



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:28 PM UTC

PDB ID : 3K34 / pdb_00003k34
Title : Human carbonic anhydrase II with a sulfonamide inhibitor
Authors : Behnke, C.A.; Le Trong, I.; Merritt, E.A.; Teller, D.C.; Stenkamp, R.E.
Deposited on : 2009-10-01
Resolution : 0.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

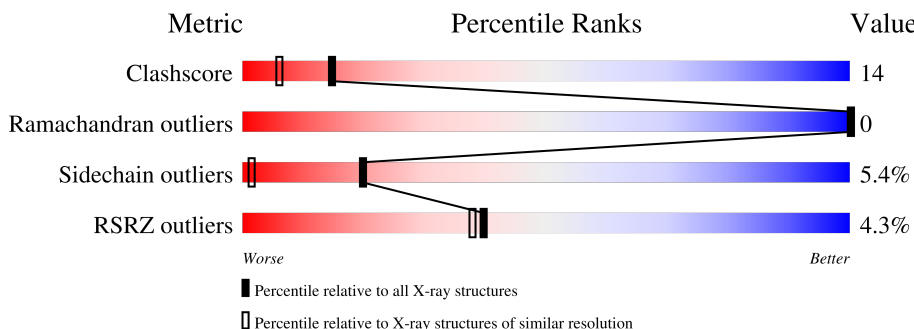
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 0.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1416 (1.00-0.80)
Ramachandran outliers	187476	1341 (1.00-0.80)
Sidechain outliers	187428	1342 (1.00-0.80)
RSRZ outliers	180081	1363 (1.00-0.80)

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	260	4% 70% 21% 5%

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
5	GOL	A	1004	-	X	X	-
5	GOL	A	1005	-	-	X	-
5	GOL	A	1006	-	X	-	-

2 Entry composition [i](#)

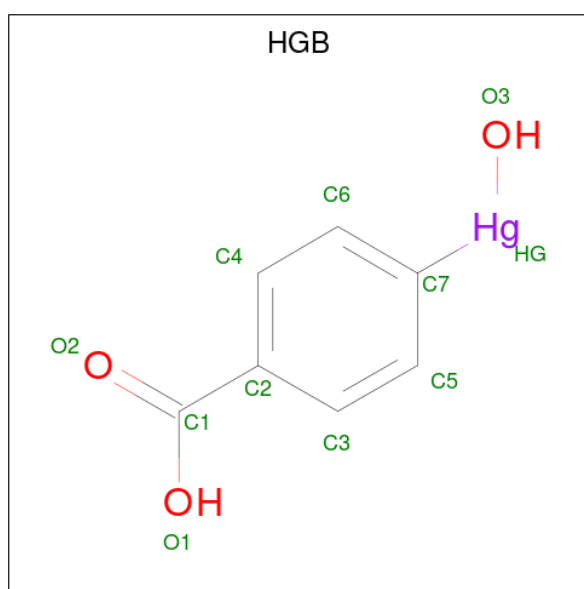
There are 6 unique types of molecules in this entry. The entry contains 2387 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	10	0
			2086	1337	359	387	3			

- Molecule 2 is 4-(HYDROXYMERCURY)BENZOIC ACID (CCD ID: HGB) (formula: $C_7H_6HgO_3$).

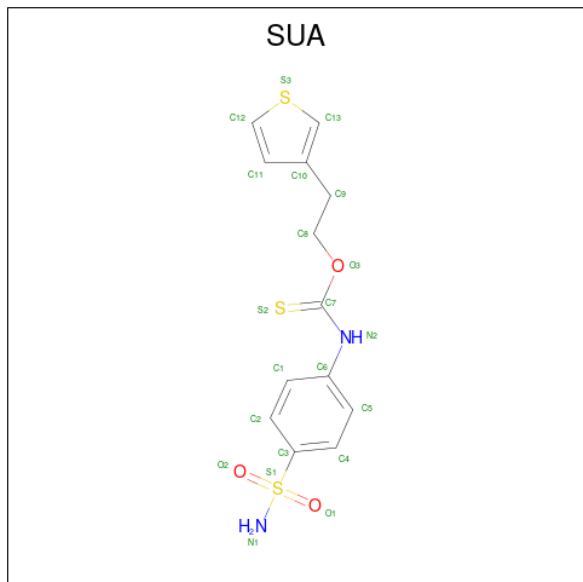


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Hg	O	0	1
			12	8	2	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

