5.88	1.58	1.50
1	B	85	TYR	CA-C	-5.87	1.45	1.52
1	A	120	HIS	CE1-NE2	5.82	1.38	1.32
1	D	117	HIS	CE1-NE2	5.76	1.38	1.32
1	D	33	HIS	CD2-NE2	-5.75	1.31	1.37
1	B	195	GLY	C-O	-5.74	1.19	1.24
1	C	8	GLY	N-CA	5.74	1.52	1.44
1	A	200	PRO	CA-C	5.65	1.57	1.52
1	C	89	GLN	C-O	5.63	1.30	1.23
1	A	93	HIS	ND1-CE1	5.61	1.38	1.32
1	A	161	HIS	CE1-NE2	5.60	1.38	1.32
1	A	23	GLY	CA-C	-5.58	1.45	1.51
1	C	148	MET	CA-C	-5.57	1.45	1.52
1	B	218	SER	CA-C	-5.54	1.45	1.53
1	A	8	GLY	N-CA	5.54	1.52	1.44
1	D	93	HIS	CG-CD2	5.53	1.42	1.35
1	A	118	ILE	C-O	5.52	1.30	1.24
1	B	111	HIS	ND1-CE1	5.52	1.38	1.32
1	B	185	GLU	C-O	5.52	1.30	1.23
1	C	111	HIS	CG-CD2	5.50	1.41	1.35
1	D	106	THR	N-CA	5.49	1.52	1.45
1	D	165	VAL	CA-CB	5.46	1.61	1.54
1	D	164	HIS	ND1-CE1	5.42	1.38	1.32
1	C	256	LEU	CA-C	5.42	1.59	1.52
1	B	9	PRO	CA-C	-5.40	1.44	1.52
1	C	77	HIS	CA-C	-5.39	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	TYR	N-CA	-5.33	1.39	1.46
1	A	132	ALA	C-O	-5.33	1.17	1.24
1	D	190	TYR	CA-C	-5.33	1.46	1.52
1	D	156	ASP	CA-C	5.32	1.60	1.52
1	B	235	ASP	N-CA	5.31	1.52	1.46
1	A	58	GLN	CA-C	-5.26	1.46	1.52
1	C	31	ASP	C-O	5.26	1.30	1.24
1	B	69	LYS	N-CA	5.25	1.52	1.46
1	D	194	ARG	N-CA	5.25	1.52	1.46
1	B	87	ALA	N-CA	5.24	1.52	1.46
1	C	66	HIS	CE1-NE2	5.23	1.37	1.32
1	D	23	GLY	C-O	5.22	1.29	1.24
1	C	233	HIS	N-CA	5.18	1.52	1.45
1	D	111	HIS	CE1-NE2	5.16	1.37	1.32
1	B	164	HIS	CE1-NE2	5.16	1.37	1.32
1	C	111	HIS	CE1-NE2	5.15	1.37	1.32
1	C	230	TYR	N-CA	-5.13	1.40	1.45
1	C	245	ASN	N-CA	5.09	1.52	1.46
1	C	84	ARG	NE-CZ	5.09	1.38	1.33
1	A	11	GLY	N-CA	5.08	1.51	1.45
1	C	120	HIS	CE1-NE2	5.08	1.37	1.32
1	A	111	HIS	CE1-NE2	5.06	1.37	1.32
1	D	93	HIS	CE1-NE2	5.06	1.37	1.32
1	B	77	HIS	ND1-CE1	5.04	1.37	1.32
1	C	222	LEU	N-CA	5.04	1.52	1.46
1	D	203	ASN	CA-C	-5.03	1.48	1.53
1	B	206	VAL	C-O	-5.03	1.18	1.24
1	A	158	ILE	C-O	5.02	1.28	1.23
1	A	91	HIS	CG-ND1	-5.00	1.32	1.38

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	TYR	CA-C-N	12.45	132.38	119.19
1	B	126	TYR	C-N-CA	12.45	132.38	119.19
1	B	252	PHE	N-CA-C	6.72	119.62	111.82
1	C	55	ALA	N-CA-C	-6.25	102.27	110.33
1	B	86	SER	O-C-N	6.11	130.34	123.19
1	B	252	PHE	CA-CB-CG	-6.10	107.70	113.80
1	B	157	LYS	N-CA-C	-5.94	104.88	111.71
1	C	261	PHE	CA-C-N	-5.93	114.04	122.94
1	C	261	PHE	C-N-CA	-5.93	114.04	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	69	LYS	CG-CD-CE	-5.92	97.69	111.30
1	C	175	PRO	CA-C-N	5.80	125.61	120.10
1	C	175	PRO	C-N-CA	5.80	125.61	120.10
1	B	138	GLY	N-CA-C	-5.78	105.63	113.37
1	C	53	LEU	CA-C-N	5.74	132.50	121.54
1	C	53	LEU	C-N-CA	5.74	132.50	121.54
1	C	166	LYS	N-CA-C	5.69	118.26	111.71
1	A	253	ASP	N-CA-C	5.56	117.84	110.06
1	B	206	VAL	N-CA-C	5.49	115.86	108.17
1	C	235	ASP	N-CA-C	5.40	117.87	111.33
1	A	110	GLN	N-CA-C	5.38	118.01	109.24
1	D	158	ILE	N-CA-C	-5.34	106.48	111.45
1	A	158	ILE	CB-CA-C	-5.29	105.56	111.80
1	D	100	PRO	N-CA-C	-5.22	105.43	112.48
1	D	262	SER	CA-C-N	5.16	130.99	121.70
1	D	262	SER	C-N-CA	5.16	130.99	121.70
1	A	199	THR	O-C-N	5.11	125.53	121.55
1	C	53	LEU	O-C-N	5.10	129.03	123.22
1	B	194	ARG	CA-C-N	-5.05	118.27	122.16
1	B	194	ARG	C-N-CA	-5.05	118.27	122.16
1	C	262	SER	N-CA-C	-5.03	101.21	109.40
1	B	180[A]	GLU	CA-C-O	5.01	125.55	119.38
1	B	180[B]	GLU	CA-C-O	5.01	125.55	119.38

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	2188	0	2064	41	0
1	B	2146	0	2011	23	0
1	C	2123	0	1971	36	0
1	D	2172	0	2048	22	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	22	0	0	0	0
3	B	22	0	0	0	0
3	C	22	0	0	3	0
3	D	44	0	0	8	0
4	A	12	0	18	1	0
4	B	12	0	18	6	0
4	C	8	0	12	3	0
4	D	16	0	24	7	0
5	A	273	0	0	10	1
5	B	324	0	0	7	1
5	C	276	0	0	7	0
5	D	327	0	0	2	0
All	All	9991	0	8166	122	1

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 7.

