



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 10:36 pm BST

PDB ID : 1TWW
Title : Dihydropteroate Synthetase, With Bound Substrate Analogue PtPP, From
Bacillus anthracis
Authors : Babaoglu, K.; Qi, J.; Lee, R.E.; White, S.W.
Deposited on : 2004-07-01
Resolution : 2.50 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 : 2.11
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

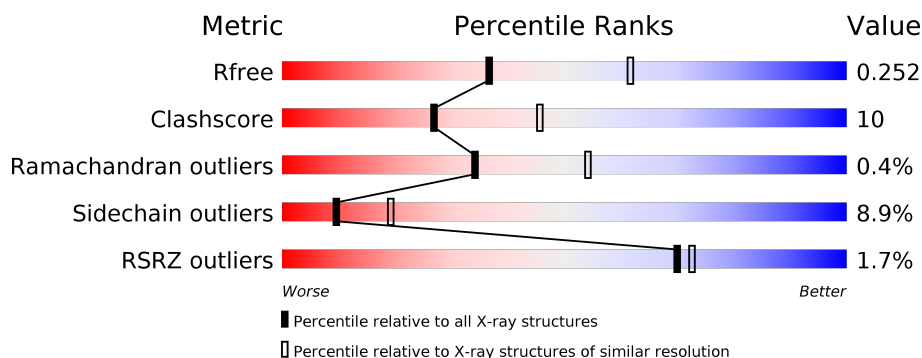
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 ≥ 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	297	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>18%</div> <div>•</div> <div>10%</div> </div> </div>
1	B	297	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>17%</div> <div>•</div> <div>12%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	279[A]	-	X	-	-
2	SO4	B	279[B]	-	X	-	-
2	SO4	B	280	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4320 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 DHPS, Dihydropteroate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2062	1295	353	398	16			
1	B	260	Total	C	N	O	S	0	0	0
			2012	1266	347	383	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q81VW8
A	-18	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-17	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-16	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-15	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-14	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-13	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-12	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-11	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-10	HIS	-	EXPRESSION TAG	UNP Q81VW8
A	-9	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-8	SER	-	EXPRESSION TAG	UNP Q81VW8
A	-7	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-6	LEU	-	EXPRESSION TAG	UNP Q81VW8
A	-5	VAL	-	EXPRESSION TAG	UNP Q81VW8
A	-4	PRO	-	EXPRESSION TAG	UNP Q81VW8
A	-3	ARG	-	EXPRESSION TAG	UNP Q81VW8
A	-2	GLY	-	EXPRESSION TAG	UNP Q81VW8
A	-1	SER	-	EXPRESSION TAG	UNP Q81VW8
A	0	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-19	MET	-	EXPRESSION TAG	UNP Q81VW8
B	-18	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-17	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-16	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-15	HIS	-	EXPRESSION TAG	UNP Q81VW8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-13	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-12	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-11	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-10	HIS	-	EXPRESSION TAG	UNP Q81VW8
B	-9	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-8	SER	-	EXPRESSION TAG	UNP Q81VW8
B	-7	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-6	LEU	-	EXPRESSION TAG	UNP Q81VW8
B	-5	VAL	-	EXPRESSION TAG	UNP Q81VW8
B	-4	PRO	-	EXPRESSION TAG	UNP Q81VW8
B	-3	ARG	-	EXPRESSION TAG	UNP Q81VW8
B	-2	GLY	-	EXPRESSION TAG	UNP Q81VW8
B	-1	SER	-	EXPRESSION TAG	UNP Q81VW8
B	0	HIS	-	EXPRESSION TAG	UNP Q81VW8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



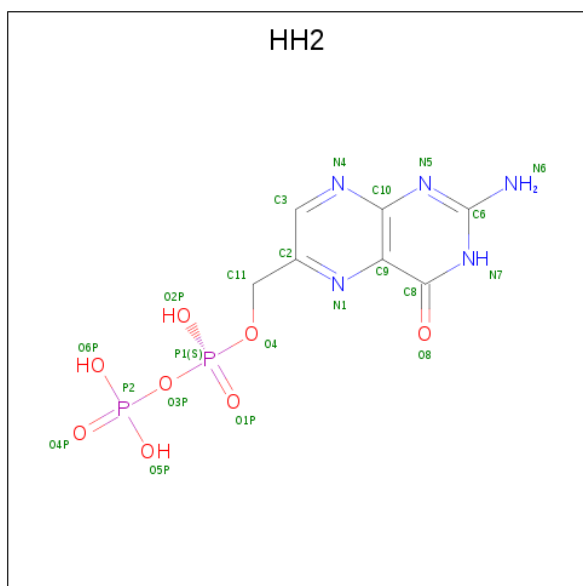
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 6 4 2	0	1
2	B	1	Total O 4 4	0	0
2	B	1	Total O S 5 4 1	0	0