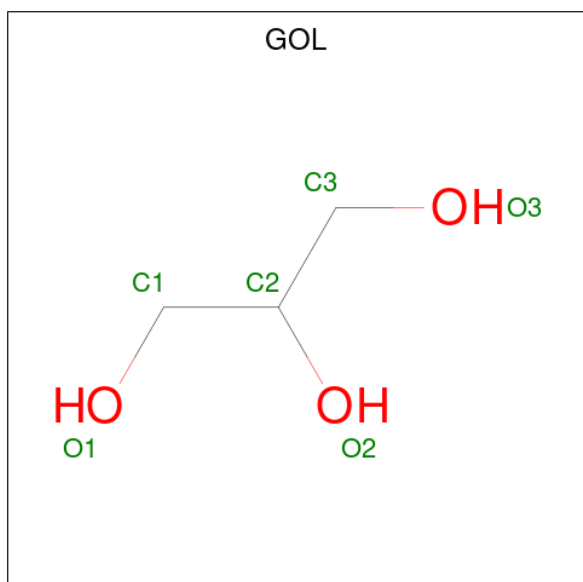
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (4-SULFAMOYL-PHENYL)-THIOCARBAMIC ACID O-(2-THIOPHEN-3-Y L-ETHYL) ESTER (CCD ID: SUA) (formula: $C_{13}H_{14}N_2O_3S_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	21	13	2	3	3	0	0

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

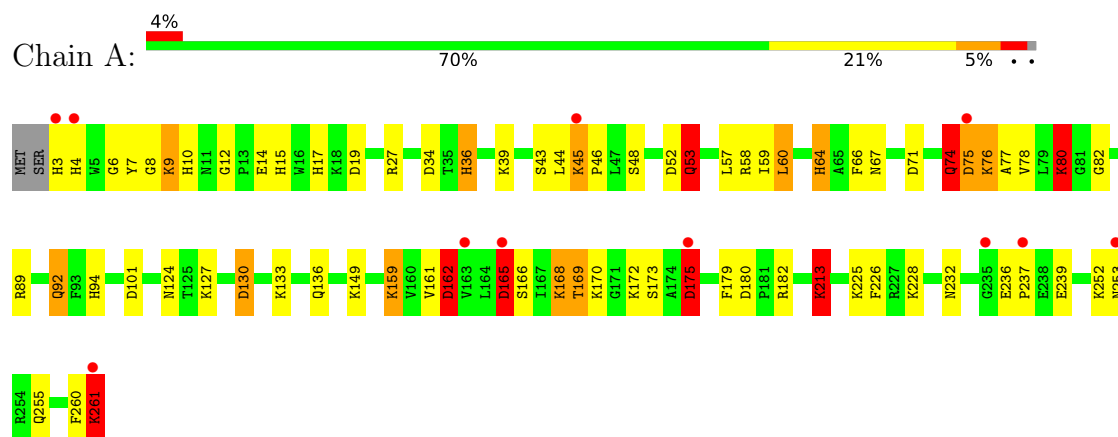
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	249	Total	O	0	0
			249	249		

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 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.05Å 41.27Å 71.82Å 90.00° 104.23° 90.00°	Depositor
Resolution (Å)	18.00 – 0.90 18.00 – 0.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (18.00-0.90) 88.2 (18.00-0.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 0.90Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.141 , 0.160 0.128 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	8.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	2387	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SUA, HGB, ZN, GOL

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	1.89	42/2199 (1.9%)	2.07	76/2978 (2.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	HIS	CE1-NE2	18.02	1.50	1.32
1	A	64	HIS	CD2-NE2	-17.83	1.18	1.37
1	A	27	ARG	CD-NE	-16.40	1.23	1.46
1	A	3	HIS	ND1-CE1	9.70	1.42	1.32
1	A	14	GLU	CD-OE2	8.59	1.41	1.25
1	A	57	LEU	CA-C	-8.13	1.44	1.52
1	A	10	HIS	ND1-CE1	8.03	1.40	1.32
1	A	130	ASP	CA-CB	7.71	1.67	1.53
1	A	27	ARG	CZ-NH2	-7.39	1.23	1.33
1	A	17	HIS	CD2-NE2	7.34	1.46	1.37
1	A	161	VAL	CA-CB	7.26	1.63	1.54
1	A	76	LYS	C-O	6.59	1.32	1.24
1	A	169	THR	CA-C	6.51	1.60	1.52
1	A	101	ASP	C-O	-6.49	1.15	1.24
1	A	9	LYS	CA-CB	6.46	1.63	1.53
1	A	159	LYS	CE-NZ	6.39	1.68	1.49
1	A	59	ILE	C-O	6.33	1.30	1.24
1	A	182	ARG	NE-CZ	6.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	ASP	CA-CB	6.07	1.62	1.53
1	A	78	VAL	CA-CB	-6.04	1.44	1.55
1	A	71	ASP	C-O	5.96	1.31	1.24
1	A	14	GLU	N-CA	5.96	1.53	1.46
1	A	89	ARG	NE-CZ	-5.96	1.26	1.33
1	A	10	HIS	CB-CG	5.82	1.58	1.50
1	A	3	HIS	C-O	5.75	1.35	1.23
1	A	253	ASN	C-O	5.71	1.32	1.23
1	A	52	ASP	C-N	-5.62	1.26	1.33
1	A	173	SER	C-O	5.58	1.30	1.23
1	A	44	LEU	C-N	5.54	1.41	1.33
1	A	60	LEU	N-CA	-5.49	1.39	1.46
1	A	15	HIS	CE1-NE2	5.40	1.38	1.32
1	A	255	GLN	C-N	-5.35	1.25	1.33
1	A	82	GLY	CA-C	-5.35	1.44	1.51
1	A	165	ASP	CG-OD1	5.34	1.35	1.25
1	A	162	ASP	CG-OD2	5.27	1.35	1.25
1	A	8	GLY	N-CA	5.27	1.51	1.45
1	A	159	LYS	CA-C	5.26	1.59	1.52
1	A	169	THR	C-N	5.21	1.40	1.33
1	A	253	ASN	C-N	5.15	1.40	1.33
1	A	39	LYS	CA-C	-5.10	1.46	1.52
1	A	10	HIS	N-CA	5.08	1.52	1.46
1	A	10	HIS	CE1-NE2	5.03	1.37	1.32

