



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 12:36 am BST

PDB ID : 1ZZ1  
Title : Crystal structure of a HDAC-like protein with SAHA bound  
Authors : Nielsen, T.K.; Hildmann, C.; Dickmanns, A.; Schwienhorst, A.; Ficner, R.  
Deposited on : 2005-06-13  
Resolution : 1.57 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](mailto: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.

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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 : 2.11  
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) : 2.11

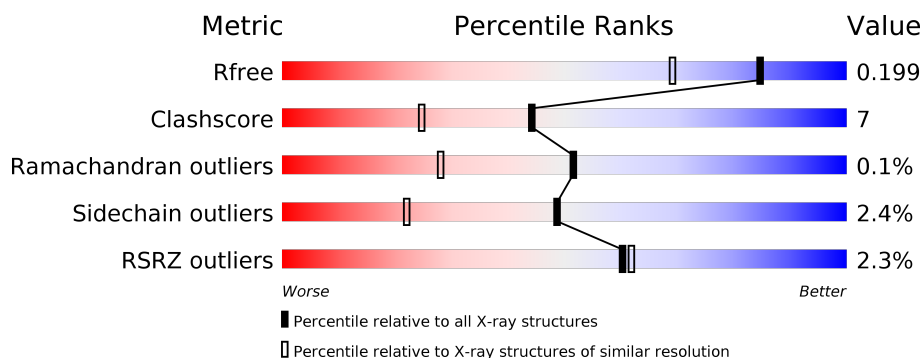
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.57 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	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	369	<div> <div>8%</div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	B	369	<div> <div>87%</div> <div>12%</div> <div>..</div> </div>
1	C	369	<div> <div>88%</div> <div>11%</div> <div>..</div> </div>
1	D	369	<div> <div>%</div> <div>89%</div> <div>9%</div> <div>..</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SHH	B	2552	-	-	X	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12576 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 Histone deacetylase-like amidohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	2	0
			2754	1728	494	514	18			
1	B	367	Total	C	N	O	S	0	5	0
			2765	1733	501	513	18			
1	C	367	Total	C	N	O	S	0	3	0
			2757	1729	494	516	18			
1	D	367	Total	C	N	O	S	0	4	0
			2762	1732	497	515	18			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP Q70I53
A	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
B	1	MET	-	INITIATING METHIONINE	UNP Q70I53
B	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
C	1	MET	-	INITIATING METHIONINE	UNP Q70I53
C	251	PRO	HIS	SEE REMARK 999	UNP Q70I53
D	1	MET	-	INITIATING METHIONINE	UNP Q70I53
D	251	PRO	HIS	SEE REMARK 999	UNP Q70I53

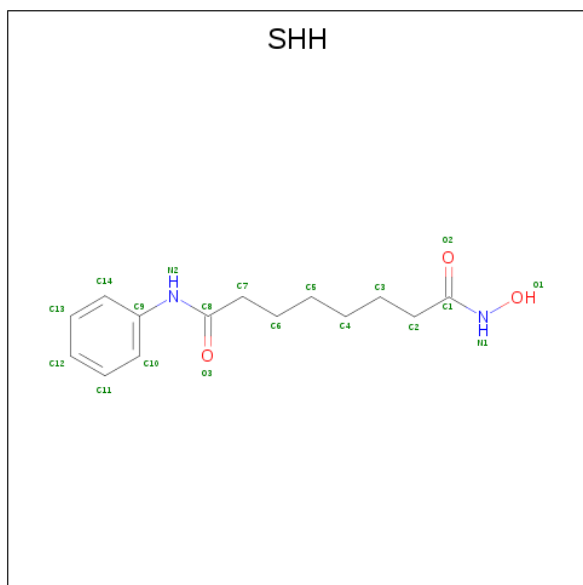
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is OCTANEDIOIC ACID HYDROXYAMIDE PHENYLAMIDE (three-letter code: SHH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 19 14 2 3	0	0
4	B	1	Total C N O 19 14 2 3	0	0
4	C	1	Total C N O 19 14 2 3	0	0
4	D	1	Total C N O 19 14 2 3	0	0

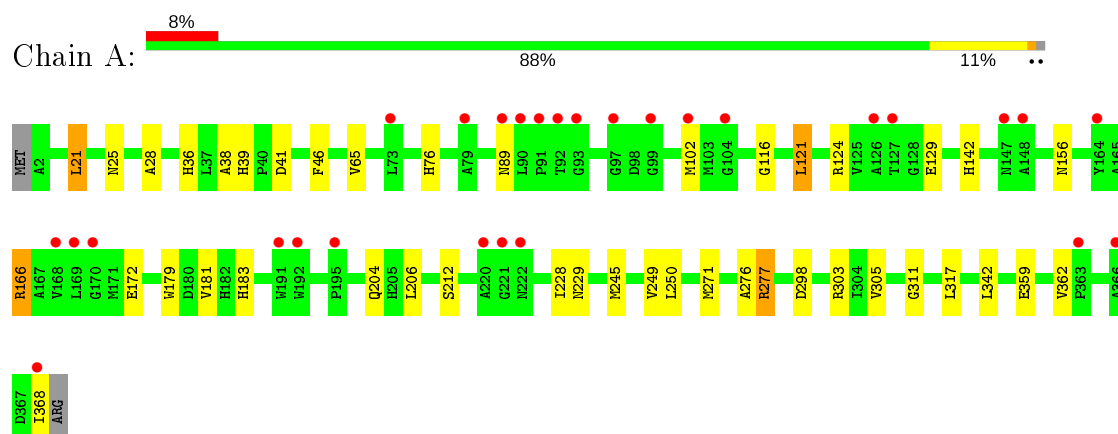
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	299	Total 299	O 299	0	0
5	B	389	Total 389	O 389	0	0
5	C	400	Total 400	O 400	0	0
5	D	362	Total 362	O 362	0	0

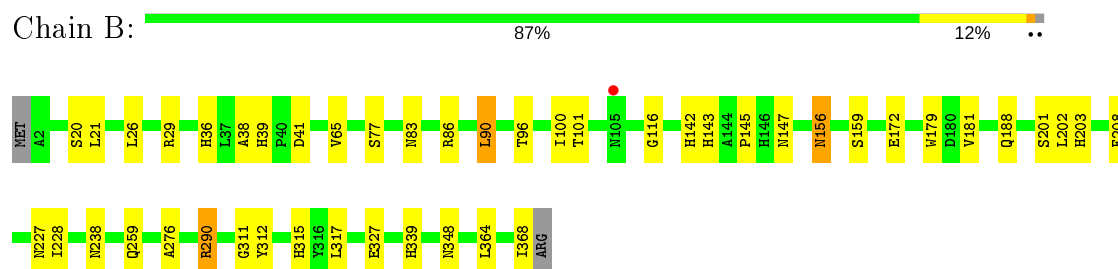
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