All (122) 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:B:42[A]:SER:OG	5:B:401:HOH:O	1.65	1.12
1:B:64:ASN:HD22	4:B:305:EDO:H22	1.15	1.11
1:D:147[B]:GLU:OE2	5:D:401:HOH:O	1.70	1.09
1:C:262:SER:O	1:C:263:GLN:HG2	1.54	1.08
1:C:58:GLN:OE1	5:C:401:HOH:O	1.77	1.03
5:A:637:HOH:O	1:C:234:MET:HE2	1.65	0.95
1:D:130[A]:SER:HA	3:D:302[A]:6YH:N17	1.87	0.90
1:C:168:LYS:HB2	1:C:231[B]:CYS:O	1.71	0.89
1:C:58:GLN:HG2	1:C:173[B]:PHE:HB3	1.55	0.88
1:A:148:MET:SD	1:A:219:GLN:HA	2.13	0.87
1:A:216:GLN:HG3	5:A:618:HOH:O	1.79	0.82
1:A:148:MET:SD	1:A:219:GLN:CA	2.69	0.80
1:C:262:SER:O	1:C:263:GLN:CG	2.31	0.79
1:C:216:GLN:HG3	5:C:550:HOH:O	1.82	0.79
1:B:69:LYS:NZ	4:B:305:EDO:H21	1.97	0.78
1:C:58:GLN:HG2	1:C:173[A]:PHE:HB3	1.64	0.77
1:C:148:MET:HE2	5:C:598:HOH:O	1.86	0.75
1:B:122:ASN:ND2	5:B:403:HOH:O	2.14	0.74
1:B:64:ASN:ND2	4:B:305:EDO:H22	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ASP:OD2	5:A:401:HOH:O	2.08	0.71
1:B:3:LYS:N	5:B:405:HOH:O	2.26	0.69
1:B:180[B]:GLU:OE2	5:B:402:HOH:O	2.11	0.69
1:C:3[A]:LYS:CG	1:C:3[A]:LYS:O	2.42	0.67
1:D:69:LYS:NZ	4:D:305[A]:EDO:H11	2.11	0.66
1:A:231[B]:CYS:SG	1:A:240:ARG:HB2	2.37	0.64
1:B:180[A]:GLU:HG3	1:B:183:LEU:HD12	1.80	0.63
1:D:69:LYS:HZ2	4:D:305[A]:EDO:H11	1.62	0.63
1:C:197:LEU:HD22	3:C:302:6YH:C6	2.29	0.62
1:D:130[A]:SER:CA	3:D:302[A]:6YH:N17	2.62	0.61
1:A:79:GLN:OE1	5:A:402:HOH:O	2.16	0.61
1:A:7[B]:PHE:CZ	1:A:240:ARG:HD2	2.36	0.61
1:A:148:MET:SD	1:A:219:GLN:HB3	2.40	0.61
1:C:75[B]:ASP:OD2	5:C:402:HOH:O	2.17	0.60
1:B:180[B]:GLU:CD	5:B:402:HOH:O	2.45	0.60
1:D:212:ARG:HH22	1:D:263:GLN:HB3	1.66	0.60
1:B:47:GLU:HB2	1:B:79:GLN:HB3	1.84	0.59
1:C:47:GLU:HB2	1:C:79:GLN:HB3	1.85	0.59
1:C:58:GLN:CG	1:C:173[A]:PHE:HB3	2.32	0.59
1:A:74:SER:O	5:A:403:HOH:O	2.18	0.57
1:C:89:GLN:HE22	4:C:303:EDO:H22	1.68	0.57
1:C:33:HIS:CE1	1:C:35:ASP:OD1	2.58	0.57
1:B:69:LYS:HZ3	4:B:305:EDO:H21	1.68	0.57
1:A:3:LYS:HA	5:A:578:HOH:O	2.05	0.56
1:C:7:PHE:CD1	1:C:8:GLY:N	2.74	0.56
1:D:89:GLN:HE21	4:D:305[B]:EDO:H12	1.69	0.56
1:B:77:HIS:CE1	1:B:86:SER:OG	2.59	0.56
1:D:212:ARG:HH12	1:D:263:GLN:CB	2.18	0.56
1:A:7[B]:PHE:HZ	1:A:240:ARG:HD2	1.71	0.55
1:D:89:GLN:NE2	4:D:305[B]:EDO:H12	2.23	0.54
1:A:194[A]:ARG:NE	1:A:207:LEU:HD13	2.24	0.53
1:A:148:MET:SD	1:A:219:GLN:CB	2.97	0.53
1:C:148:MET:CE	5:C:598:HOH:O	2.50	0.53
1:A:164:HIS:HD2	5:A:468:HOH:O	1.93	0.52
1:B:77:HIS:CE1	1:B:86:SER:HG	2.28	0.52
1:C:55:ALA:C	1:C:57:LYS:H	2.18	0.52
1:C:234:MET:CE	5:C:577:HOH:O	2.57	0.52
1:B:126:TYR:HB3	1:B:127:PRO:HD2	1.92	0.52
1:A:18[B]:LYS:HG2	1:A:18[B]:LYS:O	2.10	0.52
1:C:197:LEU:CD2	3:C:302:6YH:C6	2.89	0.51
1:A:180:GLU:HG3	1:A:183:LEU:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:LYS:N	5:D:405:HOH:O	2.44	0.51
1:D:69:LYS:HZ2	4:D:305[B]:EDO:H11	1.77	0.50
1:C:60:LEU:HD11	1:C:171:GLU:HB3	1.93	0.50
1:A:57:LYS:HE3	1:A:59:PHE:CZ	2.47	0.50
1:A:7[B]:PHE:C	1:A:7[B]:PHE:CD1	2.88	0.50
1:D:89:GLN:HE21	4:D:305[B]:EDO:C1	2.25	0.50
1:B:79:GLN:NE2	5:B:407:HOH:O	2.34	0.49
1:A:148:MET:SD	1:A:219:GLN:N	2.86	0.49
1:D:130[A]:SER:OG	3:D:302[A]:6YH:N17	2.45	0.49
1:A:252[B]:PHE:CG	1:A:252[B]:PHE:O	2.66	0.49
1:C:54:SER:C	1:C:55:ALA:O	2.53	0.48
1:D:197[B]:LEU:CD2	3:D:302[B]:6YH:C3	2.91	0.48
1:C:69:LYS:HZ2	4:C:304:EDO:H21	1.78	0.48
1:D:163[B]:GLN:HG3	1:D:164:HIS:CD2	2.48	0.48
1:D:197[B]:LEU:HD22	3:D:302[B]:6YH:C2	2.44	0.48
1:C:263:GLN:OXT	1:C:263:GLN:HG3	2.14	0.47
1:D:197[B]:LEU:HD22	3:D:302[B]:6YH:C3	2.45	0.47
1:A:7[B]:PHE:HZ	1:A:240:ARG:CD	2.26	0.47
1:D:130[A]:SER:HA	3:D:302[A]:6YH:C19	2.43	0.47
1:C:197:LEU:HD22	3:C:302:6YH:C1	2.44	0.47
1:C:7:PHE:HD1	1:C:8:GLY:N	2.13	0.46
1:A:103:SER:O	1:A:111:HIS:HD2	1.99	0.46
1:C:69:LYS:NZ	4:C:304:EDO:H21	2.30	0.46
1:A:216:GLN:HG3	5:A:556:HOH:O	2.16	0.46
1:C:55:ALA:O	1:C:57:LYS:N	2.48	0.46
1:B:58:GLN:HG3	1:B:173:PHE:CD1	2.52	0.45
1:B:99:ASP:OD1	1:B:101:HIS:HD2	1.98	0.45
1:B:189[B]:GLU:OE2	5:B:404:HOH:O	2.20	0.45
1:C:55:ALA:HB2	5:C:429:HOH:O	2.16	0.45
1:D:197[B]:LEU:CD2	3:D:302[B]:6YH:C2	2.94	0.44
1:A:3:LYS:HE2	1:A:66:HIS:NE2	2.32	0.44
1:A:7[B]:PHE:O	1:A:8:GLY:C	2.61	0.44
1:A:49:GLN:OE1	1:A:77:HIS:NE2	2.44	0.44
1:A:88:THR:HG23	1:A:89:GLN:HG3	2.00	0.44
1:A:90:LEU:HD12	1:A:90:LEU:C	2.42	0.44
1:B:69:LYS:HZ1	4:B:305:EDO:H21	1.79	0.44
1:C:262:SER:O	1:C:263:GLN:CB	2.66	0.44
1:C:52:ASN:HA	1:C:178:ASN:HA	2.00	0.43
1:A:18[B]:LYS:O	1:A:18[B]:LYS:CG	2.65	0.43
1:A:148:MET:HE2	1:A:148:MET:HB3	1.73	0.43
1:D:180:GLU:HG3	1:D:183:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:ILE:HD12	1:B:36:ILE:C	2.44	0.43
1:B:49[B]:GLN:NE2	1:B:79:GLN:HB2	2.34	0.43
1:D:69:LYS:HD3	4:D:305[A]:EDO:H12	2.01	0.43
1:A:194[A]:ARG:CZ	1:A:207:LEU:HD13	2.49	0.42
1:A:7[B]:PHE:HD1	1:A:8:GLY:N	2.17	0.42
1:B:122:ASN:OD1	1:B:124:ASP:HB2	2.19	0.42
1:A:69:LYS:NZ	4:A:305:EDO:H21	2.35	0.42
1:C:149:GLY:O	1:C:218:SER:HA	2.20	0.42
1:A:60:LEU:HD11	1:A:171[A]:GLU:HB3	2.02	0.42
1:C:58:GLN:CD	1:C:173[A]:PHE:HB3	2.44	0.42
1:D:192:ARG:HD2	1:D:207:LEU:HD11	2.02	0.42
1:A:164:HIS:CD2	5:A:468:HOH:O	2.71	0.41
1:B:69:LYS:CE	4:B:305:EDO:H21	2.48	0.41
1:A:99:ASP:OD1	1:A:101:HIS:HD2	2.03	0.41
1:C:90:LEU:C	1:C:90:LEU:HD12	2.45	0.41
1:A:163:GLN:HG2	5:A:579:HOH:O	2.21	0.41
1:A:174:VAL:HA	1:A:175:PRO:HD3	1.92	0.41
1:C:7:PHE:CD1	1:C:7:PHE:C	2.99	0.40
1:A:231[B]:CYS:SG	1:A:240:ARG:NH1	2.94	0.40
1:A:52:ASN:HA	1:A:178:ASN:HA	2.04	0.40
1:A:40:ASP:OD1	1:A:42:SER:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:417:HOH:O	5:B:462:HOH:O[2_555]	2.13	0.07