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	ASP	CA-CB-CG	33.46	146.06	112.60
1	A	74	GLN	OE1-CD-NE2	30.99	153.59	122.60
1	A	175	ASP	CA-CB-CG	-17.79	94.81	112.60
1	A	162	ASP	CB-CG-OD2	12.48	147.11	118.40
1	A	52	ASP	CA-CB-CG	12.27	124.87	112.60
1	A	64	HIS	ND1-CE1-NE2	-12.16	96.24	108.40
1	A	27	ARG	CG-CD-NE	12.07	138.55	112.00
1	A	27	ARG	NE-CZ-NH2	-11.72	108.65	119.20
1	A	74	GLN	CG-CD-OE1	-10.81	99.18	120.80
1	A	80	LYS	CD-CE-NZ	10.26	144.72	111.90
1	A	182	ARG	NE-CZ-NH2	-9.96	110.23	119.20
1	A	3	HIS	CA-CB-CG	-9.87	103.94	113.80
1	A	3	HIS	CA-C-O	-9.61	104.46	120.80
1	A	27	ARG	CD-NE-CZ	9.55	137.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	ARG	NE-CZ-NH1	8.92	130.42	121.50
1	A	76	LYS	O-C-N	-8.86	110.80	122.59
1	A	77	ALA	N-CA-CB	-8.64	96.11	109.94
1	A	159	LYS	CG-CD-CE	8.53	130.92	111.30
1	A	130	ASP	OD1-CG-OD2	-8.48	102.54	122.90
1	A	3	HIS	O-C-N	8.45	136.52	123.00
1	A	175	ASP	OD1-CG-OD2	7.75	141.49	122.90
1	A	252	LYS	CB-CG-CD	7.68	128.96	111.30
1	A	237	PRO	N-CA-CB	7.33	109.83	103.31
1	A	236	GLU	O-C-N	-7.22	114.70	121.20
1	A	170	LYS	CD-CE-NZ	7.16	134.82	111.90
1	A	261	LYS	CA-CB-CG	-7.15	99.80	114.10
1	A	3	HIS	CA-C-N	7.14	134.28	122.07
1	A	3	HIS	C-N-CA	7.14	134.28	122.07
1	A	36	HIS	CA-CB-CG	-6.99	106.81	113.80
1	A	236	GLU	CA-C-N	6.99	126.96	119.76
1	A	236	GLU	C-N-CA	6.99	126.96	119.76
1	A	175	ASP	CB-CG-OD1	-6.94	102.44	118.40
1	A	225	LYS	CB-CG-CD	6.91	127.19	111.30
1	A	4	HIS	CA-CB-CG	6.80	120.60	113.80
1	A	213	LYS	CG-CD-CE	-6.64	96.02	111.30
1	A	10	HIS	ND1-CG-CD2	6.59	112.69	106.10
1	A	75	ASP	CB-CG-OD1	6.57	133.52	118.40
1	A	10	HIS	ND1-CE1-NE2	-6.57	101.83	108.40
1	A	162	ASP	OD1-CG-OD2	-6.48	107.36	122.90
1	A	74	GLN	CB-CG-CD	-6.33	101.84	112.60
1	A	53	GLN	OE1-CD-NE2	-6.31	116.29	122.60
1	A	149	LYS	CG-CD-CE	6.29	125.77	111.30
1	A	136	GLN	OE1-CD-NE2	6.25	128.85	122.60
1	A	175	ASP	CB-CA-C	-6.23	99.38	109.72
1	A	237	PRO	CB-CA-C	-6.16	103.52	111.46
1	A	239	GLU	OE1-CD-OE2	6.15	137.66	122.90
1	A	74	GLN	CG-CD-NE2	-6.12	107.23	116.40
1	A	19	ASP	CA-CB-CG	-6.08	106.52	112.60
1	A	232	ASN	CA-C-O	5.92	128.80	121.81
1	A	64	HIS	CB-CG-CD2	5.87	138.83	131.20
1	A	239	GLU	CB-CG-CD	5.80	122.45	112.60
1	A	162	ASP	CB-CG-OD1	-5.75	105.17	118.40
1	A	53	GLN	CB-CG-CD	5.69	122.27	112.60
1	A	130	ASP	CB-CG-OD1	5.67	131.44	118.40
1	A	76	LYS	CA-CB-CG	-5.64	102.82	114.10
1	A	179	PHE	CA-CB-CG	-5.57	108.23	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CB-CG-CD2	-5.51	124.04	131.20
1	A	253	ASN	O-C-N	5.49	130.25	122.68
1	A	74	GLN	O-C-N	5.47	129.79	123.17
1	A	53	GLN	CG-CD-OE1	5.46	131.73	120.80
1	A	180	ASP	CA-CB-CG	-5.41	107.19	112.60
1	A	9	LYS	O-C-N	5.40	127.84	122.12
1	A	165	ASP	OD1-CG-OD2	5.39	135.84	122.90
1	A	58	ARG	NE-CZ-NH1	5.34	126.84	121.50
1	A	14	GLU	CG-CD-OE1	-5.33	106.14	118.40
1	A	165	ASP	CA-C-O	-5.32	113.06	119.49
1	A	75	ASP	OD1-CG-OD2	-5.31	110.15	122.90
1	A	175	ASP	O-C-N	5.29	129.38	122.87
1	A	182	ARG	CD-NE-CZ	-5.28	117.00	124.40
1	A	226	PHE	CB-CG-CD1	5.27	129.66	120.70
1	A	43	SER	CA-CB-OG	5.24	121.57	111.10
1	A	168	LYS	CD-CE-NZ	5.22	128.62	111.90
1	A	8	GLY	O-C-N	-5.16	116.20	122.71
1	A	10	HIS	CE1-NE2-CD2	5.12	114.12	109.00
1	A	59	ILE	O-C-N	-5.11	117.63	123.10
1	A	14	GLU	CB-CG-CD	5.04	121.17	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	34	ASP	Sidechain
1	A	64	HIS	Sidechain