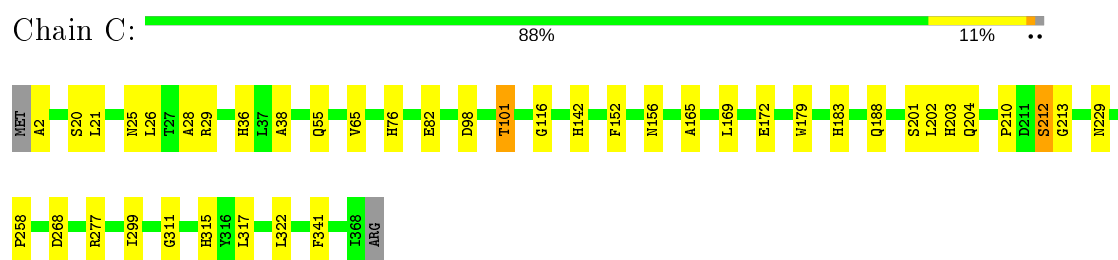
- Molecule 1: Histone deacetylase-like amidohydrolase



- Molecule 1: Histone deacetylase-like amidohydrolase

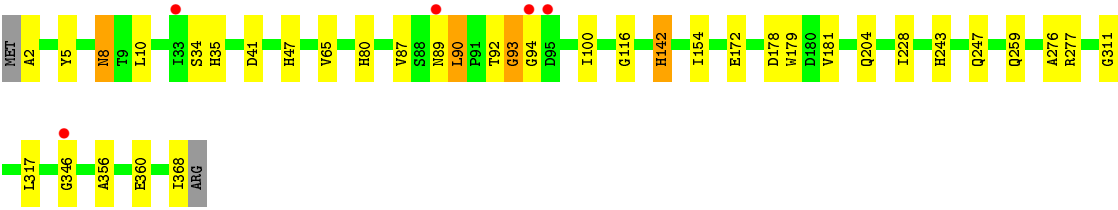


- Molecule 1: Histone deacetylase-like amidohydrolase



- Molecule 1: Histone deacetylase-like amidohydrolase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.61Å 94.72Å 123.92Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	38.38 – 1.57 46.01 – 1.57	Depositor EDS
% Data completeness (in resolution range)	84.6 (38.38-1.57) 84.6 (46.01-1.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.83 (at 1.57Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.172 , 0.201 0.169 , 0.199	Depositor DCC
$R_{free}$ test set	9071 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	12.9	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.61% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SHH, ZN, K

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.56	0/2830	0.68	2/3861 (0.1%)
1	B	0.61	0/2860	0.75	2/3899 (0.1%)
1	C	0.63	0/2838	0.74	1/3871 (0.0%)
1	D	0.72	2/2847 (0.1%)	0.74	1/3883 (0.0%)
All	All	0.63	2/11375 (0.0%)	0.73	6/15514 (0.0%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	GLY	C-N	-17.33	0.94	1.34
1	D	92	THR	C-N	-8.18	1.18	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	290	ARG	NE-CZ-NH2	-7.57	116.52	120.30
1	D	93	GLY	O-C-N	-7.36	110.69	123.20
1	B	290	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	277	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	277	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	268	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	93	GLY	Mainchain

## 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	2754	0	2665	27	0
1	B	2765	0	2678	51	0
1	C	2757	0	2665	43	0
1	D	2762	0	2674	25	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	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	19	0	19	0	0
4	B	19	0	18	24	0
4	C	19	0	19	0	0
4	D	19	0	19	2	0
5	A	299	0	0	1	0
5	B	389	0	0	4	0
5	C	400	0	0	5	0
5	D	362	0	0	4	0
All	All	12576	0	10757	144	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 7.