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	270/263 (103%)	265 (98%)	5 (2%)	0	100	100
1	B	266/263 (101%)	260 (98%)	6 (2%)	0	100	100
1	C	265/263 (101%)	254 (96%)	11 (4%)	0	100	100
1	D	268/263 (102%)	262 (98%)	6 (2%)	0	100	100
All	All	1069/1052 (102%)	1041 (97%)	28 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	243/235 (103%)	237 (98%)	6 (2%)	42	10
1	B	238/235 (101%)	231 (97%)	7 (3%)	37	8
1	C	232/235 (99%)	226 (97%)	6 (3%)	40	9
1	D	242/235 (103%)	240 (99%)	2 (1%)	73	47
All	All	955/940 (102%)	934 (98%)	21 (2%)	44	13

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	42	SER
1	A	148	MET
1	A	156	ASP
1	A	166	LYS
1	A	238	SER
1	B	3	LYS
1	B	84	ARG
1	B	89	GLN
1	B	125	LEU
1	B	130	SER
1	B	137	GLU
1	B	156	ASP

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Mol	Chain	Res	Type
1	C	35	ASP
1	C	54	SER
1	C	58	GLN
1	C	89	GLN
1	C	148	MET
1	C	156	ASP
1	D	89	GLN
1	D	156	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	33	HIS
1	A	38	GLN
1	A	164	HIS
1	B	38	GLN
1	B	96	ASN
1	B	101	HIS
1	B	134	ASN
1	B	244	ASN
1	B	250	GLN
1	C	13	ASN
1	C	49	GLN
1	C	58	GLN
1	C	79	GLN
1	C	82	GLN
1	C	110	GLN
1	C	233	HIS
1	C	250	GLN
1	D	13	ASN
1	D	101	HIS
1	D	164	HIS
1	D	213	ASN
1	D	219	GLN
1	D	250	GLN

5.3.3 RNA ⓘ

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 21 ligands modelled in this entry, 4 are monoatomic - leaving 17 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	EDO	A	304	-	3,3,3	0.50	0	2,2,2	0.64	0
3	6YH	D	302[A]	2	24,24,24	2.79	8 (33%)	34,35,35	1.96	9 (26%)
4	EDO	C	303	-	3,3,3	0.52	0	2,2,2	0.73	0
4	EDO	A	305	-	3,3,3	0.61	0	2,2,2	0.30	0
4	EDO	D	305[A]	-	3,3,3	0.75	0	2,2,2	1.07	0
3	6YH	D	302[B]	2	24,24,24	1.91	6 (25%)	34,35,35	2.40	14 (41%)
4	EDO	B	303	-	3,3,3	0.87	0	2,2,2	0.28	0
4	EDO	D	305[B]	-	3,3,3	1.11	0	2,2,2	0.77	0
4	EDO	D	303	-	3,3,3	0.93	0	2,2,2	0.10	0
4	EDO	B	304	-	3,3,3	0.33	0	2,2,2	0.54	0
3	6YH	C	302	2	24,24,24	1.94	8 (33%)	34,35,35	2.18	13 (38%)
4	EDO	B	305	-	3,3,3	0.78	0	2,2,2	0.97	0
4	EDO	C	304	-	3,3,3	0.76	0	2,2,2	0.61	0
4	EDO	A	303	-	3,3,3	0.68	0	2,2,2	0.20	0
4	EDO	D	304	-	3,3,3	0.65	0	2,2,2	0.39	0
3	6YH	B	302	2	24,24,24	1.83	7 (29%)	34,35,35	2.46	14 (41%)
3	6YH	A	302	2	24,24,24	2.05	7 (29%)	34,35,35	2.02	11 (32%)