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	2086	0	2031	50	4
2	A	12	0	4	0	0
3	A	1	0	0	0	0
4	A	21	0	12	5	0
5	A	18	0	18	8	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	249	0	0	12	6
All	All	2387	0	2065	59	7

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 14.

All (59) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:CE	1:A:159:LYS:NZ	1.68	1.54
5:A:1006:GOL:C1	5:A:1006:GOL:C2	1.95	1.45
5:A:1005:GOL:O1	5:A:1005:GOL:C1	1.69	1.39
5:A:1004:GOL:O1	5:A:1004:GOL:C1	1.77	1.30
1:A:45:LYS:NZ	1:A:46:PRO:HD2	1.53	1.23
1:A:45:LYS:NZ	1:A:45:LYS:HB3	1.56	1.14
1:A:45:LYS:HZ2	1:A:45:LYS:CB	1.67	1.06
1:A:124:ASN:HD21	1:A:127[B]:LYS:HE3	1.18	1.05
1:A:45:LYS:NZ	1:A:46:PRO:CD	2.21	1.03
1:A:45:LYS:HZ1	1:A:46:PRO:HD2	0.89	1.03
1:A:45:LYS:HZ1	1:A:46:PRO:CD	1.73	1.02
1:A:124:ASN:ND2	1:A:127[B]:LYS:HE3	1.76	1.00
1:A:45:LYS:NZ	1:A:45:LYS:CB	2.20	0.99
1:A:45:LYS:HB3	1:A:45:LYS:HZ2	0.81	0.97
1:A:130:ASP:OD2	1:A:133[B]:LYS:NZ	2.01	0.93
1:A:36:HIS:HD2	6:A:2197:HOH:O	1.57	0.88
1:A:261:LYS:O	1:A:261:LYS:HG3	1.66	0.85
1:A:124:ASN:HD21	1:A:127[B]:LYS:CE	1.94	0.80
5:A:1005:GOL:O1	5:A:1005:GOL:C2	2.32	0.78
1:A:36:HIS:CD2	6:A:2197:HOH:O	2.34	0.78
1:A:213:LYS:HE3	1:A:260:PHE:CE1	2.19	0.77
1:A:130:ASP:OD1	1:A:133[B]:LYS:NZ	2.22	0.72
1:A:162:ASP:OD1	6:A:2243:HOH:O	2.09	0.70
5:A:1006:GOL:C1	5:A:1006:GOL:O2	2.41	0.68
4:A:1003:SUA:S2	6:A:2235:HOH:O	2.53	0.66
1:A:45:LYS:CB	1:A:45:LYS:HZ3	2.09	0.65
1:A:7:TYR:O	6:A:2383:HOH:O	2.14	0.64
1:A:165:ASP:OD1	1:A:165:ASP:N	2.21	0.60
1:A:76:LYS:HE2	6:A:2247:HOH:O	2.02	0.59
1:A:162:ASP:CB	6:A:2243:HOH:O	2.51	0.58
1:A:168:LYS:NZ	1:A:228:LYS:O	2.37	0.58
1:A:213:LYS:HE3	1:A:260:PHE:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HB3	1:A:80:LYS:HG2	1.86	0.56
1:A:169:THR:OG1	1:A:172[B]:LYS:HD2	2.07	0.55
1:A:124:ASN:HD21	1:A:127[B]:LYS:NZ	2.06	0.54
5:A:1005:GOL:C1	5:A:1005:GOL:HO1	2.12	0.53
1:A:130:ASP:CG	1:A:133[B]:LYS:NZ	2.67	0.53
1:A:159:LYS:NZ	1:A:159:LYS:CD	2.64	0.53
1:A:162:ASP:HA	6:A:2243:HOH:O	2.08	0.52
1:A:45:LYS:HZ2	1:A:46:PRO:HD2	1.68	0.51
1:A:166:SER:O	1:A:172[A]:LYS:HE2	2.12	0.50
1:A:67:ASN:HD22	1:A:94:HIS:HB3	1.75	0.50
1:A:175:ASP:HB3	6:A:2420:HOH:O	2.12	0.48
1:A:162:ASP:CA	6:A:2243:HOH:O	2.60	0.48
5:A:1004:GOL:O1	5:A:1004:GOL:C3	2.63	0.46
1:A:159:LYS:HE3	6:A:2238:HOH:O	2.16	0.45
1:A:45:LYS:NZ	1:A:46:PRO:HD3	2.26	0.44
1:A:60:LEU:O	1:A:66:PHE:HA	2.18	0.44
1:A:92:GLN:HE21	4:A:1003:SUA:H92	1.83	0.44
1:A:92:GLN:HE21	4:A:1003:SUA:C9	2.30	0.43
1:A:92:GLN:HG2	4:A:1003:SUA:C9	2.49	0.42
1:A:92:GLN:HG2	4:A:1003:SUA:H91	2.01	0.42
1:A:6:GLY:O	1:A:12:GLY:HA2	2.20	0.41
5:A:1005:GOL:O1	5:A:1005:GOL:C3	2.68	0.41
1:A:124:ASN:CG	1:A:127[B]:LYS:HE3	2.41	0.41
1:A:168:LYS:NZ	6:A:2072:HOH:O	2.23	0.41
1:A:74:GLN:HE21	1:A:74:GLN:HB2	1.10	0.41
1:A:67:ASN:ND2	1:A:94:HIS:HB3	2.37	0.40