All (144) 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:100:ILE:HD13	4:B:2552:SHH:C7	1.82	1.09
1:A:36:HIS:HD2	1:A:38:ALA:H	1.05	1.02
1:B:100:ILE:HD13	4:B:2552:SHH:H71	1.41	0.99
1:B:172:GLU:H	1:B:259[A]:GLN:HE22	1.07	0.93
1:C:204:GLN:HE22	1:C:277:ARG:H	1.16	0.93
1:D:204:GLN:HE22	1:D:277:ARG:H	1.13	0.92
1:B:208:PHE:CE1	4:B:2552:SHH:O3	2.21	0.92
1:A:76:HIS:HE1	1:A:156:ASN:H	1.15	0.92
1:C:36:HIS:HD2	1:C:38:ALA:H	1.11	0.92
1:B:36:HIS:HD2	1:B:38:ALA:H	1.10	0.91
1:B:36:HIS:CD2	1:B:38:ALA:H	1.89	0.91
1:A:204:GLN:HE22	1:A:277:ARG:H	1.13	0.90
1:A:36:HIS:CD2	1:A:38:ALA:H	1.92	0.88
1:B:39:HIS:HD2	1:B:41:ASP:H	1.22	0.88
1:B:100:ILE:HD13	4:B:2552:SHH:C8	2.05	0.87
1:C:76:HIS:HE1	1:C:156:ASN:H	1.18	0.87
1:B:100:ILE:HG21	4:B:2552:SHH:HN2	1.39	0.86
1:C:36:HIS:CD2	1:C:38:ALA:H	1.95	0.83
1:A:39:HIS:HD2	1:A:41:ASP:H	1.26	0.81
1:B:100:ILE:CD1	4:B:2552:SHH:C7	2.59	0.80
1:B:100:ILE:CD1	4:B:2552:SHH:H71	2.12	0.78
1:B:172:GLU:N	1:B:259[A]:GLN:HE22	1.81	0.77
1:A:76:HIS:CE1	1:A:156:ASN:H	2.02	0.76
4:B:2552:SHH:H72	1:C:341:PHE:CE1	2.21	0.75
1:C:76:HIS:CE1	1:C:156:ASN:H	2.04	0.74
1:B:83:ASN:HD21	1:B:86:ARG:HH21	1.33	0.73
1:C:2:ALA:N	5:C:3043:HOH:O	2.20	0.73
1:D:204:GLN:NE2	1:D:277:ARG:H	1.86	0.73
1:C:25:ASN:HD22	1:C:28:ALA:H	1.36	0.73
1:B:208:PHE:HE1	4:B:2552:SHH:O3	1.70	0.72
1:A:204:GLN:NE2	1:A:277:ARG:H	1.87	0.70
1:A:359:GLU:HG2	5:A:2614:HOH:O	1.90	0.70
1:D:228:ILE:HD11	1:D:368:ILE:HD11	1.75	0.69
1:B:100:ILE:CD1	4:B:2552:SHH:C6	2.71	0.69
1:B:39:HIS:CD2	1:B:41:ASP:H	2.10	0.68
1:D:5:TYR:OH	1:D:47:HIS:HD2	1.75	0.68
1:B:339:HIS:CE1	5:B:2938:HOH:O	2.46	0.68
1:B:36:HIS:HD2	1:B:38:ALA:N	1.89	0.68
1:B:86:ARG:O	1:B:90:LEU:HD13	1.93	0.67
1:B:96:THR:HG22	1:B:101:THR:O	1.93	0.67
4:B:2552:SHH:C8	1:C:341:PHE:CE1	2.77	0.67
1:C:188:GLN:HE22	1:C:229:ASN:HD21	1.40	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:HIS:HD2	5:D:2874:HOH:O	1.79	0.66
1:C:210:PRO:O	5:C:2782:HOH:O	2.13	0.66
1:A:124:ARG:HD3	1:A:129:GLU:OE1	1.96	0.66
1:A:25:ASN:HD22	1:A:28:ALA:H	1.43	0.65
1:C:101:THR:CG2	1:C:152:PHE:H	2.09	0.64
1:B:315:HIS:HE1	5:C:2790:HOH:O	1.79	0.64
1:C:101:THR:HG21	1:C:152:PHE:H	1.63	0.64
5:B:2637:HOH:O	1:C:315:HIS:HE1	1.81	0.63
1:B:100:ILE:CD1	4:B:2552:SHH:H62	2.29	0.63
1:B:228[A]:ILE:HD11	1:B:368:ILE:HD11	1.81	0.62
1:A:36:HIS:HD2	1:A:38:ALA:N	1.88	0.62
1:D:8:ASN:HD22	1:D:10:LEU:H	1.47	0.62
1:C:201:SER:OG	1:C:203:HIS:HD2	1.83	0.62
1:D:100:ILE:HD13	4:D:2752:SHH:O3	1.99	0.62
1:A:204:GLN:HE22	1:A:277:ARG:N	1.93	0.61
1:A:39:HIS:CD2	1:A:41:ASP:H	2.14	0.61
1:A:166:ARG:HH21	1:A:172:GLU:HA	1.67	0.60
1:D:100:ILE:HD13	4:D:2752:SHH:C8	2.31	0.60
1:C:183:HIS:HD2	1:C:212:SER:OG	1.85	0.60
1:C:204:GLN:NE2	1:C:277:ARG:H	1.94	0.59
4:B:2552:SHH:C7	1:C:341:PHE:CE1	2.85	0.59
1:B:96:THR:HG23	5:B:2675:HOH:O	2.02	0.59
1:A:183:HIS:HD2	1:A:212:SER:OG	1.86	0.59
1:B:100:ILE:HD13	4:B:2552:SHH:N2	2.19	0.57
1:A:65:VAL:O	1:A:116:GLY:HA3	2.03	0.57
1:B:315:HIS:HD2	1:C:20:SER:OG	1.88	0.57
1:D:204:GLN:HE22	1:D:277:ARG:N	1.93	0.57
4:B:2552:SHH:H72	1:C:341:PHE:CZ	2.40	0.57
1:C:82[B]:GLU:OE2	5:C:2938:HOH:O	2.18	0.57
1:D:34[A]:SER:OG	5:D:2798:HOH:O	2.16	0.56
1:D:65:VAL:O	1:D:116:GLY:HA3	2.05	0.56
1:C:25:ASN:ND2	1:C:28:ALA:H	2.04	0.55
1:D:2:ALA:N	5:D:3021:HOH:O	2.40	0.54
1:D:181:VAL:HG11	1:D:276:ALA:HB2	1.89	0.54
1:A:183:HIS:HE1	1:A:229:ASN:HD21	1.58	0.51
1:B:100:ILE:HD12	4:B:2552:SHH:H62	1.91	0.51
4:B:2552:SHH:O3	1:C:341:PHE:CE1	2.63	0.51
1:D:35:HIS:HE1	1:D:41:ASP:OD2	1.93	0.51
1:A:359:GLU:O	1:A:362:VAL:HG22	2.11	0.51
1:A:228:ILE:HD11	1:A:368:ILE:HD11	1.93	0.51
1:C:36:HIS:HD2	1:C:38:ALA:N	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:HIS:HE1	1:C:188:GLN:NE2	2.09	0.50
1:C:165:ALA:HA	1:C:169:LEU:HD12	1.94	0.50
1:C:98:ASP:OD2	1:C:101:THR:HG23	2.11	0.50
1:B:65:VAL:O	1:B:116:GLY:HA3	2.11	0.49
1:A:245:MET:HA	1:A:249:VAL:HB	1.93	0.49
1:B:20:SER:OG	1:C:315:HIS:HD2	1.96	0.49
1:C:21:LEU:O	1:C:36:HIS:HE1	1.94	0.49
1:D:311:GLY:HA3	1:D:317:LEU:HD12	1.95	0.49
1:D:47:HIS:HE1	5:D:2853:HOH:O	1.95	0.49
4:B:2552:SHH:O3	1:C:341:PHE:HE1	1.96	0.49
1:D:87:VAL:HA	1:D:90:LEU:HD22	1.94	0.49
1:D:356:ALA:O	1:D:360:GLU:HG3	2.13	0.49
1:B:201:SER:OG	1:B:203:HIS:HD2	1.96	0.49
1:A:271:MET:HG2	1:A:342:LEU:HD22	1.96	0.48
1:D:181:VAL:HG11	1:D:276:ALA:CB	2.44	0.48
1:C:183:HIS:CD2	1:C:212:SER:OG	2.67	0.48
1:B:238:ASN:HD22	1:B:348:ASN:HD21	1.61	0.48
1:B:208:PHE:CG	4:B:2552:SHH:H52	2.49	0.48
1:C:65:VAL:O	1:C:116:GLY:HA3	2.14	0.47
1:B:364:LEU:HD12	1:B:364:LEU:N	2.30	0.47
1:B:172:GLU:H	1:B:259[A]:GLN:NE2	1.92	0.47
1:B:290:ARG:NH2	1:B:327:GLU:O	2.48	0.47
1:A:21:LEU:O	1:A:36:HIS:HE1	1.98	0.47
1:B:188:GLN:NE2	1:B:227:ASN:HD21	2.14	0.46
1:B:208:PHE:CZ	4:B:2552:SHH:H61	2.50	0.46
1:A:181:VAL:HG11	1:A:276:ALA:HB2	1.97	0.46
1:A:311:GLY:HA3	1:A:317:LEU:HD12	1.97	0.46
1:B:21:LEU:O	1:B:36:HIS:HE1	1.98	0.45
1:A:311:GLY:HA3	1:A:317:LEU:CD1	2.45	0.45
1:B:156:ASN:HD22	1:B:159:SER:H	1.64	0.45
1:B:208:PHE:CE1	4:B:2552:SHH:H61	2.52	0.44
1:C:55:GLN:HG3	1:C:322:LEU:HD11	1.99	0.44
1:C:183:HIS:CE1	1:C:188:GLN:NE2	2.85	0.44
1:C:204:GLN:HE22	1:C:277:ARG:N	1.99	0.44
1:A:121:LEU:HD13	1:A:305:VAL:HG13	2.00	0.44
1:D:8:ASN:ND2	1:D:10:LEU:H	2.14	0.44
1:B:100:ILE:CG2	4:B:2552:SHH:HN2	2.21	0.43
1:D:80:HIS:HE1	1:D:154:ILE:O	2.01	0.43
1:C:101:THR:HB	1:C:152:PHE:HA	2.01	0.43
1:C:258:PRO:HD2	1:C:299:ILE:HD12	2.00	0.43
1:C:317:LEU:C	1:C:317:LEU:HD23	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:2552:SHH:C8	1:C:341:PHE:HE1	2.29	0.43
1:B:172:GLU:N	1:B:259[A]:GLN:NE2	2.59	0.43
1:C:2:ALA:N	5:C:2970:HOH:O	2.52	0.42
1:B:77:SER:OG	1:B:147:ASN:ND2	2.44	0.42
1:B:83:ASN:ND2	1:B:86:ARG:HH21	2.09	0.42
1:D:172:GLU:H	1:D:259:GLN:NE2	2.18	0.42
1:C:311:GLY:HA3	1:C:317:LEU:HD12	2.02	0.42
1:D:89:ASN:HD22	1:D:89:ASN:HA	1.65	0.42
1:B:181:VAL:HG11	1:B:276:ALA:CB	2.50	0.41
1:D:142:HIS:ND1	1:D:178:ASP:OD2	2.54	0.41
1:B:26:LEU:O	1:B:29:ARG:HD3	2.20	0.41
1:B:312:TYR:HH	4:B:2552:SHH:C1	2.33	0.41
1:A:183:HIS:CE1	1:A:229:ASN:HD21	2.38	0.41
1:B:143:HIS:O	1:B:145:PRO:HD3	2.21	0.41
1:B:311:GLY:HA3	1:B:317:LEU:HD12	2.02	0.41
1:B:259[A]:GLN:HE21	1:B:259[A]:GLN:HB2	1.76	0.40
1:D:243:HIS:CE1	1:D:247:GLN:HG3	2.56	0.40
1:C:203:HIS:HE1	1:C:213:GLY:O	2.04	0.40
1:B:339:HIS:ND1	5:B:2938:HOH:O	2.37	0.40
1:C:26:LEU:O	1:C:29:ARG:HD3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	367/369 (100%)	358 (98%)	9 (2%)	0	100	100
1	B	370/369 (100%)	360 (97%)	10 (3%)	0	100	100
1	C	368/369 (100%)	359 (98%)	9 (2%)	0	100	100
1	D	369/369 (100%)	358 (97%)	10 (3%)	1 (0%)	41	21
All	All	1474/1476 (100%)	1435 (97%)	38 (3%)	1 (0%)	51	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	346	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/282 (100%)	270 (96%)	12 (4%)	29	7
1	B	285/282 (101%)	280 (98%)	5 (2%)	59	34
1	C	283/282 (100%)	277 (98%)	6 (2%)	53	27
1	D	284/282 (101%)	280 (99%)	4 (1%)	67	45
All	All	1134/1128 (100%)	1107 (98%)	27 (2%)	49	22