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	EDO	A	304	-	-	0/1/1/1	-
3	6YH	D	302[A]	2	-	7/14/14/14	0/3/3/3
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	D	305[A]	-	-	0/1/1/1	-
3	6YH	D	302[B]	2	-	4/14/14/14	0/3/3/3
4	EDO	B	303	-	-	0/1/1/1	-
4	EDO	D	305[B]	-	-	0/1/1/1	-
4	EDO	D	303	-	-	0/1/1/1	-
4	EDO	B	304	-	-	0/1/1/1	-
3	6YH	C	302	2	-	5/14/14/14	0/3/3/3
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	C	304	-	-	1/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
4	EDO	D	304	-	-	0/1/1/1	-
3	6YH	B	302	2	-	2/14/14/14	0/3/3/3
3	6YH	A	302	2	-	2/14/14/14	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302[A]	6YH	O9-S7	9.27	1.60	1.43
3	D	302[B]	6YH	O9-S7	4.96	1.52	1.43
3	D	302[A]	6YH	O8-S7	4.90	1.52	1.43
3	A	302	6YH	O8-S7	4.87	1.52	1.43
3	A	302	6YH	O9-S7	4.35	1.51	1.43
3	C	302	6YH	C2-C3	3.79	1.44	1.38
3	D	302[B]	6YH	O8-S7	3.71	1.50	1.43
3	D	302[A]	6YH	C1-S7	3.67	1.82	1.77
3	B	302	6YH	C2-C3	3.59	1.44	1.38
3	A	302	6YH	C16-N17	3.58	1.38	1.31
3	C	302	6YH	C1-S7	3.45	1.82	1.77
3	D	302[A]	6YH	S7-N10	3.38	1.67	1.60
3	B	302	6YH	O9-S7	3.38	1.49	1.43
3	C	302	6YH	O8-S7	3.30	1.49	1.43
3	D	302[A]	6YH	C16-N17	3.23	1.37	1.31
3	C	302	6YH	O9-S7	3.22	1.49	1.43
3	C	302	6YH	C16-N17	3.02	1.37	1.31
3	B	302	6YH	C16-N17	3.00	1.37	1.31
3	B	302	6YH	C1-S7	2.96	1.81	1.77
3	D	302[B]	6YH	C16-N17	2.66	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302[A]	6YH	C13-N14	2.60	1.49	1.46
3	D	302[B]	6YH	C6-C5	2.46	1.42	1.38
3	C	302	6YH	C13-N14	2.43	1.49	1.46
3	D	302[B]	6YH	C1-S7	2.42	1.80	1.77
3	B	302	6YH	C21-C20	2.35	1.42	1.38
3	C	302	6YH	O12-C11	2.33	1.26	1.22
3	A	302	6YH	S7-N10	-2.33	1.55	1.60
3	B	302	6YH	C22-C21	2.32	1.43	1.38
3	D	302[A]	6YH	C13-C11	2.30	1.56	1.52
3	D	302[A]	6YH	C22-C21	2.26	1.43	1.38
3	D	302[B]	6YH	C22-C21	2.22	1.43	1.38
3	A	302	6YH	C2-C1	-2.18	1.35	1.38
3	A	302	6YH	C21-C20	2.13	1.42	1.38
3	B	302	6YH	C22-C23	2.13	1.42	1.38
3	A	302	6YH	C6-C1	2.10	1.42	1.38
3	C	302	6YH	C19-N17	-2.01	1.36	1.39

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302[B]	6YH	C2-C1-S7	-6.43	110.99	119.72
3	D	302[A]	6YH	C19-C18-N14	5.81	108.88	105.40
3	B	302	6YH	C6-C1-C2	5.07	127.08	120.47
3	B	302	6YH	O9-S7-N10	5.07	114.67	107.35
3	A	302	6YH	C19-C18-N14	5.06	108.43	105.40
3	D	302[B]	6YH	C6-C1-S7	5.04	126.57	119.72
3	C	302	6YH	C13-C11-C4	4.87	123.76	117.67
3	B	302	6YH	C3-C2-C1	-4.64	114.93	119.44
3	A	302	6YH	O9-S7-N10	4.51	113.85	107.35
3	C	302	6YH	C19-C18-N14	4.45	108.06	105.40
3	D	302[B]	6YH	C19-C18-N14	4.42	108.05	105.40
3	D	302[B]	6YH	O12-C11-C13	4.40	126.27	120.28
3	B	302	6YH	C19-C18-N14	4.18	107.90	105.40
3	B	302	6YH	C5-C4-C3	4.09	123.78	118.57
3	B	302	6YH	C5-C6-C1	-4.09	115.46	119.44
3	D	302[A]	6YH	O12-C11-C13	3.92	125.62	120.28
3	C	302	6YH	O12-C11-C4	-3.89	115.52	120.73
3	A	302	6YH	O8-S7-O9	-3.80	112.95	118.80
3	B	302	6YH	O12-C11-C4	-3.76	115.70	120.73
3	C	302	6YH	O8-S7-N10	3.70	112.69	107.35
3	B	302	6YH	N14-C16-N17	-3.59	110.84	114.16
3	C	302	6YH	O8-S7-O9	-3.45	113.49	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	6YH	C13-C11-C4	3.42	121.95	117.67
3	D	302[A]	6YH	N14-C16-N17	-3.31	111.10	114.16
3	D	302[A]	6YH	O9-S7-N10	3.27	112.06	107.35
3	D	302[B]	6YH	O8-S7-O9	-3.25	113.80	118.80
3	D	302[A]	6YH	O12-C11-C4	-3.22	116.42	120.73
3	C	302	6YH	O8-S7-C1	-3.18	103.75	107.35
3	C	302	6YH	C5-C4-C11	-3.11	113.62	120.60
3	A	302	6YH	O12-C11-C4	-2.97	116.75	120.73
3	C	302	6YH	C6-C1-S7	-2.95	115.71	119.72
3	A	302	6YH	C2-C1-S7	-2.94	115.73	119.72
3	D	302[A]	6YH	O8-S7-O9	-2.90	114.33	118.80
3	A	302	6YH	C6-C1-C2	2.83	124.16	120.47
3	D	302[B]	6YH	N14-C16-N17	-2.83	111.55	114.16
3	D	302[B]	6YH	O8-S7-N10	2.70	111.24	107.35
3	D	302[B]	6YH	O8-S7-C1	-2.68	104.32	107.35
3	D	302[B]	6YH	C5-C4-C3	2.64	121.92	118.57
3	D	302[B]	6YH	O9-S7-N10	2.54	111.01	107.35
3	A	302	6YH	C13-C11-C4	2.51	120.81	117.67
3	A	302	6YH	C13-N14-C16	2.51	129.75	127.27
3	B	302	6YH	C2-C1-S7	-2.51	116.32	119.72
3	C	302	6YH	C3-C2-C1	-2.50	117.00	119.44
3	B	302	6YH	C6-C1-S7	-2.41	116.45	119.72
3	A	302	6YH	C6-C5-C4	-2.37	118.26	120.80
3	D	302[B]	6YH	C13-N14-C18	2.36	128.63	126.32
3	B	302	6YH	O9-S7-C1	-2.36	104.68	107.35
3	D	302[A]	6YH	C1-S7-N10	-2.35	105.13	108.40
3	C	302	6YH	C6-C1-C2	2.33	123.51	120.47
3	D	302[A]	6YH	O8-S7-N10	2.32	110.70	107.35
3	A	302	6YH	C5-C4-C3	2.26	121.44	118.57
3	C	302	6YH	C3-C4-C11	2.25	125.64	120.60
3	C	302	6YH	O9-S7-C1	2.24	109.88	107.35
3	A	302	6YH	N14-C16-N17	-2.22	112.11	114.16
3	B	302	6YH	C1-S7-N10	-2.22	105.31	108.40
3	D	302[B]	6YH	O12-C11-C4	-2.21	117.77	120.73
3	D	302[B]	6YH	C6-C5-C4	-2.15	118.51	120.80
3	D	302[B]	6YH	C13-N14-C16	-2.12	125.17	127.27
3	B	302	6YH	C2-C3-C4	-2.12	118.54	120.80
3	C	302	6YH	C18-N14-C16	-2.04	104.84	106.19
3	D	302[A]	6YH	O8-S7-C1	-2.02	105.07	107.35