All (7) 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:1004:GOL:O1	6:A:2112:HOH:O[2_546]	1.13	1.07
5:A:1004:GOL:C1	6:A:2117:HOH:O[2_546]	1.39	0.81
1:A:130:ASP:CG	6:A:2208:HOH:O[1_565]	1.51	0.69
6:A:2084:HOH:O	6:A:2233:HOH:O[1_655]	1.65	0.55
1:A:130:ASP:OD2	6:A:2208:HOH:O[1_565]	1.66	0.54
1:A:130:ASP:CB	6:A:2208:HOH:O[1_565]	1.74	0.46
1:A:53:GLN:NE2	1:A:165:ASP:OD2[2_455]	2.09	0.11

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	266/260 (102%)	256 (96%)	10 (4%)	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	233/225 (104%)	221 (95%)	12 (5%)	21	1

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	45	LYS
1	A	53	GLN
1	A	74	GLN
1	A	75	ASP
1	A	80	LYS
1	A	92	GLN
1	A	162	ASP
1	A	165	ASP
1	A	175	ASP
1	A	213	LYS
1	A	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	36	HIS
1	A	53	GLN
1	A	67	ASN
1	A	74	GLN
1	A	137	GLN
1	A	249	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HGB	A	265[B]	6,1	0,1,11	-	-	-		
4	SUA	A	1003	3	22,22,22	6.61	6 (27%)	30,30,30	3.28	9 (30%)
5	GOL	A	1005	-	5,5,5	3.54	2 (40%)	5,5,5	2.72	3 (60%)
5	GOL	A	1006	-	5,5,5	5.27	2 (40%)	5,5,5	3.30	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	A	1004	-	5,5,5	5.47	4 (80%)	5,5,5	2.88	1 (20%)
2	HGB	A	265[A]	6,1	7,10,11	1.93	1 (14%)	11,13,14	2.35	5 (45%)