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	46	PHE
1	A	89	ASN
1	A	102	MET
1	A	121	LEU
1	A	142	HIS
1	A	166	ARG
1	A	179	TRP
1	A	206	LEU
1	A	250	LEU
1	A	298	ASP
1	A	303	ARG
1	B	90	LEU
1	B	142	HIS
1	B	156	ASN
1	B	179	TRP
1	B	202	LEU
1	C	101	THR
1	C	142	HIS

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Mol	Chain	Res	Type
1	C	172	GLU
1	C	179	TRP
1	C	202	LEU
1	C	212	SER
1	D	8	ASN
1	D	90	LEU
1	D	142	HIS
1	D	179	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	36	HIS
1	A	39	HIS
1	A	76	HIS
1	A	147	ASN
1	A	183	HIS
1	A	204	GLN
1	A	227	ASN
1	A	229	ASN
1	A	308	GLN
1	B	36	HIS
1	B	39	HIS
1	B	58	HIS
1	B	83	ASN
1	B	138	ASN
1	B	147	ASN
1	B	156	ASN
1	B	188	GLN
1	B	203	HIS
1	B	222	ASN
1	B	229	ASN
1	B	247	GLN
1	B	287	GLN
1	B	308	GLN
1	B	315	HIS
1	B	348	ASN
1	C	25	ASN
1	C	36	HIS
1	C	55	GLN
1	C	76	HIS

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Mol	Chain	Res	Type
1	C	147	ASN
1	C	183	HIS
1	C	188	GLN
1	C	203	HIS
1	C	204	GLN
1	C	227	ASN
1	C	308	GLN
1	C	315	HIS
1	D	8	ASN
1	D	35	HIS
1	D	47	HIS
1	D	80	HIS
1	D	89	ASN
1	D	138	ASN
1	D	147	ASN
1	D	204	GLN
1	D	229	ASN
1	D	259	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 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	$\# Z  > 2$
4	SHH	A	2452	2	19,19,19	1.13	2 (10%)	21,22,22	1.42	4 (19%)
4	SHH	C	2652	2	19,19,19	0.94	2 (10%)	21,22,22	1.30	1 (4%)
4	SHH	B	2552	2	19,19,19	2.26	3 (15%)	21,22,22	1.53	6 (28%)
4	SHH	D	2752	2	19,19,19	0.99	2 (10%)	21,22,22	1.19	2 (9%)

