



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 5, 2024 – 01:20 am GMT

PDB ID : 5FL5
Title : Three dimensional structure of human carbonic anhydrase IX in complex with 5-(1-(4-Methoxyphenyl)-1H-1,2,3-triazol-4-yl)thiophene-2- sulfonamide
Authors : Leitans, J.; Tars, K.; Zalubovskis, R.
Deposited on : 2015-10-21
Resolution : 2.05 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

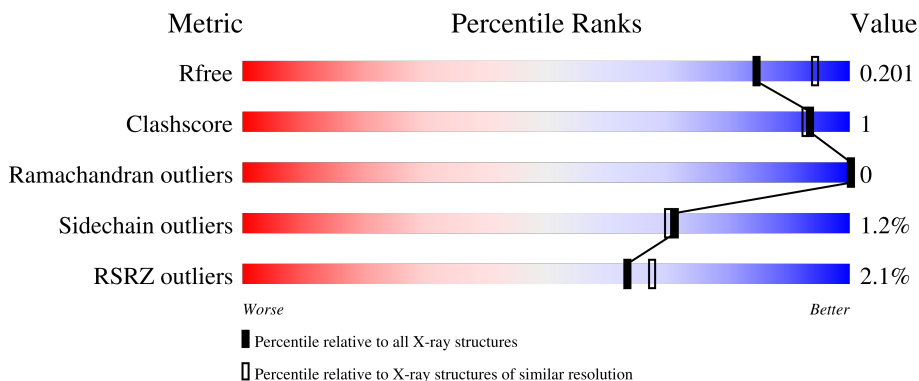
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	257	 94%
1	B	257	 93%
1	C	257	 91%
1	D	257	 93%

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
6	TRS	B	1267	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 8842 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.

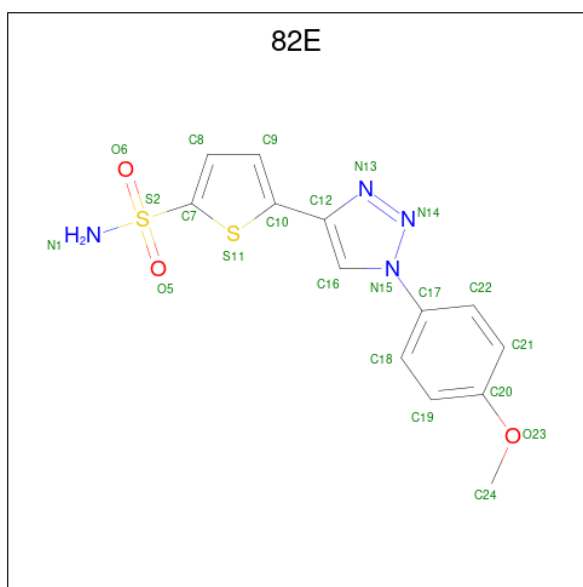
- Molecule 1 is a protein called CARBONIC ANHYDRASE IX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	251	Total 1941	C 1237	N 346	O 354	S 4	0	0	0
1	B	251	Total 1915	C 1223	N 336	O 352	S 4	0	0	0
1	C	251	Total 1919	C 1225	N 336	O 354	S 4	0	0	0
1	D	251	Total 1931	C 1232	N 343	O 352	S 4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP Q16790
A	4	PRO	-	expression tag	UNP Q16790
A	42	SER	CYS	engineered mutation	UNP Q16790
B	3	GLY	-	expression tag	UNP Q16790
B	4	PRO	-	expression tag	UNP Q16790
B	42	SER	CYS	engineered mutation	UNP Q16790
C	3	GLY	-	expression tag	UNP Q16790
C	4	PRO	-	expression tag	UNP Q16790
C	42	SER	CYS	engineered mutation	UNP Q16790
D	3	GLY	-	expression tag	UNP Q16790
D	4	PRO	-	expression tag	UNP Q16790
D	42	SER	CYS	engineered mutation	UNP Q16790