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302[A]	6YH	C11-C13-N14-C18
3	D	302[A]	6YH	C11-C13-N14-C16
4	A	305	EDO	O1-C1-C2-O2
4	B	305	EDO	O1-C1-C2-O2
3	D	302[B]	6YH	C6-C1-S7-N10
3	C	302	6YH	C2-C1-S7-N10
3	C	302	6YH	C6-C1-S7-N10
3	D	302[B]	6YH	C2-C1-S7-N10
3	C	302	6YH	C6-C1-S7-O9
3	D	302[B]	6YH	C2-C1-S7-O9
3	D	302[A]	6YH	C6-C1-S7-O9
3	C	302	6YH	C2-C1-S7-O9
3	D	302[B]	6YH	C6-C1-S7-O9
3	D	302[A]	6YH	C2-C1-S7-O9
3	A	302	6YH	C2-C1-S7-O9
3	A	302	6YH	C6-C1-S7-O9
3	B	302	6YH	C6-C1-S7-O9
4	C	304	EDO	O1-C1-C2-O2
3	D	302[A]	6YH	C6-C1-S7-N10
3	B	302	6YH	C2-C1-S7-O9
3	C	302	6YH	O12-C11-C4-C3
3	D	302[A]	6YH	C13-C11-C4-C5
3	D	302[A]	6YH	C2-C1-S7-N10

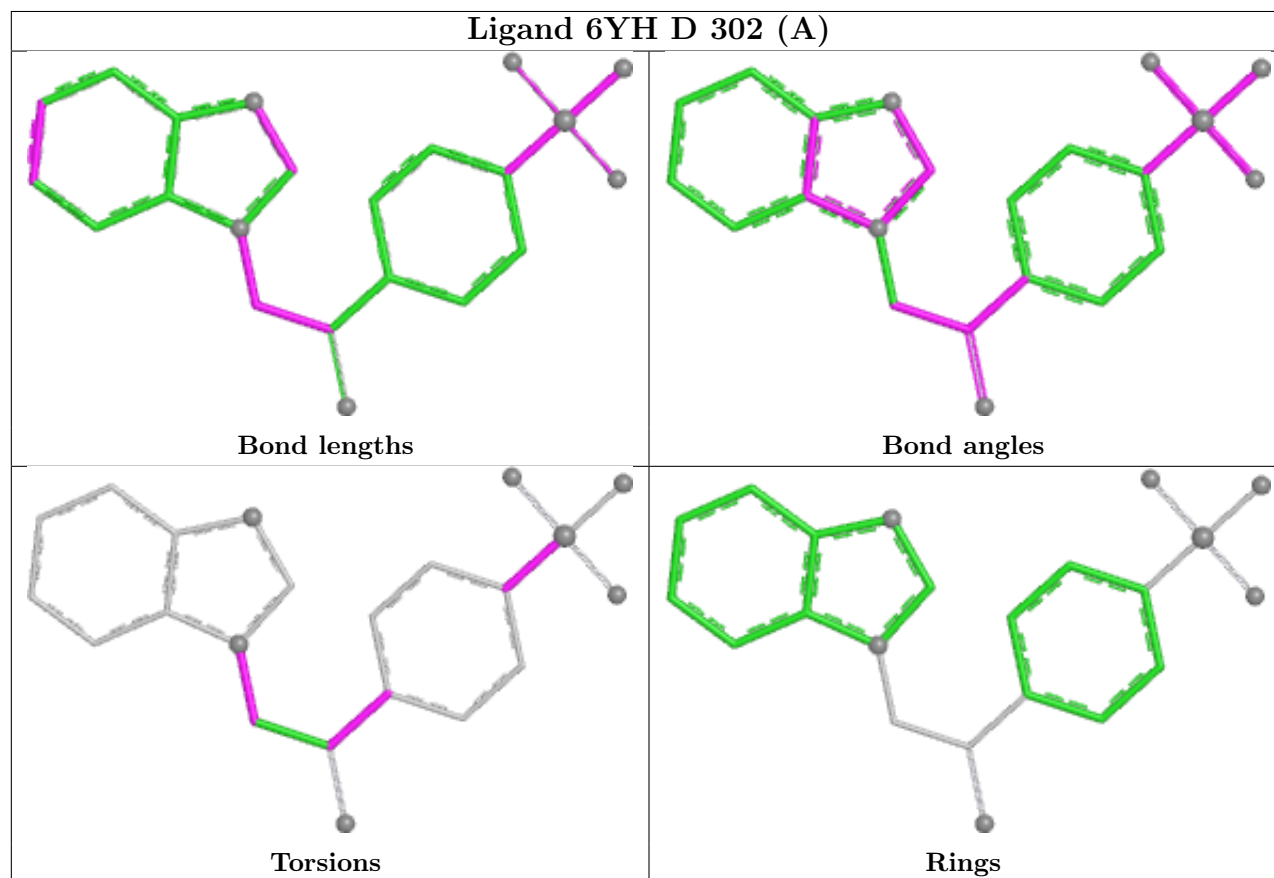
There are no ring outliers.

9 monomers are involved in 28 short contacts:

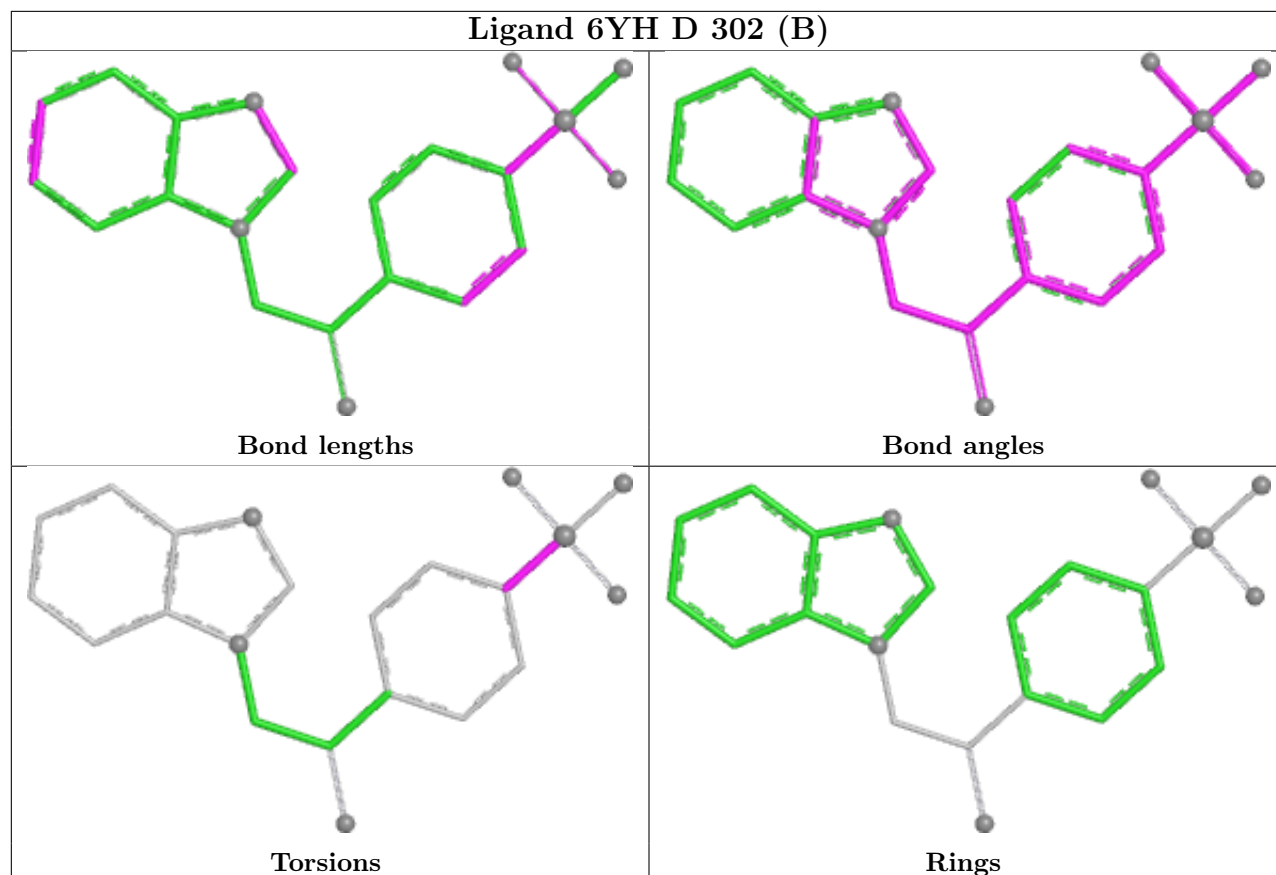
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302[A]	6YH	4	0
4	C	303	EDO	1	0
4	A	305	EDO	1	0
4	D	305[A]	EDO	3	0
3	D	302[B]	6YH	4	0
4	D	305[B]	EDO	4	0
3	C	302	6YH	3	0
4	B	305	EDO	6	0
4	C	304	EDO	2	0

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.