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	SHH	A	2452	2	-	5/15/15/15	0/1/1/1
4	SHH	C	2652	2	-	7/15/15/15	0/1/1/1
4	SHH	B	2552	2	-	10/15/15/15	0/1/1/1
4	SHH	D	2752	2	-	3/15/15/15	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2552	SHH	C1-N1	-8.62	1.22	1.32
4	A	2452	SHH	C1-N1	-3.49	1.28	1.32
4	B	2552	SHH	O1-N1	3.34	1.48	1.40
4	D	2752	SHH	C1-N1	-2.70	1.29	1.32
4	A	2452	SHH	C9-N2	-2.65	1.36	1.41
4	D	2752	SHH	C9-N2	-2.60	1.36	1.41
4	C	2652	SHH	C9-N2	-2.56	1.36	1.41
4	B	2552	SHH	C9-N2	-2.33	1.36	1.41
4	C	2652	SHH	C1-N1	-2.07	1.30	1.32

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2652	SHH	O2-C1-N1	-5.28	116.79	123.27
4	A	2452	SHH	O2-C1-N1	-4.41	117.85	123.27
4	D	2752	SHH	O2-C1-N1	-3.29	119.23	123.27
4	B	2552	SHH	C7-C8-N2	3.04	119.94	114.59
4	B	2552	SHH	C9-N2-C8	-3.03	122.20	127.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2552	SHH	O2-C1-N1	-2.70	119.95	123.27
4	A	2452	SHH	O1-N1-C1	-2.61	115.93	119.79
4	B	2552	SHH	O2-C1-C2	2.58	126.73	122.02
4	B	2552	SHH	C3-C2-C1	2.29	119.68	113.26
4	D	2752	SHH	O1-N1-C1	-2.25	116.47	119.79
4	A	2452	SHH	O2-C1-C2	2.21	126.06	122.02
4	B	2552	SHH	C4-C3-C2	-2.09	105.66	113.19
4	A	2452	SHH	C9-N2-C8	-2.07	123.87	127.50

There are no chirality outliers.

All (25) torsion outliers are listed below:

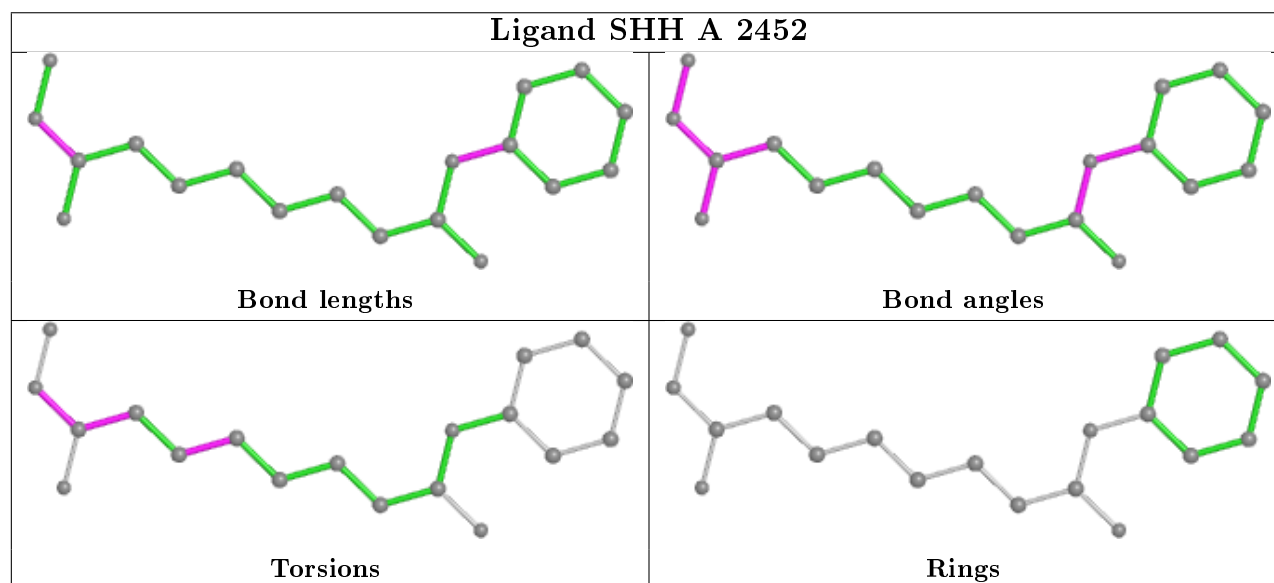
Mol	Chain	Res	Type	Atoms
4	C	2652	SHH	O2-C1-N1-O1
4	C	2652	SHH	C2-C1-N1-O1
4	A	2452	SHH	O2-C1-N1-O1
4	A	2452	SHH	C2-C1-N1-O1
4	D	2752	SHH	O2-C1-N1-O1
4	D	2752	SHH	C2-C1-N1-O1
4	B	2552	SHH	O2-C1-N1-O1
4	B	2552	SHH	C2-C1-N1-O1
4	C	2652	SHH	C5-C6-C7-C8
4	B	2552	SHH	C5-C6-C7-C8
4	B	2552	SHH	C14-C9-N2-C8
4	B	2552	SHH	C10-C9-N2-C8
4	B	2552	SHH	C4-C5-C6-C7
4	B	2552	SHH	C3-C4-C5-C6
4	B	2552	SHH	N1-C1-C2-C3
4	B	2552	SHH	C1-C2-C3-C4
4	B	2552	SHH	O2-C1-C2-C3
4	A	2452	SHH	N1-C1-C2-C3
4	D	2752	SHH	N1-C1-C2-C3
4	C	2652	SHH	O2-C1-C2-C3
4	C	2652	SHH	C2-C3-C4-C5
4	A	2452	SHH	C2-C3-C4-C5
4	C	2652	SHH	C6-C7-C8-O3
4	C	2652	SHH	N1-C1-C2-C3
4	A	2452	SHH	O2-C1-C2-C3

There are no ring outliers.