- Molecule 3 is 6-HYDROXYMETHYLPTERIN-DIPHOSPHATE (three-letter code: HH2) (formula: $C_7H_9N_5O_8P_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O P 22 7 5 8 2	0	0
3	B	1	Total C N O P 22 7 5 8 2	0	0

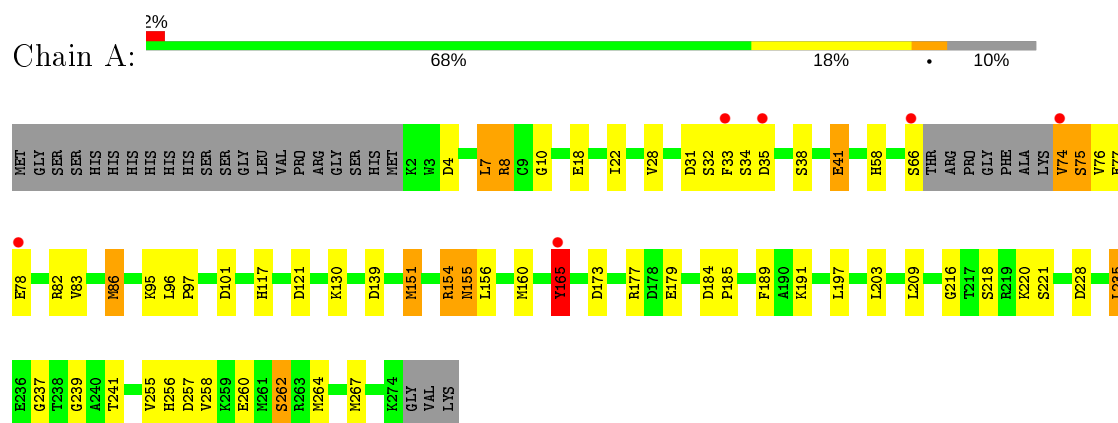
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	83	Total O 83 83	0	0
4	B	79	Total O 79 79	0	0

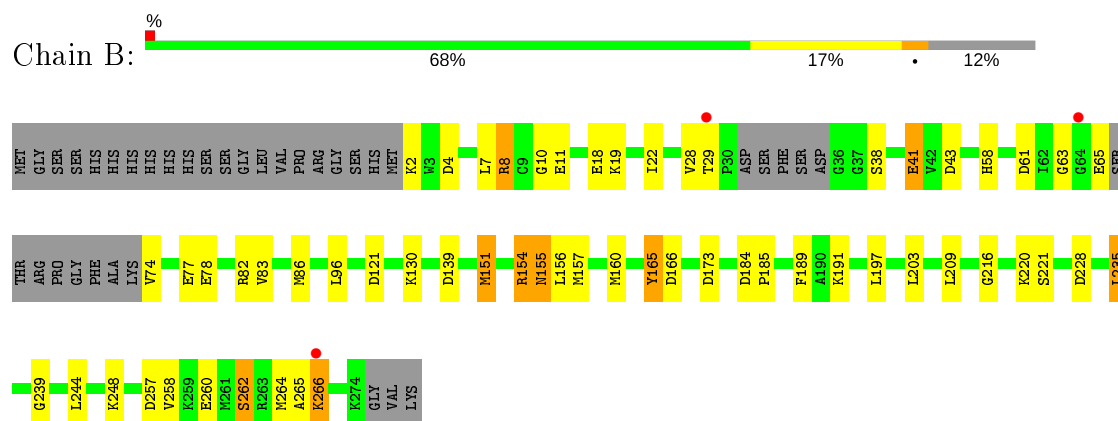
3 Residue-property plots [i](#)

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: DHPS, Dihydropteroate synthase



• Molecule 1: DHPS, Dihydropteroate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	98.24Å 98.24Å 262.61Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 41.99 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.7 (50.00-2.50) 96.7 (41.99-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.211 , 0.254 0.213 , 0.252	Depositor DCC
R_{free} test set	1311 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.769	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 32.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4320	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 47.11 % 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 1.0392e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HH2, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	3/2092 (0.1%)	0.99	10/2821 (0.4%)
1	B	0.88	3/2039 (0.1%)	1.02	10/2747 (0.4%)
All	All	0.86	6/4131 (0.1%)	1.01	20/5568 (0.4%)

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	B	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	266	LYS	C-N	12.42	1.62	1.34
1	B	151	MET	SD-CE	7.83	2.21	1.77
1	B	265	ALA	C-N	6.48	1.49	1.34
1	A	165	TYR	CZ-OH	6.25	1.48	1.37
1	A	165	TYR	CD1-CE1	6.22	1.48	1.39
1	A	267	MET	SD-CE	-5.55	1.46	1.77