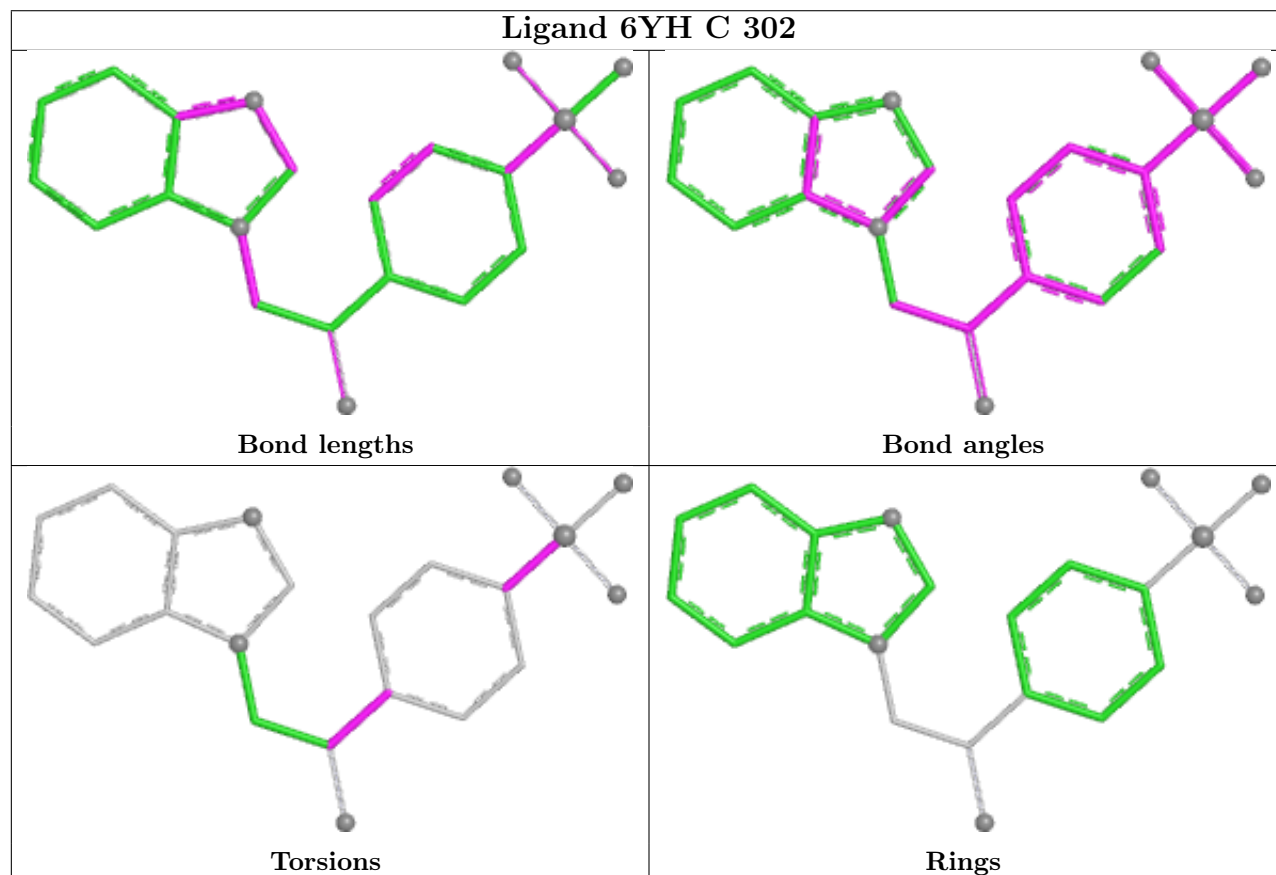
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.



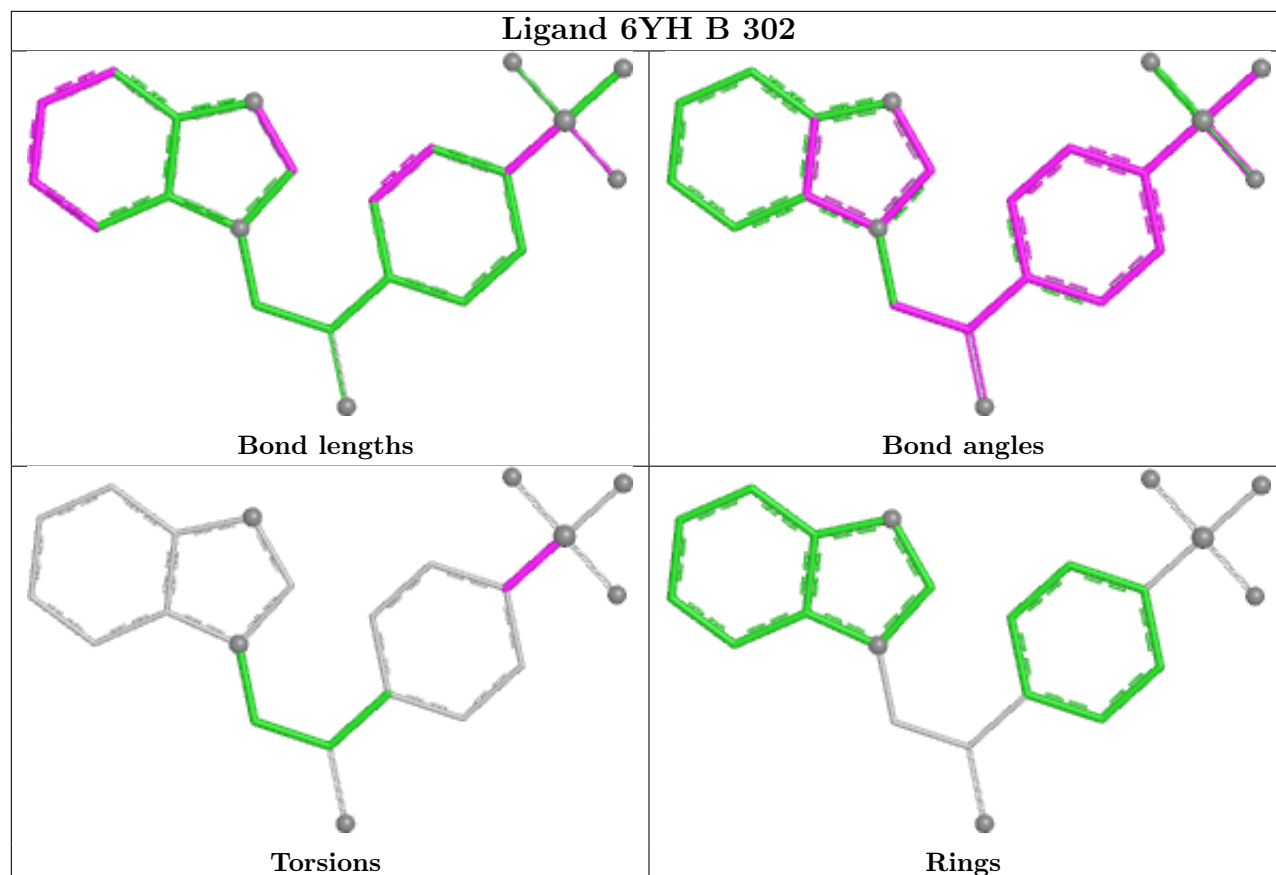
Ligand 6YH D 302 (B)