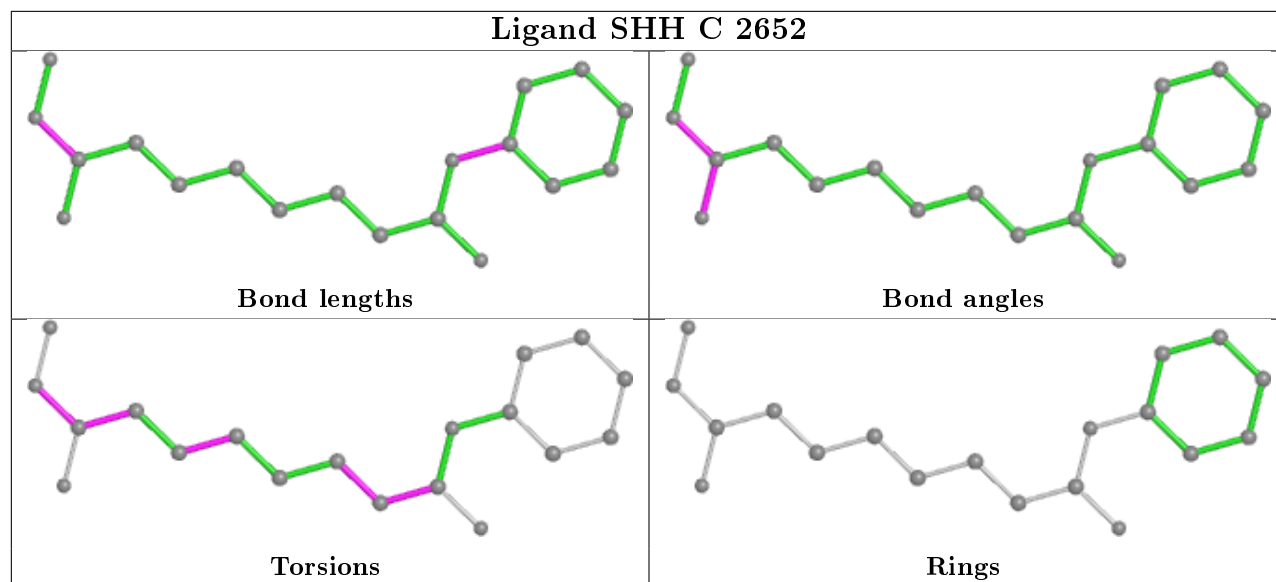
2 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	2552	SHH	24	0
4	D	2752	SHH	2	0

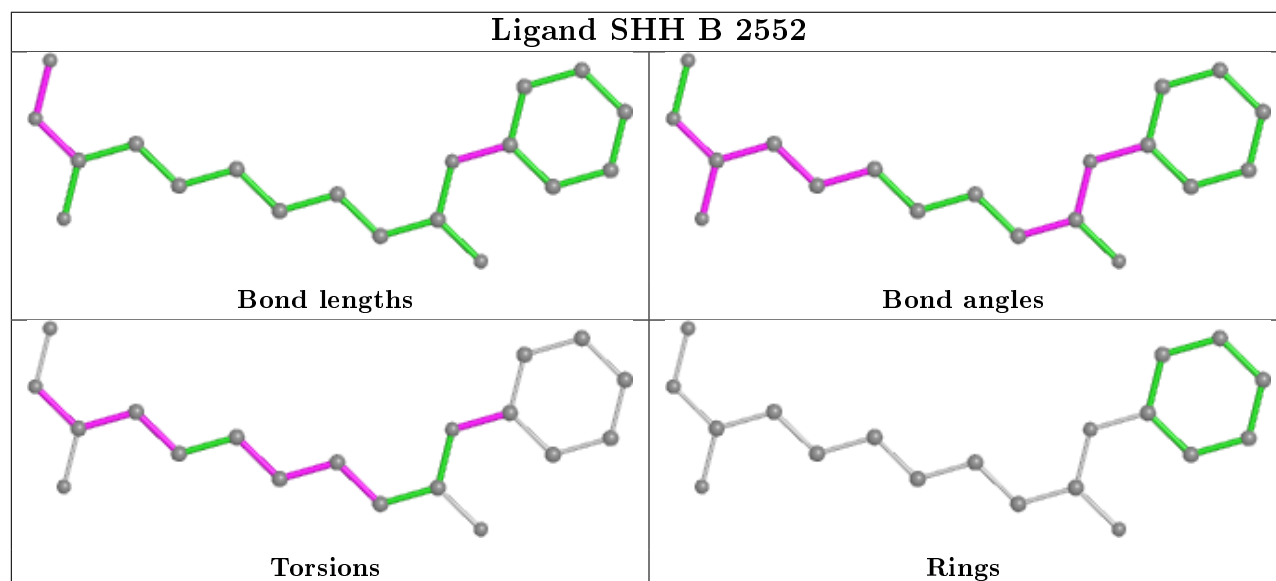
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



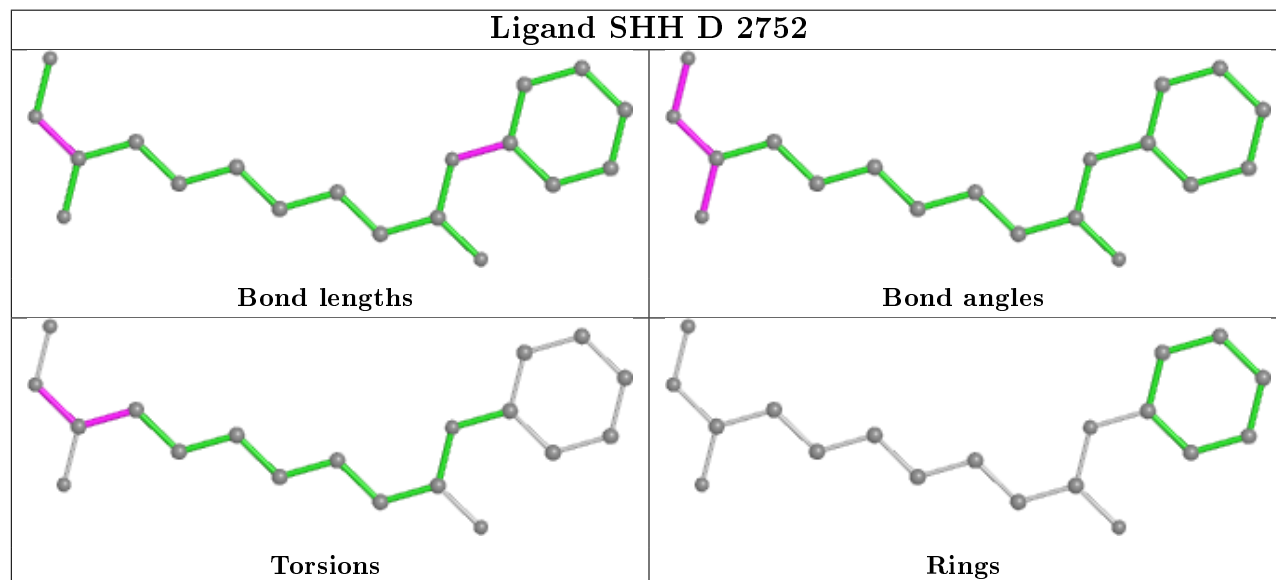
## Ligand SHH C 2652



## Ligand SHH B 2552



## Ligand SHH D 2752



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	92:THR	C	93:GLY	N	1.18
1	D	94:GLY	C	95:ASP	N	0.94