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	SUA	A	1003	3	-	4/16/16/16	0/2/2/2
5	GOL	A	1005	-	-	0/4/4/4	-
5	GOL	A	1006	-	-	2/4/4/4	-
5	GOL	A	1004	-	-	2/4/4/4	-
2	HGB	A	265[A]	6,1	-	0/4/4/6	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1003	SUA	C7-N2	-28.95	1.11	1.34
5	A	1006	GOL	C1-C2	11.41	1.95	1.51
5	A	1004	GOL	O1-C1	8.43	1.77	1.42
5	A	1004	GOL	C3-C2	-6.79	1.25	1.51
4	A	1003	SUA	O3-C7	6.51	1.41	1.33
5	A	1005	GOL	O1-C1	6.41	1.69	1.42
4	A	1003	SUA	C13-C10	5.05	1.46	1.36
4	A	1003	SUA	C7-S2	4.55	1.74	1.66
5	A	1004	GOL	O2-C2	4.38	1.56	1.43
2	A	265[A]	HGB	C2-C1	4.07	1.58	1.49
5	A	1005	GOL	O3-C3	3.80	1.58	1.42
5	A	1004	GOL	O3-C3	-3.52	1.27	1.42
4	A	1003	SUA	C6-N2	-3.10	1.35	1.41
5	A	1006	GOL	O1-C1	-2.14	1.33	1.42
4	A	1003	SUA	C9-C8	2.03	1.57	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	SUA	C8-O3-C7	-9.37	111.70	119.04
4	A	1003	SUA	O3-C7-N2	9.15	130.07	112.20
4	A	1003	SUA	O3-C7-S2	-8.19	118.48	125.07
5	A	1004	GOL	O2-C2-C3	6.09	134.39	109.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1003	SUA	S2-C7-N2	-5.48	111.45	122.94
5	A	1006	GOL	O2-C2-C3	5.26	130.97	109.18
5	A	1006	GOL	O2-C2-C1	-4.53	90.43	109.18
5	A	1005	GOL	O1-C1-C2	-4.39	90.62	110.38
2	A	265[A]	HGB	O2-C1-C2	-4.37	110.01	121.46
2	A	265[A]	HGB	C6-C4-C2	-3.20	117.38	120.80
4	A	1003	SUA	O3-C8-C9	-2.91	101.52	108.39
5	A	1005	GOL	O3-C3-C2	-2.89	97.37	110.38
4	A	1003	SUA	C6-N2-C7	2.86	135.00	130.07
2	A	265[A]	HGB	C4-C6-C7	2.60	126.52	121.53
5	A	1005	GOL	C3-C2-C1	2.50	120.97	111.80
2	A	265[A]	HGB	O1-C1-O2	2.47	128.67	123.35
2	A	265[A]	HGB	O1-C1-C2	2.43	121.07	114.84
4	A	1003	SUA	O1-S1-N1	2.31	110.69	107.35
4	A	1003	SUA	C9-C10-C13	-2.23	122.02	125.43
4	A	1003	SUA	O2-S1-N1	2.19	110.51	107.35
5	A	1006	GOL	C3-C2-C1	2.16	119.73	111.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1003	SUA	C13-C10-C9-C8
5	A	1006	GOL	C1-C2-C3-O3
5	A	1004	GOL	O1-C1-C2-C3
5	A	1006	GOL	O2-C2-C3-O3
4	A	1003	SUA	C11-C10-C9-C8
5	A	1004	GOL	O2-C2-C3-O3
4	A	1003	SUA	C4-C3-S1-O2
4	A	1003	SUA	C2-C3-S1-O2

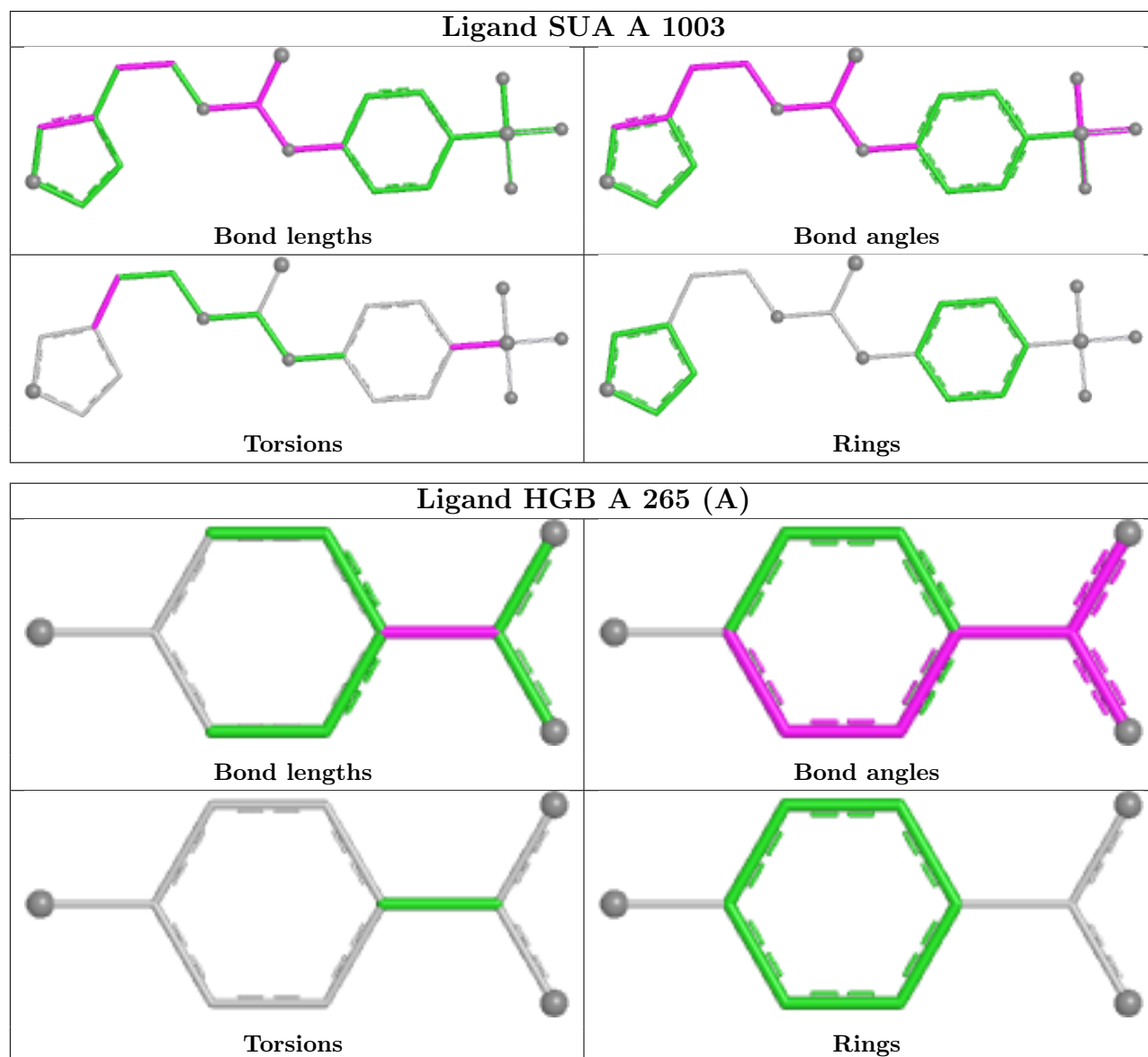
There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1003	SUA	5	0
5	A	1005	GOL	4	0
5	A	1006	GOL	2	0
5	A	1004	GOL	2	2