- Molecule 2 is 5-[1-(4-methoxyphenyl)-1,2,3-triazol-4-yl]thiophene-2-sulfonamide (three-letter code: 82E) (formula: C₁₃H₁₂N₄O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	Total	C	N	O	S	0	0
			22	13	4	3	2		
2	B	1	Total	C	N	O	S	0	0
			22	13	4	3	2		
2	C	1	Total	C	N	O	S	0	0
			22	13	4	3	2		
2	D	1	Total	C	N	O	S	0	0
			22	13	4	3	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

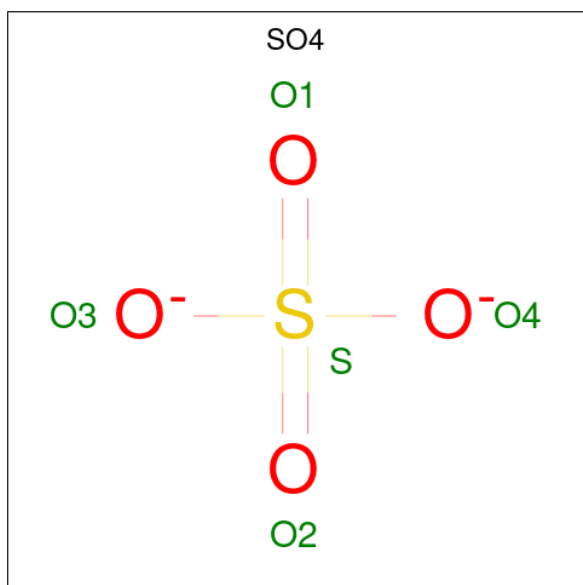
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



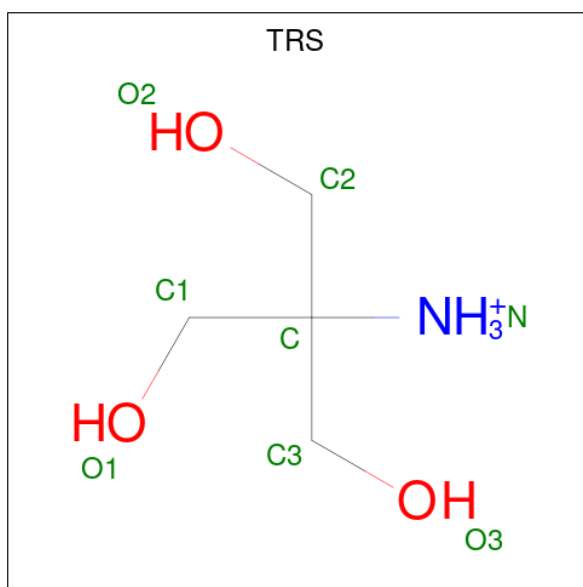
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C₄H₁₂NO₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	A	1	8	4	1	3	0	0
6	B	1	8	4	1	3	0	0
6	D	1	8	4	1	3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	290	290	290	0	0
7	B	250	250	250	0	0
7	C	180	180	180	0	0
7	D	181	181	181	0	0

3 Residue-property plots [i](#)

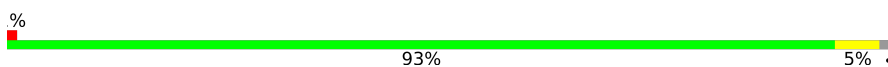
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

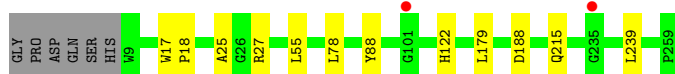
- Molecule 1: CARBONIC ANHYDRASE IX

Chain A: 



- Molecule 1: CARBONIC ANHYDRASE IX

Chain B: 