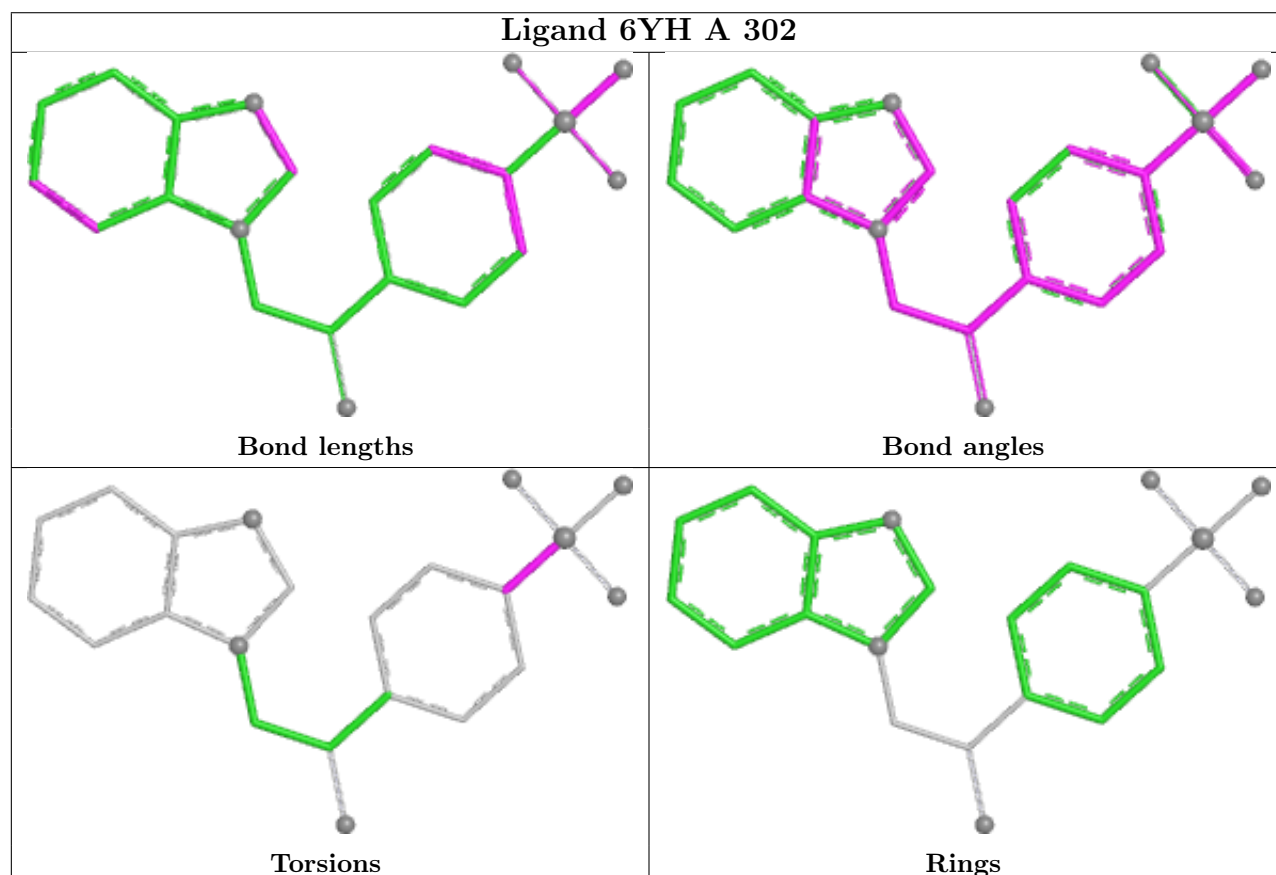
Ligand 6YH C 302



Ligand 6YH B 302



Ligand 6YH A 302



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	261/263 (99%)	-0.06	3 (1%) 78 81	5, 15, 32, 49	11 (4%)
1	B	261/263 (99%)	-0.19	11 (4%) 40 43	5, 12, 31, 45	7 (2%)
1	C	261/263 (99%)	0.18	15 (5%) 29 31	5, 18, 34, 61	7 (2%)
1	D	261/263 (99%)	-0.43	2 (0%) 82 86	5, 12, 24, 62	9 (3%)
All	All	1044/1052 (99%)	-0.12	31 (2%) 52 56	5, 14, 31, 62	34 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7[A]	PHE	6.3
1	C	55	ALA	4.8
1	C	56	ASN	4.8
1	C	54	SER	3.9
1	C	7	PHE	3.5
1	C	235	ASP	3.4
1	B	252	PHE	3.3
1	B	131	THR	3.0
1	B	125	LEU	3.0
1	C	3[A]	LYS	3.0
1	C	8	GLY	2.8
1	B	81	LEU	2.7
1	C	57	LYS	2.7
1	C	174	VAL	2.6
1	B	127	PRO	2.5
1	C	58	GLN	2.5
1	B	132	ALA	2.3
1	C	173[A]	PHE	2.3
1	B	137	GLU	2.3
1	C	237	PRO	2.3
1	A	35	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	148	MET	2.2
1	B	124	ASP	2.2
1	A	56	ASN	2.1
1	B	3	LYS	2.1
1	D	263	GLN	2.1
1	B	136	SER	2.1
1	C	262	SER	2.1
1	D	75	ASP	2.1
1	B	129	ALA	2.0
1	C	35	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 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
4	EDO	D	305[A]	4/4	0.68	0.21	20,20,26,32	4
4	EDO	D	305[B]	4/4	0.68	0.21	19,20,22,22	4
4	EDO	C	304	4/4	0.72	0.18	39,40,44,46	0
4	EDO	A	305	4/4	0.80	0.13	34,37,40,42	0
4	EDO	B	305	4/4	0.86	0.11	20,24,25,29	0
4	EDO	C	303	4/4	0.87	0.13	32,36,38,41	0
3	6YH	D	302[A]	22/22	0.90	0.16	13,34,50,54	22
4	EDO	D	303	4/4	0.90	0.10	23,23,24,31	0
3	6YH	D	302[B]	22/22	0.90	0.16	8,17,19,19	22
4	EDO	A	304	4/4	0.90	0.09	25,25,28,28	0
4	EDO	A	303	4/4	0.91	0.09	27,28,28,29	0
4	EDO	B	303	4/4	0.91	0.09	23,27,29,31	0
3	6YH	C	302	22/22	0.94	0.13	13,37,53,57	0