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 ⓘ

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	258/260 (99%)	0.16	11 (4%) 40 38	6, 12, 26, 44	10 (3%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	ASN	3.6
1	A	3	HIS	3.5
1	A	45	LYS	2.8
1	A	175	ASP	2.7
1	A	4	HIS	2.7
1	A	235	GLY	2.5
1	A	165	ASP	2.5
1	A	75	ASP	2.4
1	A	163	VAL	2.1
1	A	261	LYS	2.1
1	A	237	PRO	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.

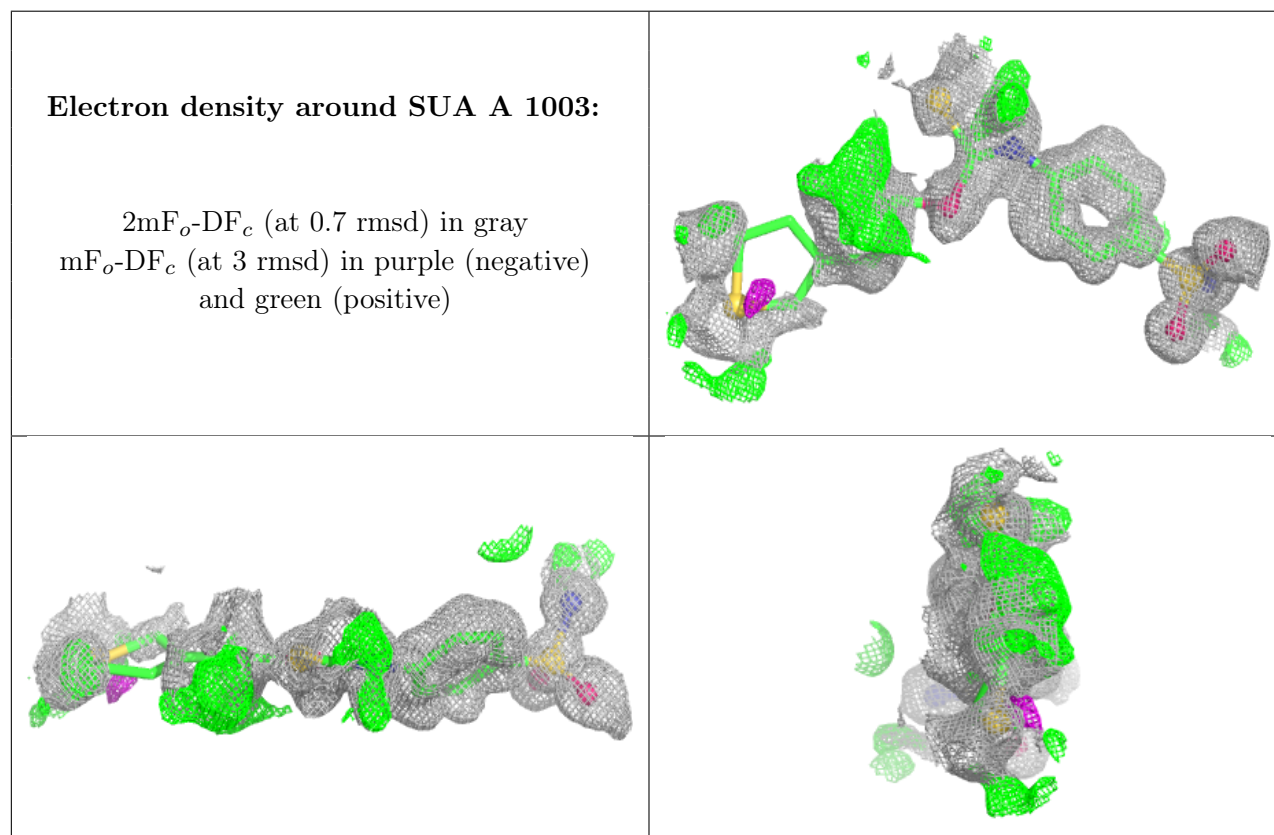
6.4 Ligands [i](#)