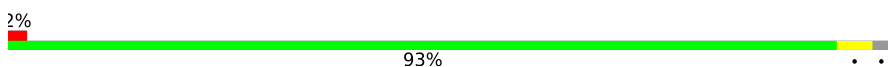


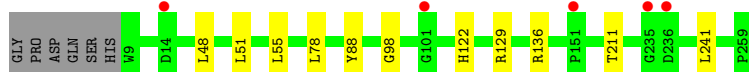
- Molecule 1: CARBONIC ANHYDRASE IX

Chain C: 



- Molecule 1: CARBONIC ANHYDRASE IX

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	152.38Å 152.38Å 170.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.10 – 2.05 38.10 – 2.05	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.10-2.05) 100.0 (38.10-2.05)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.158 , 0.196 0.167 , 0.201	Depositor DCC
R_{free} test set	4640 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtrriage
Anisotropy	0.004	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.022 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8842	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, GOL, TRS, 82E

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	0/1999	0.76	3/2730 (0.1%)
1	B	0.53	0/1973	0.72	0/2700
1	C	0.51	0/1977	0.70	0/2705
1	D	0.49	0/1989	0.68	1/2718 (0.0%)
All	All	0.52	0/7938	0.72	4/10853 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ARG	NE-CZ-NH2	-9.72	115.44	120.30
1	A	62	ARG	NE-CZ-NH1	7.76	124.18	120.30
1	A	86	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	136	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1941	0	1893	3	1
1	B	1915	0	1845	7	0
1	C	1919	0	1849	8	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1931	0	1878	4	0
2	A	22	0	11	0	0
2	B	22	0	11	0	0
2	C	22	0	12	1	0
2	D	22	0	11	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	8	0	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	0	0
5	A	40	0	0	0	0
5	B	25	0	0	1	0
5	C	15	0	0	0	0
5	D	15	0	0	0	0
6	A	8	0	12	0	0
6	B	8	0	12	1	0
6	D	8	0	12	0	0
7	A	290	0	0	0	0
7	B	250	0	0	0	0
7	C	180	0	0	1	0
7	D	181	0	0	0	0
All	All	8842	0	7578	22	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 1.

All (22) 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:C:55:LEU:HD21	1:C:78:LEU:HD11	1.85	0.59
1:A:55:LEU:HD21	1:A:78:LEU:HD11	1.86	0.57
1:D:55:LEU:HD21	1:D:78:LEU:HD11	1.88	0.55
1:B:18:PRO:HB3	1:B:25:ALA:HB2	1.89	0.54
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.91	0.52
1:B:17:TRP:CD2	6:B:1267:TRS:H21	2.47	0.49
1:B:27:ARG:N	5:B:1264:SO4:O2	2.40	0.48
1:C:94:HIS:C	1:C:95:LEU:HD12	2.34	0.48
1:B:55:LEU:HD21	1:B:78:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:H	1:B:215:GLN:HE22	1.62	0.46
1:D:98:GLY:HA2	1:D:241:LEU:HD23	1.98	0.45
1:D:88:TYR:HB3	1:D:122:HIS:HB3	1.98	0.45
1:C:88:TYR:HB3	1:C:122:HIS:HB3	1.99	0.45
1:C:134:LEU:HD11	2:C:265:82E:C21	2.47	0.44
1:B:88:TYR:HB3	1:B:122:HIS:HB3	2.00	0.43
1:C:150:GLY:HA3	1:C:218:MET:HG3	2.00	0.43
1:C:49:GLU:O	1:C:80:MET:HA	2.20	0.42
1:D:48:LEU:HD11	1:D:211:THR:HG21	2.01	0.42
1:A:48:LEU:HD21	1:A:211:THR:HG21	2.02	0.41
1:C:157:TYR:CE1	1:C:217:VAL:HG11	2.56	0.41
1:B:188:ASP:N	1:B:215:GLN:HE22	2.18	0.41
1:C:158:GLU:HB3	7:C:2121:HOH:O	2.21	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)
1:A:62:ARG:NH2	1:C:134:LEU:O[5_455]	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	249/257 (97%)	246 (99%)	3 (1%)	0	100	100
1	B	249/257 (97%)	243 (98%)	6 (2%)	0	100	100
1	C	249/257 (97%)	244 (98%)	5 (2%)	0	100	100
1	D	249/257 (97%)	241 (97%)	8 (3%)	0	100	100
All	All	996/1028 (97%)	974 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	203/210 (97%)	201 (99%)	2 (1%)	76	75
1	B	198/210 (94%)	196 (99%)	2 (1%)	76	75
1	C	199/210 (95%)	195 (98%)	4 (2%)	55	50
1	D	201/210 (96%)	199 (99%)	2 (1%)	76	75
All	All	801/840 (95%)	791 (99%)	10 (1%)	71	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	LEU
1	A	239	LEU
1	B	179	LEU
1	B	239	LEU
1	C	46	ARG
1	C	179	LEU
1	C	218	MET
1	C	239	LEU
1	D	51	LEU
1	D	129	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	68	HIS
1	A	71	GLN
1	A	159	GLN
1	B	37	GLN
1	B	71	GLN
1	B	215	GLN
1	C	37	GLN
1	C	71	GLN