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	367/369 (99%)	0.21	28 (7%) 13 13	10, 17, 27, 30	0
1	B	367/369 (99%)	-0.18	1 (0%) 94 94	8, 13, 23, 26	0
1	C	367/369 (99%)	-0.41	0 100 100	7, 12, 23, 28	0
1	D	367/369 (99%)	-0.28	5 (1%) 75 77	9, 15, 25, 29	0
All	All	1468/1476 (99%)	-0.17	34 (2%) 60 62	7, 14, 25, 30	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	170	GLY	4.6
1	A	222	ASN	4.0
1	A	97	GLY	3.6
1	A	220	ALA	3.6
1	A	92	THR	3.3
1	A	90	LEU	3.1
1	A	79	ALA	3.0
1	A	91	PRO	3.0
1	A	366	ALA	2.9
1	D	94	GLY	2.9
1	A	89	ASN	2.9
1	A	99	GLY	2.7
1	A	221	GLY	2.7
1	A	93	GLY	2.7
1	A	192	TRP	2.6
1	A	148	ALA	2.6
1	A	164	TYR	2.5
1	A	168	VAL	2.5
1	A	127	THR	2.5
1	D	33	ILE	2.4
1	A	191	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	89	ASN	2.4
1	D	346	GLY	2.3
1	A	126	ALA	2.2
1	B	105	ASN	2.2
1	A	102	MET	2.1
1	A	195	PRO	2.1
1	A	363	PRO	2.1
1	A	169	LEU	2.1
1	A	104	GLY	2.0
1	A	73	LEU	2.0
1	D	95	ASP	2.0
1	A	368	ILE	2.0
1	A	147	ASN	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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.

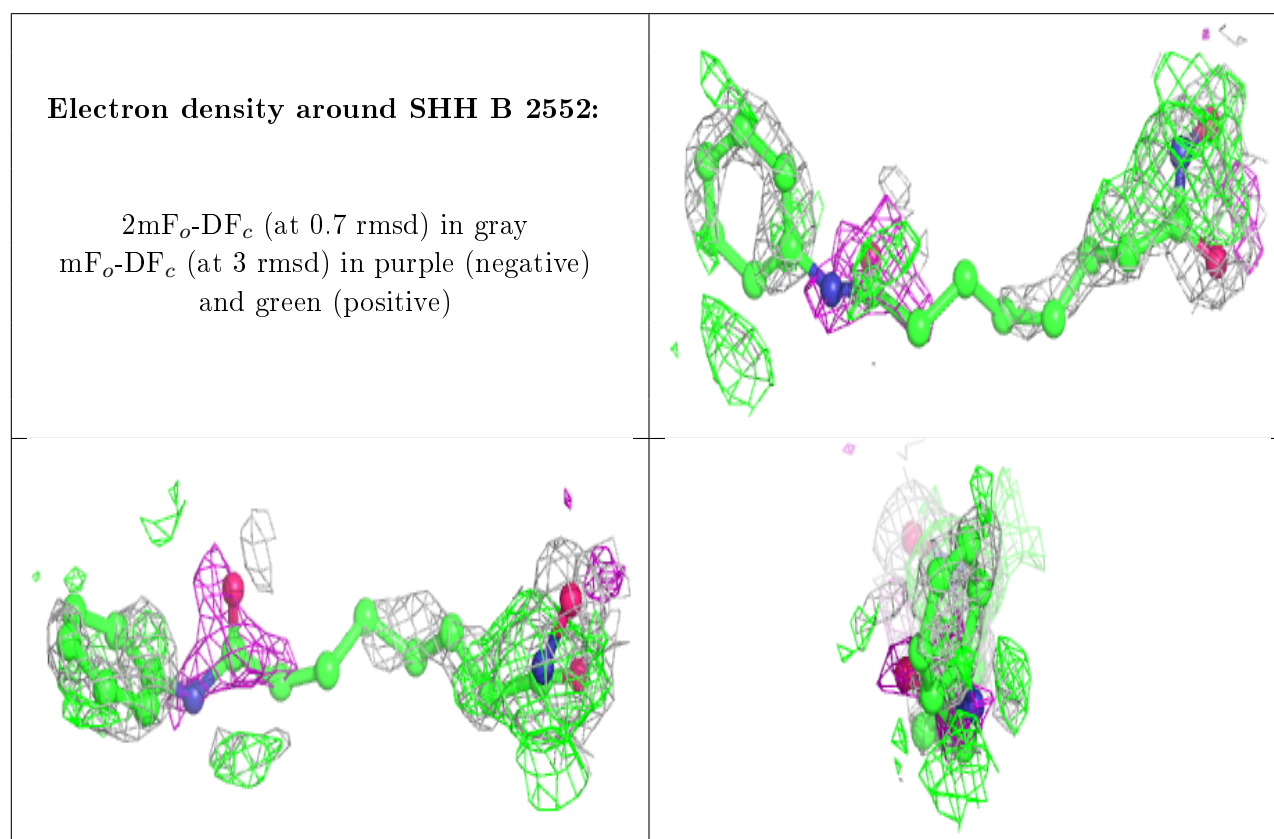
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SHH	B	2552	19/19	0.71	0.46	2,24,28,29	19
4	SHH	A	2452	19/19	0.77	0.32	6,13,21,25	18
4	SHH	C	2652	19/19	0.85	0.33	2,15,24,27	19
4	SHH	D	2752	19/19	0.87	0.29	5,13,19,20	19
3	K	A	2449	1/1	0.96	0.06	31,31,31,31	0
3	K	D	2749	1/1	0.96	0.12	25,25,25,25	0
2	ZN	C	2651	1/1	0.99	0.04	14,14,14,14	1
3	K	B	2549	1/1	0.99	0.07	22,22,22,22	0
3	K	C	2649	1/1	0.99	0.04	18,18,18,18	0
3	K	B	2550	1/1	1.00	0.03	9,9,9,9	0