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	LYS	O-C-N	-17.39	94.87	122.70
1	A	184	ASP	CB-CG-OD2	9.50	126.85	118.30
1	A	121	ASP	CB-CG-OD2	8.81	126.23	118.30
1	B	173	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	173	ASP	CB-CG-OD2	7.93	125.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ASP	CB-CG-OD2	7.34	124.90	118.30
1	B	184	ASP	CB-CG-OD2	7.30	124.88	118.30
1	A	4	ASP	CB-CG-OD2	6.22	123.90	118.30
1	A	101	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	228	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	4	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	166	ASP	CB-CG-OD1	5.84	123.55	118.30
1	B	43	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	139	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	139	ASP	CB-CG-OD2	5.42	123.18	118.30
1	B	61	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	7	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	35	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	228	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	151	MET	CB-CG-SD	-5.17	96.88	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	266	LYS	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	2062	0	2069	46	0
1	B	2012	0	2028	33	0
2	A	20	0	0	0	0
2	B	20	0	0	5	0
3	A	22	0	6	1	0
3	B	22	0	6	0	0
4	A	83	0	0	7	0
4	B	79	0	0	5	0
All	All	4320	0	4109	84	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 10.

All (84) 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:157:MET:CE	1:B:157:MET:SD	2.03	1.47
1:B:151:MET:CE	1:B:151:MET:SD	2.21	1.28
1:A:165:TYR:CE1	1:A:209:LEU:CD2	2.43	1.01
1:A:28:VAL:HG12	1:A:28:VAL:O	1.63	0.96
2:B:280:SO4:O3	2:B:280:SO4:O2	1.82	0.95
1:A:165:TYR:CE1	1:A:209:LEU:HD22	2.05	0.90
1:B:165:TYR:CE1	1:B:209:LEU:CD2	2.55	0.90
1:A:28:VAL:HG13	1:A:86:MET:CE	2.02	0.89
2:B:280:SO4:O3	2:B:280:SO4:O1	1.93	0.87
1:B:154:ARG:HH11	1:B:154:ARG:HG2	1.42	0.83
1:A:22:ILE:H	1:A:58:HIS:HD1	1.26	0.83
1:A:154:ARG:HG2	1:A:154:ARG:HH11	1.44	0.80
1:A:179:GLU:OE1	4:A:320:HOH:O	1.99	0.80
1:B:165:TYR:CE1	1:B:209:LEU:HD22	2.18	0.78
1:B:22:ILE:H	1:B:58:HIS:HD1	1.36	0.74
1:B:155:ASN:HD22	1:B:155:ASN:C	1.92	0.72
1:A:28:VAL:HG13	1:A:86:MET:HE1	1.70	0.72
1:A:28:VAL:CG1	1:A:86:MET:CE	2.69	0.70
1:A:28:VAL:HG13	1:A:86:MET:HE2	1.72	0.69
1:B:11:GLU:OE2	4:B:295:HOH:O	2.12	0.68
1:A:28:VAL:HG22	1:A:86:MET:HE1	1.75	0.67
1:A:28:VAL:CG1	1:A:86:MET:HE2	2.28	0.64
1:A:28:VAL:CG1	1:A:86:MET:HE1	2.27	0.64
1:B:28:VAL:HG21	1:B:63:GLY:O	1.98	0.63
1:A:155:ASN:C	1:A:155:ASN:HD22	2.02	0.62
1:A:185:PRO:HG3	1:A:203:LEU:HD21	1.82	0.62
1:B:78:GLU:CB	1:B:78:GLU:OE1	2.48	0.62