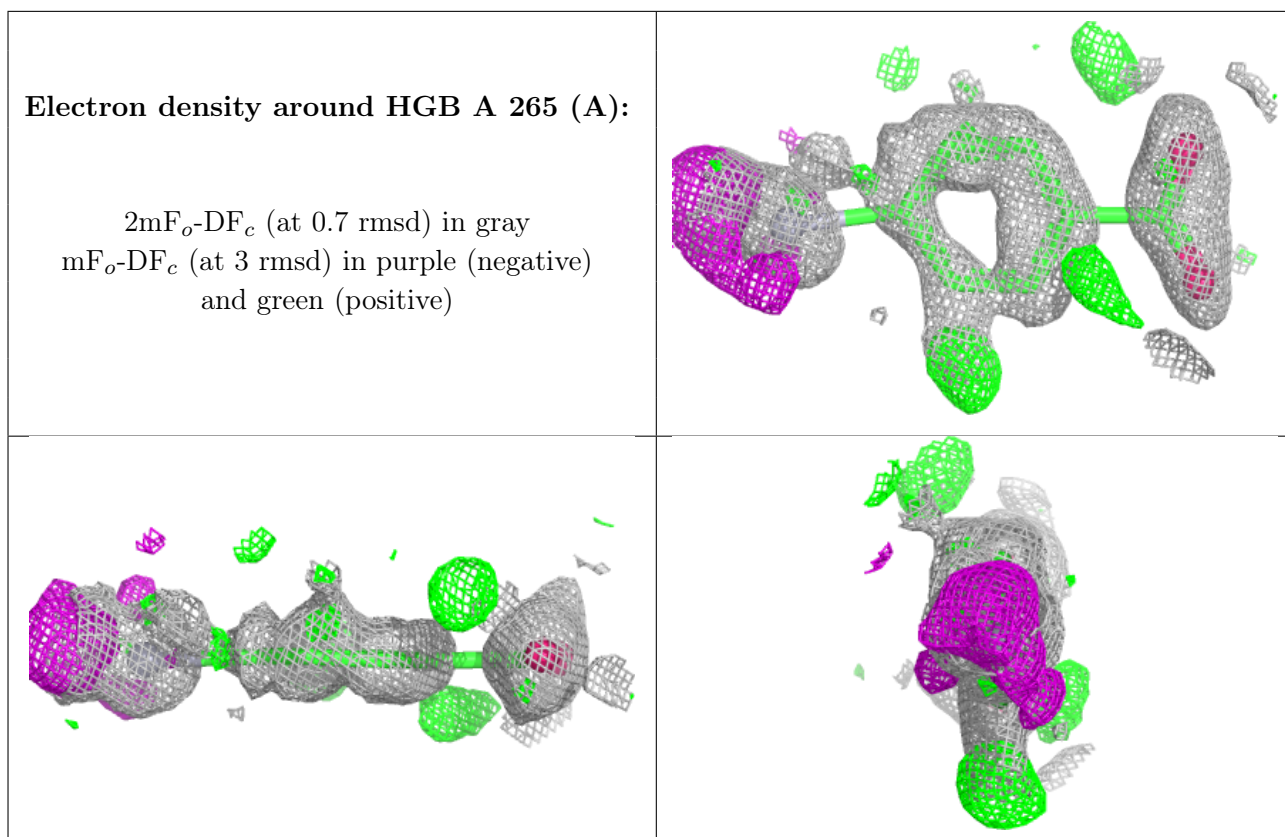
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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
5	GOL	A	1006	6/6	0.92	0.12	15,24,29,39	0
5	GOL	A	1005	6/6	0.93	0.10	21,26,28,28	0
5	GOL	A	1004	6/6	0.93	0.09	21,24,43,57	0
4	SUA	A	1003	21/21	0.98	0.11	6,14,40,59	10
2	HGB	A	265[B]	2/11	1.00	0.05	7,7,7,9	2
3	ZN	A	1002	1/1	1.00	0.01	5,5,5,5	0
2	HGB	A	265[A]	10/11	1.00	0.05	8,13,15,19	10

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.