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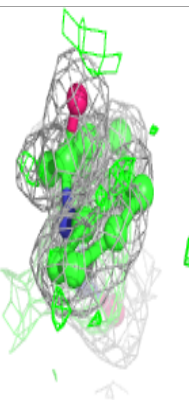
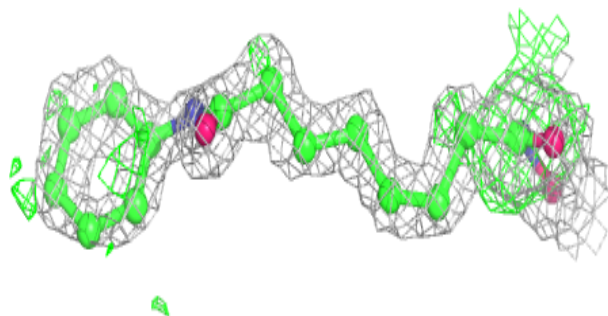
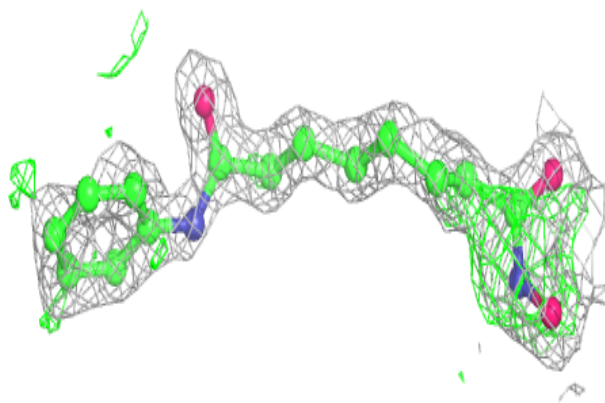
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	A	2450	1/1	1.00	0.03	15,15,15,15	0
2	ZN	B	2551	1/1	1.00	0.03	15,15,15,15	1
3	K	C	2650	1/1	1.00	0.03	10,10,10,10	0
2	ZN	A	2451	1/1	1.00	0.03	21,21,21,21	1
2	ZN	D	2751	1/1	1.00	0.05	17,17,17,17	1
3	K	D	2750	1/1	1.00	0.03	12,12,12,12	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.

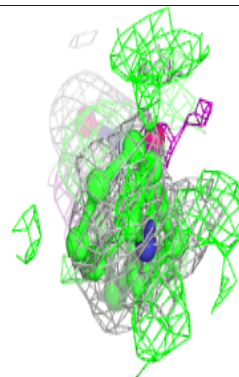
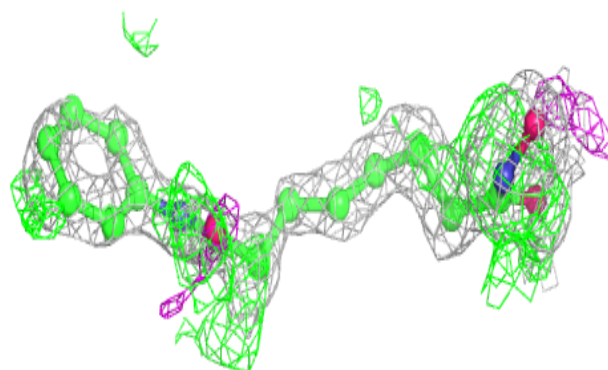
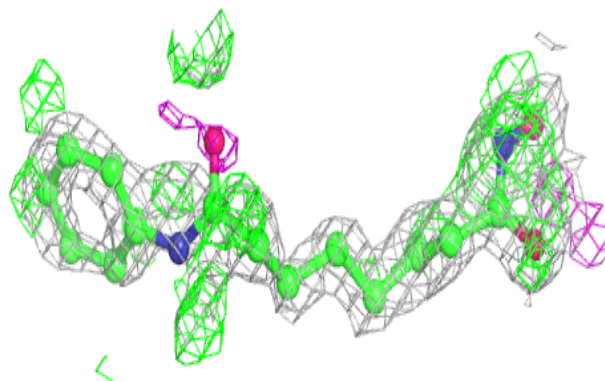


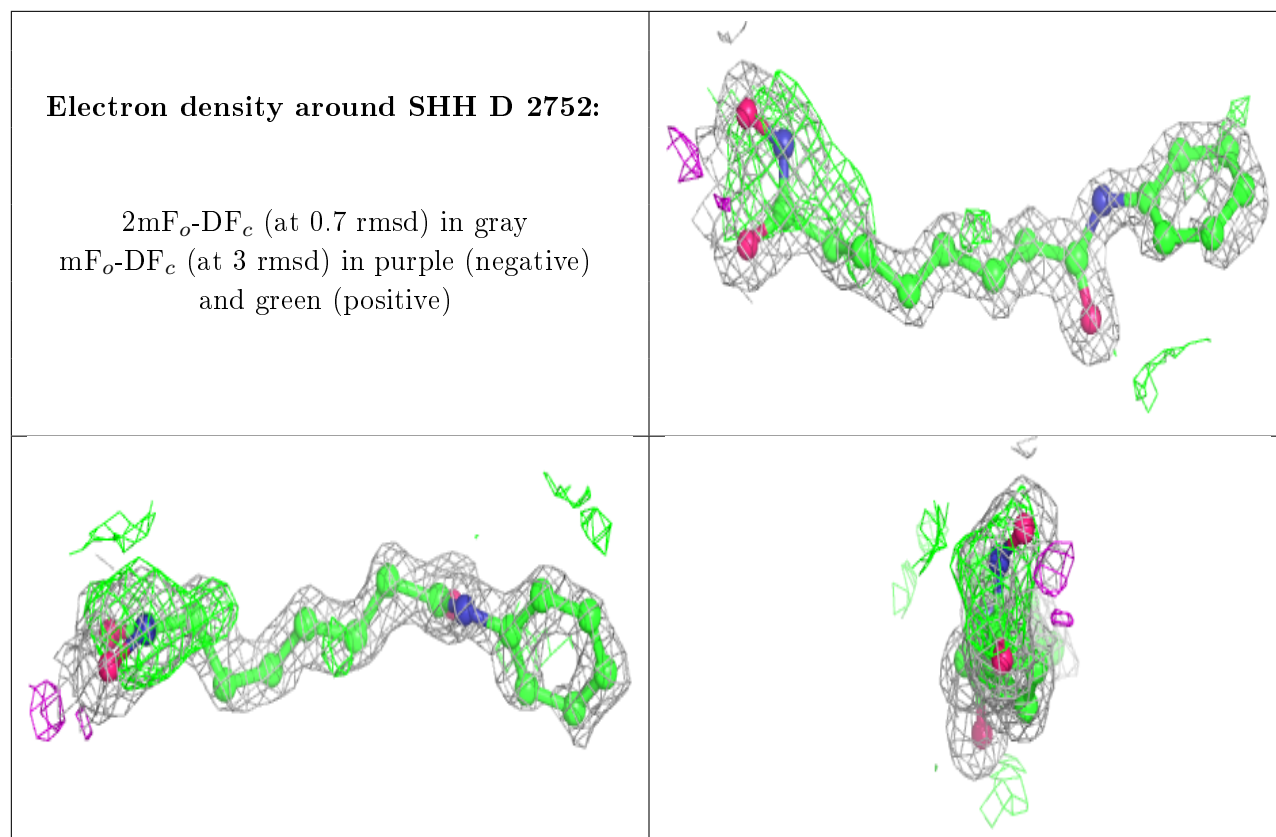
**Electron density around SHH A 2452:**

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

**Electron density around SHH C 2652:**

$2mF_o-DF_c$  (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.