1:B:156:LEU:O	1:B:160:MET:HG3	2.00	0.62
2:B:280:SO4:O2	2:B:280:SO4:O4	2.17	0.62
1:B:157:MET:HG2	4:B:340:HOH:O	1.98	0.61
1:A:28:VAL:O	1:A:28:VAL:CG1	2.36	0.61
1:B:165:TYR:CZ	1:B:209:LEU:HD22	2.35	0.61
1:A:28:VAL:CG2	1:A:86:MET:HE1	2.30	0.60
1:B:19:LYS:NZ	1:B:58:HIS:NE2	2.49	0.60
1:A:74:VAL:O	1:A:75:SER:HB3	2.01	0.59
1:B:78:GLU:CB	1:B:78:GLU:CD	2.71	0.58
1:A:156:LEU:O	1:A:160:MET:HG3	2.05	0.56
1:B:185:PRO:HG3	1:B:203:LEU:HD21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:SO4:O2	2:B:280:SO4:O1	2.23	0.56
1:A:32:SER:O	1:A:33:PHE:HB2	2.07	0.55
1:A:165:TYR:CZ	1:A:209:LEU:HD22	2.42	0.54
1:A:165:TYR:CE1	1:A:209:LEU:HD21	2.43	0.52
1:A:258:VAL:O	1:A:262:SER:HB2	2.10	0.51
1:B:155:ASN:ND2	1:B:155:ASN:C	2.63	0.51
1:A:8:ARG:NH2	1:A:10:GLY:O	2.44	0.51
1:A:235:LEU:HD21	1:A:260:GLU:HG2	1.93	0.50
1:B:154:ARG:HD2	4:B:339:HOH:O	2.11	0.50
1:A:130:LYS:HG3	4:A:335:HOH:O	2.10	0.50
1:B:38:SER:OG	1:B:41:GLU:HG3	2.12	0.50
1:A:151:MET:CE	4:A:337:HOH:O	2.59	0.50
1:B:8:ARG:NH2	1:B:10:GLY:O	2.45	0.49
1:B:239:GLY:HA3	1:B:264:MET:HE1	1.94	0.48
1:A:165:TYR:CE1	1:A:209:LEU:HD23	2.43	0.48
1:B:244:LEU:HD11	1:B:248:LYS:HE2	1.96	0.48
1:A:95:LYS:HA	1:A:95:LYS:HD3	1.64	0.47
1:A:151:MET:HE3	4:A:337:HOH:O	2.13	0.47
1:A:165:TYR:HE1	1:A:209:LEU:CD2	2.19	0.47
2:B:280:SO4:O4	2:B:280:SO4:O1	2.33	0.46
1:B:235:LEU:HD21	1:B:260:GLU:HG2	1.96	0.46
1:A:31:ASP:CG	1:A:41:GLU:HG2	2.36	0.46
1:B:65:GLU:HG2	4:B:331:HOH:O	2.15	0.46
1:A:165:TYR:HB3	4:A:353:HOH:O	2.15	0.45
1:A:58:HIS:O	1:A:97:PRO:HD2	2.16	0.45
1:A:239:GLY:HA3	1:A:264:MET:HE1	1.98	0.45
1:B:189:PHE:O	1:B:191:LYS:HG3	2.17	0.45
1:B:165:TYR:CE1	1:B:209:LEU:HD21	2.47	0.45
1:A:165:TYR:CD2	4:A:353:HOH:O	2.56	0.45
1:A:154:ARG:HG2	1:A:154:ARG:NH1	2.24	0.43
1:A:235:LEU:HD12	1:A:257:ASP:CG	2.39	0.43
1:A:31:ASP:OD2	1:A:38:SER:OG	2.36	0.43
1:B:258:VAL:O	1:B:262:SER:HB2	2.19	0.42
1:B:235:LEU:HD12	1:B:257:ASP:CG	2.39	0.42
1:A:97:PRO:HA	1:A:117:HIS:ND1	2.35	0.42
1:A:216:GLY:O	1:A:220:LYS:HE3	2.20	0.42
1:B:216:GLY:O	1:B:220:LYS:HE3	2.19	0.42
1:B:130:LYS:HG3	4:B:317:HOH:O	2.20	0.42
1:A:218:SER:HB2	1:A:255:VAL:HA	2.03	0.41
1:B:154:ARG:HH11	1:B:154:ARG:CG	2.22	0.41
1:A:237:GLY:O	1:A:241:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:ARG:HB3	4:A:320:HOH:O	2.20	0.40
1:A:189:PHE:O	1:A:191:LYS:HG3	2.21	0.40
1:B:19:LYS:HE3	1:B:58:HIS:NE2	2.35	0.40
1:B:19:LYS:CE	1:B:58:HIS:NE2	2.85	0.40
1:A:256:HIS:NE2	3:A:282:HH2:O5P	2.50	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	262/297 (88%)	254 (97%)	7 (3%)	1 (0%)	34	54
1	B	254/297 (86%)	250 (98%)	3 (1%)	1 (0%)	34	54
All	All	516/594 (87%)	504 (98%)	10 (2%)	2 (0%)	34	54