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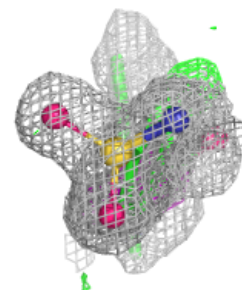
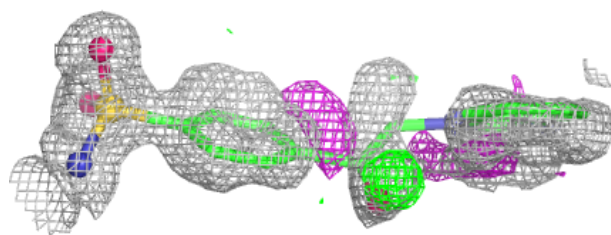
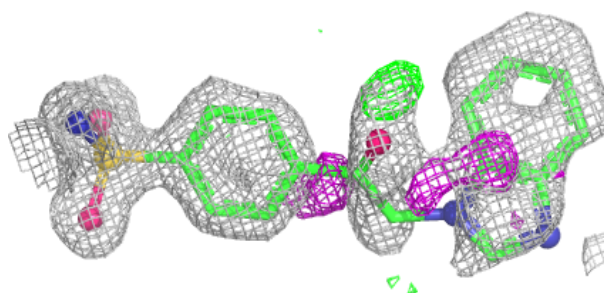
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	6YH	A	302	22/22	0.96	0.10	11,31,44,44	0
4	EDO	D	304	4/4	0.96	0.08	18,19,20,20	0
4	EDO	B	304	4/4	0.97	0.05	15,15,17,18	0
3	6YH	B	302	22/22	0.97	0.11	9,26,55,56	0
2	ZN	B	301	1/1	1.00	0.01	6,6,6,6	0
2	ZN	C	301	1/1	1.00	0.01	10,10,10,10	0
2	ZN	D	301	1/1	1.00	0.00	7,7,7,7	0
2	ZN	A	301	1/1	1.00	0.01	8,8,8,8	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.

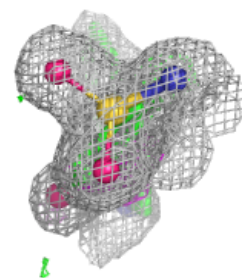
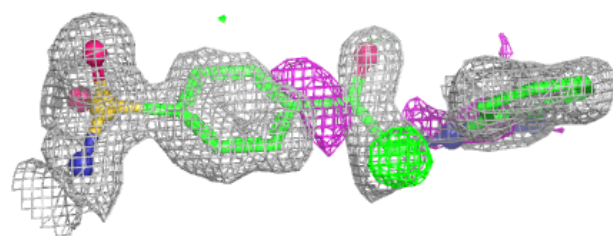
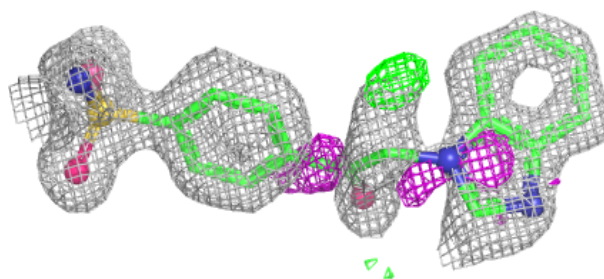
Electron density around 6YH D 302 (A):

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

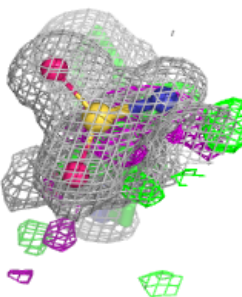
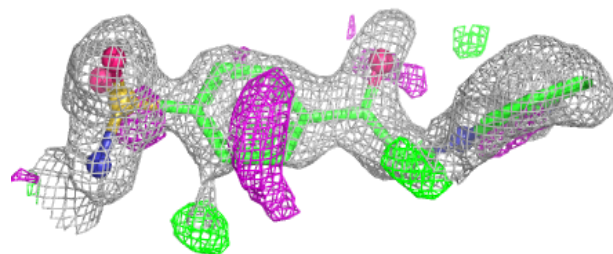
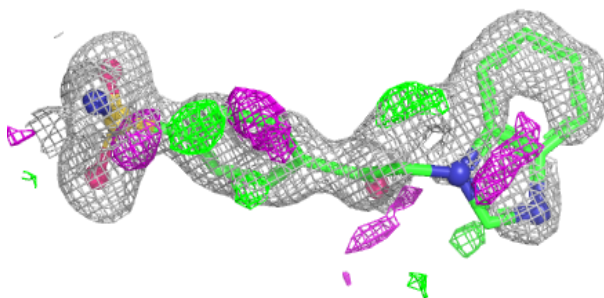


Electron density around 6YH D 302 (B):

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

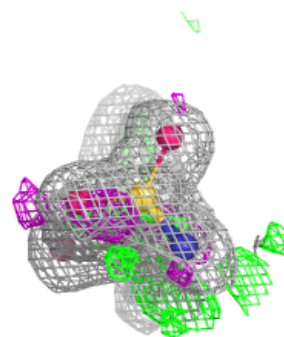
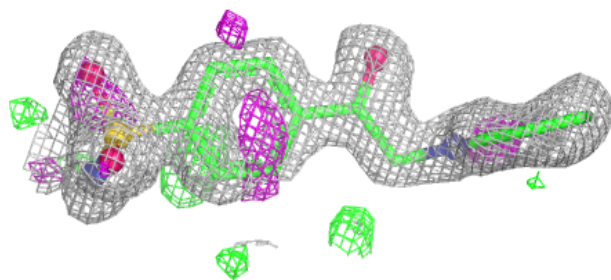
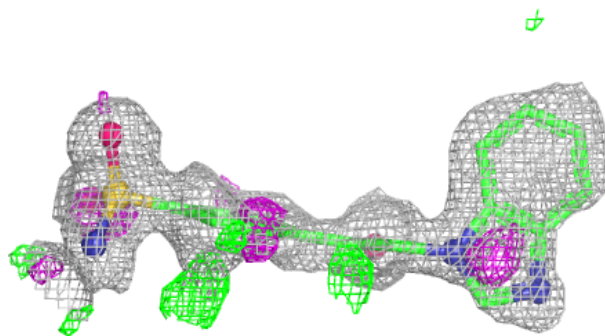
**Electron density around 6YH C 302:**

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

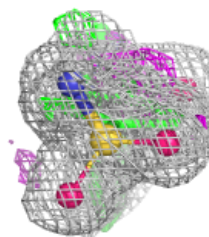
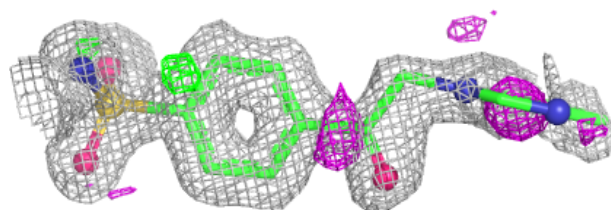
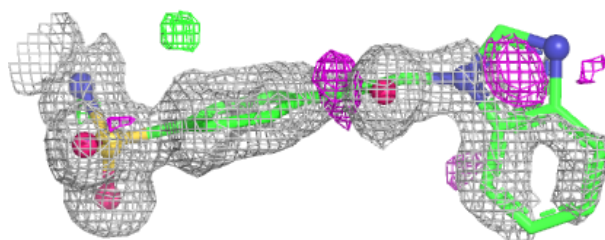


Electron density around 6YH A 302:

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

**Electron density around 6YH B 302:**

$2mF_o-DF_c$ (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.