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	B	29	THR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/247 (90%)	201 (90%)	21 (10%)	8	17
1	B	214/247 (87%)	196 (92%)	18 (8%)	11	21
All	All	436/494 (88%)	397 (91%)	39 (9%)	9	19

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	ARG
1	A	18	GLU
1	A	34	SER
1	A	41	GLU
1	A	66	SER
1	A	74	VAL
1	A	76	VAL
1	A	77	GLU
1	A	78	GLU
1	A	82	ARG
1	A	83	VAL
1	A	86	MET
1	A	96	LEU
1	A	154	ARG
1	A	155	ASN
1	A	165	TYR
1	A	197	LEU
1	A	221	SER
1	A	235	LEU
1	A	262	SER
1	B	2	LYS
1	B	7	LEU
1	B	8	ARG
1	B	18	GLU
1	B	41	GLU
1	B	74	VAL
1	B	77	GLU
1	B	82	ARG
1	B	83	VAL
1	B	86	MET
1	B	96	LEU
1	B	154	ARG
1	B	155	ASN
1	B	165	TYR

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Mol	Chain	Res	Type
1	B	197	LEU
1	B	221	SER
1	B	235	LEU
1	B	262	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	155	ASN
1	A	180	ASN
1	B	88	GLN
1	B	137	HIS
1	B	152	ASN
1	B	155	ASN
1	B	180	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	280	-	4,4,4	0.22	0	6,6,6	0.31	0
2	SO4	A	278	-	4,4,4	0.18	0	6,6,6	0.49	0
2	SO4	B	279[A]	-	4,4,4	0.24	0	6,6,6	5.17	6 (100%)
2	SO4	B	279[B]	-	4,4,4	0.16	0	6,6,6	5.18	6 (100%)
2	SO4	A	281	-	4,4,4	0.15	0	6,6,6	0.34	0
2	SO4	B	281	-	4,4,4	0.11	0	6,6,6	0.74	0
3	HH2	B	282	-	21,23,23	1.27	2 (9%)	27,35,35	2.40	9 (33%)
3	HH2	A	282	-	21,23,23	1.22	3 (14%)	27,35,35	2.15	11 (40%)
2	SO4	A	279	-	4,4,4	0.29	0	6,6,6	0.46	0
2	SO4	B	278	-	4,4,4	0.24	0	6,6,6	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HH2	A	282	-	-	4/12/12/12	0/2/2/2
3	HH2	B	282	-	-	4/12/12/12	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	282	HH2	O8-C8	3.64	1.33	1.24
3	A	282	HH2	O8-C8	3.13	1.32	1.24
3	B	282	HH2	C2-N1	2.46	1.36	1.32
3	A	282	HH2	C2-N1	2.39	1.36	1.32
3	A	282	HH2	C8-N7	2.11	1.36	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	279[B]	SO4	O4-S-O3	-7.27	78.03	109.06
2	B	279[A]	SO4	O4-S-O3	-7.16	78.48	109.06
2	B	279[A]	SO4	O4-S-O2	-5.26	81.88	109.31
2	B	279[B]	SO4	O4-S-O2	-5.21	82.13	109.31
2	B	279[B]	SO4	O3-S-O1	-5.03	83.05	109.31
3	B	282	HH2	C2-C3-N4	-5.00	118.22	123.13
3	B	282	HH2	N4-C10-N5	4.94	121.46	115.82
2	B	279[A]	SO4	O3-S-O1	-4.94	83.53	109.31
2	B	279[A]	SO4	O3-S-O2	4.59	133.25	109.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	279[B]	SO4	O4-S-O1	4.55	133.07	109.31
3	B	282	HH2	C3-N4-C10	4.54	121.25	116.69
2	B	279[A]	SO4	O4-S-O1	4.29	131.69	109.31
2	B	279[B]	SO4	O3-S-O2	4.22	131.31	109.31
2	B	279[A]	SO4	O2-S-O1	-4.16	78.73	109.43
2	B	279[B]	SO4	O2-S-O1	-4.12	78.99	109.43
3	A	282	HH2	C9-C8-N7	-4.10	117.82	123.43
3	B	282	HH2	C9-C8-N7	-3.96	118.02	123.43
3	B	282	HH2	N5-C6-N7	-3.93	121.98	127.22
3	A	282	HH2	N5-C6-N7	-3.83	122.12	127.22
3	A	282	HH2	C2-C3-N4	-3.71	119.49	123.13
3	A	282	HH2	N4-C10-N5	3.56	119.89	115.82
3	B	282	HH2	C6-N5-C10	3.55	119.41	115.36
3	A	282	HH2	C3-N4-C10	3.25	119.96	116.69
3	A	282	HH2	C6-N5-C10	3.18	118.98	115.36
3	A	282	HH2	C8-N7-C6	3.17	120.97	115.93
3	A	282	HH2	P1-O3P-P2	-2.90	122.87	132.83
3	B	282	HH2	C8-N7-C6	2.78	120.34	115.93
3	B	282	HH2	C10-C9-N1	-2.59	119.39	122.33
3	A	282	HH2	O6P-P2-O5P	2.42	116.88	107.64
3	B	282	HH2	C8-C9-C10	2.34	121.50	119.95
3	A	282	HH2	C10-C9-N1	-2.05	120.01	122.33
3	A	282	HH2	O2P-P1-O1P	2.04	122.34	112.24

There are no chirality outliers.

All (8) torsion outliers are listed below:

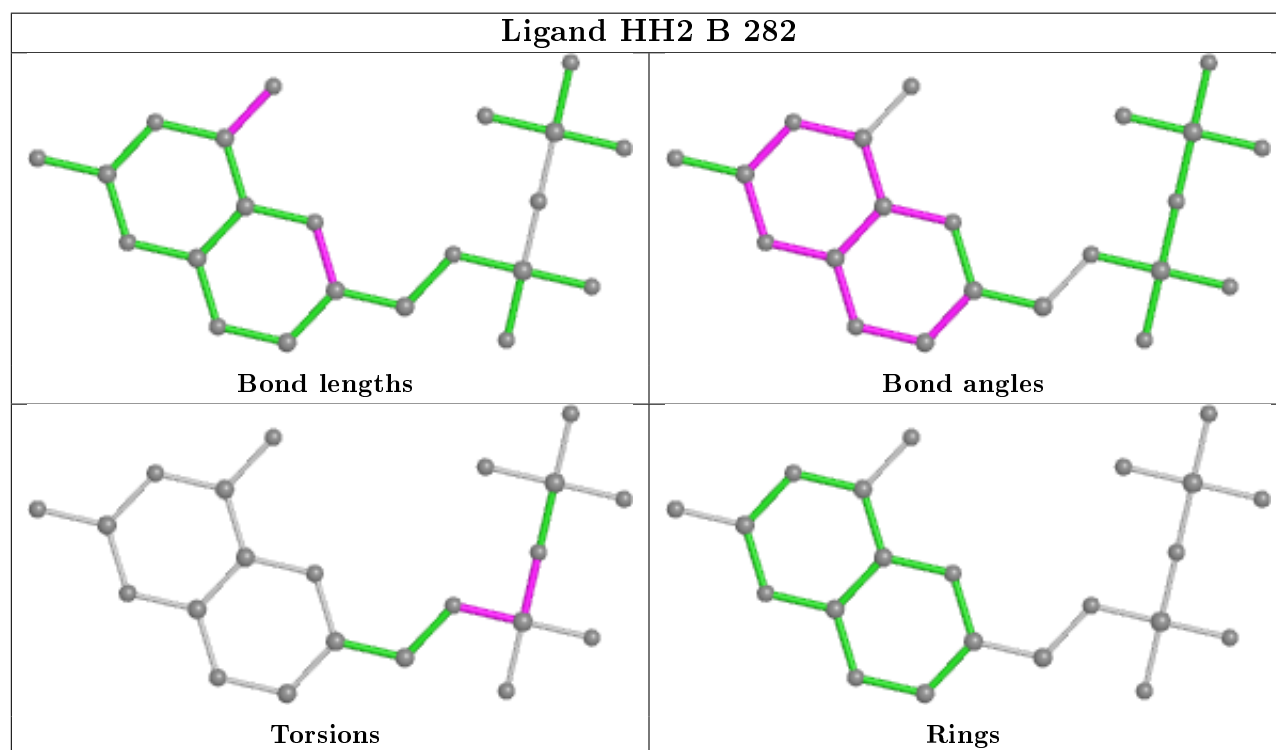
Mol	Chain	Res	Type	Atoms
3	A	282	HH2	C11-O4-P1-O1P
3	B	282	HH2	C11-O4-P1-O1P
3	B	282	HH2	P2-O3P-P1-O4
3	A	282	HH2	P2-O3P-P1-O4
3	B	282	HH2	C11-O4-P1-O3P
3	A	282	HH2	C11-O4-P1-O2P
3	B	282	HH2	C11-O4-P1-O2P
3	A	282	HH2	C11-O4-P1-O3P

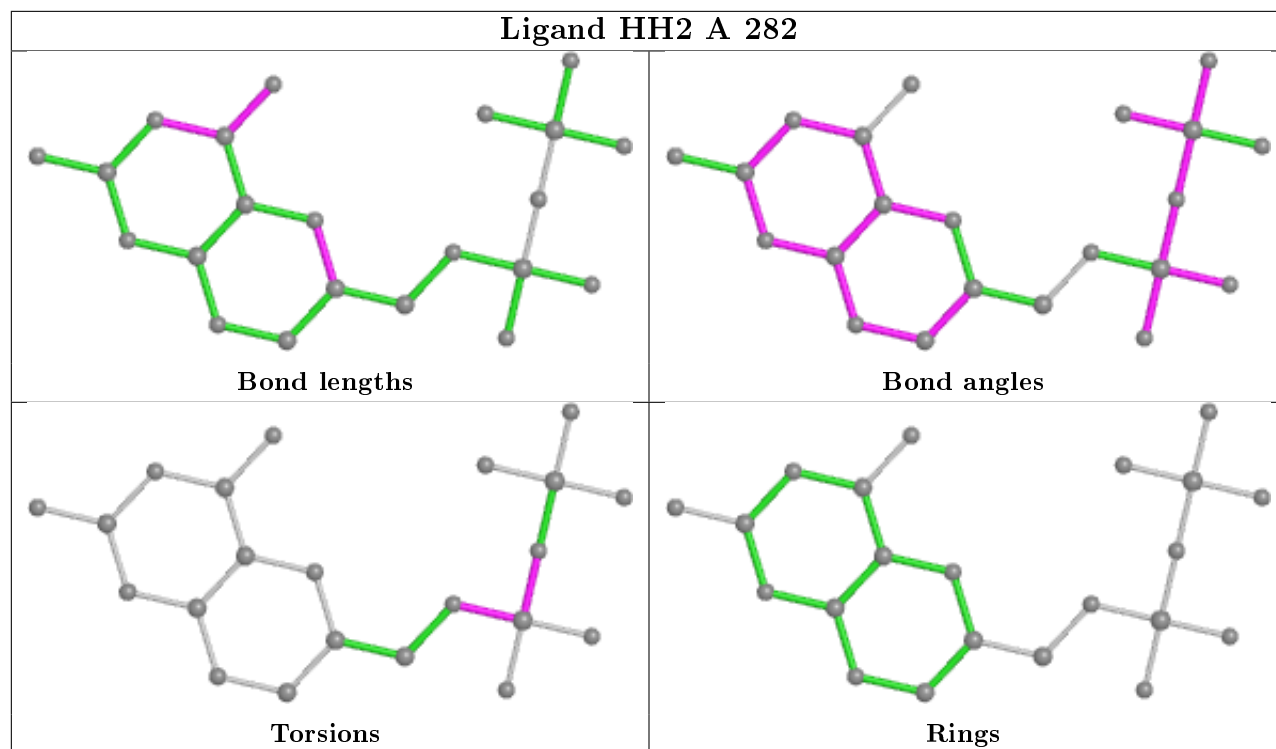
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	282	HH2	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	266:LYS	C	267:MET	N	1.62

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	266/297 (89%)	-0.24	6 (2%) 60 63	13, 21, 44, 57	0
1	B	260/297 (87%)	-0.23	3 (1%) 79 80	12, 20, 38, 79	0
All	All	526/594 (88%)	-0.24	9 (1%) 70 72	12, 20, 41, 79	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	64	GLY	3.1
1	A	35	ASP	3.1
1	A	165	TYR	2.9
1	A	66	SER	2.6
1	A	33	PHE	2.6
1	A	74	VAL	2.3
1	A	78	GLU	2.1
1	B	29	THR	2.1
1	B	266	LYS	2.1

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 carbohydrates in this entry.

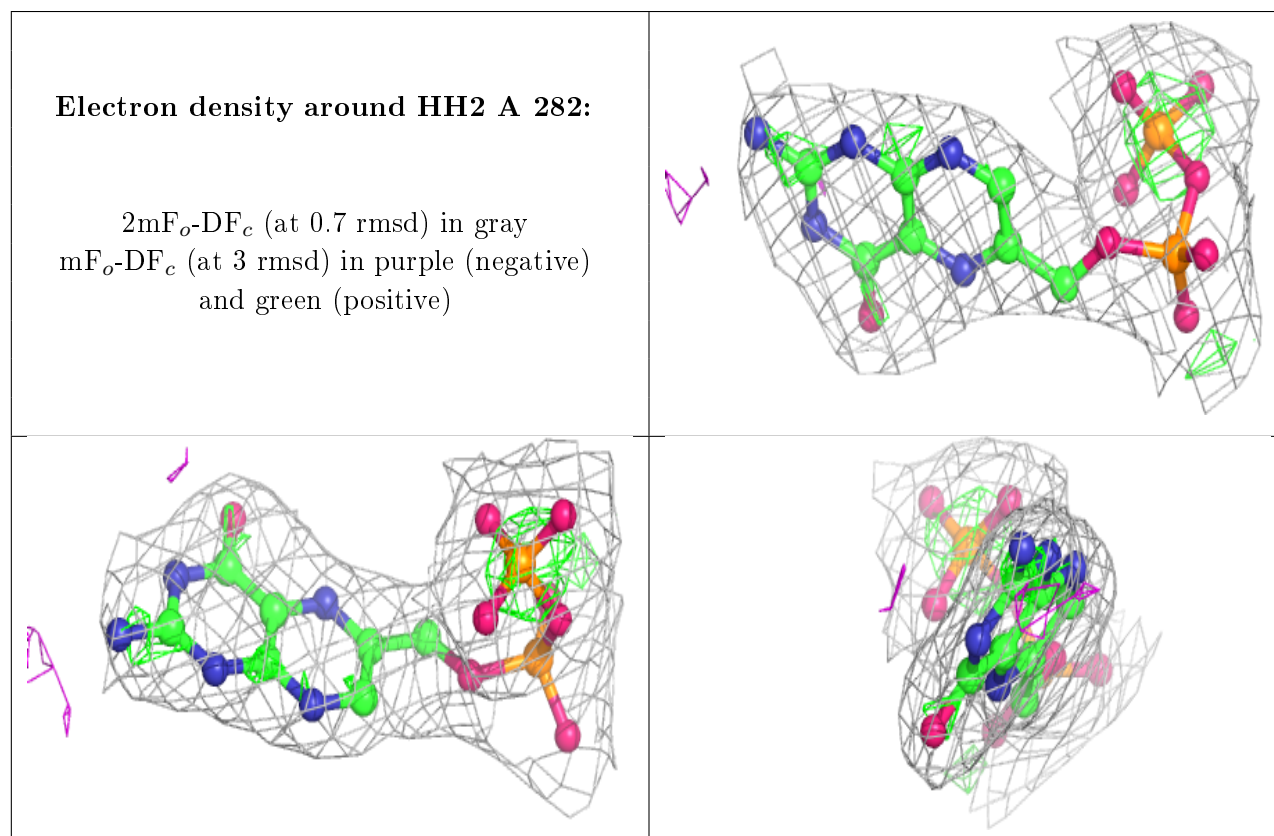
6.4 Ligands [i](#)

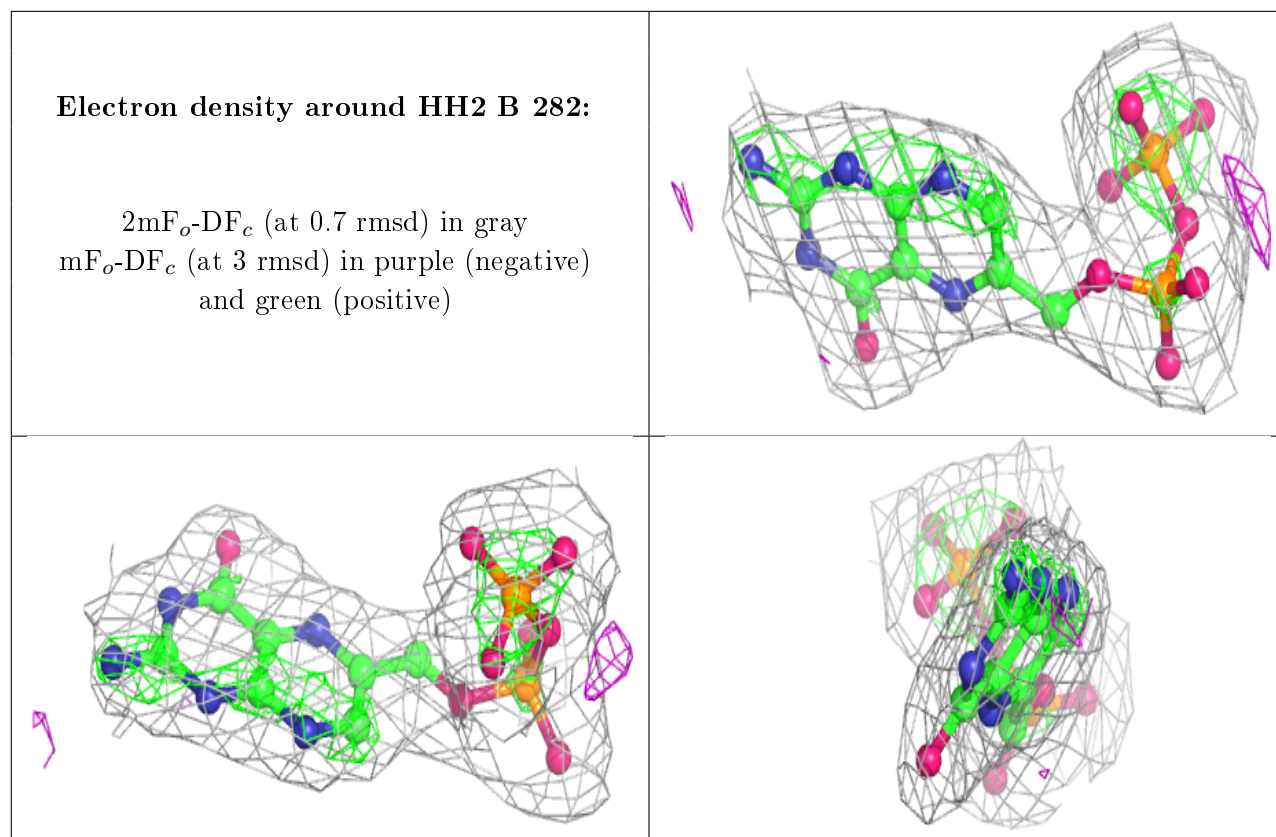
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
2	SO4	B	279[A]	5/5	0.86	0.18	93,93,93,95	1
2	SO4	B	279[B]	5/5	0.86	0.18	93,93,93,93	1
2	SO4	A	280	5/5	0.88	0.21	52,52,54,54	5
2	SO4	A	281	5/5	0.92	0.15	71,73,75,75	0
3	HH2	A	282	22/22	0.93	0.26	79,86,95,96	0
2	SO4	B	281	5/5	0.93	0.13	65,68,69,69	0
2	SO4	A	279	5/5	0.93	0.25	69,71,75,75	0
2	SO4	B	280	4/5	0.94	0.20	19,22,30,39	4
3	HH2	B	282	22/22	0.95	0.23	75,81,89,93	0
2	SO4	A	278	5/5	0.95	0.15	65,66,68,69	0
2	SO4	B	278	5/5	0.96	0.18	66,67,69,70	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.