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Mol	Chain	Res	Type
1	C	159	GLN
1	D	54	GLN
1	D	71	GLN
1	D	159	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 4 are monoatomic - leaving 30 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	$\# Z > 2$
5	SO4	A	1268	-	4,4,4	0.48	0	6,6,6	0.33	0
4	GOL	B	1261	-	5,5,5	0.32	0	5,5,5	0.53	0
5	SO4	B	1266	-	4,4,4	0.45	0	6,6,6	0.55	0
6	TRS	A	1270	-	7,7,7	0.36	0	9,9,9	0.52	0
5	SO4	C	1262	-	4,4,4	0.31	0	6,6,6	0.55	0
5	SO4	A	1269	-	4,4,4	0.36	0	6,6,6	0.44	0
5	SO4	C	1264	-	4,4,4	0.39	0	6,6,6	0.53	0
2	82E	B	267	3	20,24,24	2.17	5 (25%)	19,35,35	3.41	12 (63%)
5	SO4	C	1263	-	4,4,4	0.46	0	6,6,6	0.60	0
5	SO4	B	1264	-	4,4,4	0.31	0	6,6,6	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	D	1263	-	4,4,4	0.48	0	6,6,6	0.35	0
4	GOL	A	1261	-	5,5,5	0.22	0	5,5,5	0.71	0
5	SO4	A	1267	-	4,4,4	0.31	0	6,6,6	0.36	0
5	SO4	A	1263	-	4,4,4	0.20	0	6,6,6	0.37	0
2	82E	D	269	3	20,24,24	1.96	4 (20%)	19,35,35	2.70	9 (47%)
5	SO4	A	1266	-	4,4,4	0.51	0	6,6,6	0.76	0
5	SO4	B	1262	-	4,4,4	0.39	0	6,6,6	0.11	0
5	SO4	B	1263	-	4,4,4	0.38	0	6,6,6	0.44	0
4	GOL	C	1261	-	5,5,5	0.33	0	5,5,5	0.73	0
5	SO4	A	1265	-	4,4,4	0.37	0	6,6,6	0.37	0
2	82E	A	266	3	20,24,24	1.88	3 (15%)	19,35,35	2.67	10 (52%)
4	GOL	D	1261	-	5,5,5	0.25	0	5,5,5	0.52	0
5	SO4	D	1262	-	4,4,4	0.35	0	6,6,6	0.52	0
6	TRS	D	1265	-	7,7,7	0.30	0	9,9,9	0.46	0
5	SO4	D	1264	-	4,4,4	0.35	0	6,6,6	0.67	0
5	SO4	A	1262	-	4,4,4	0.37	0	6,6,6	0.35	0
2	82E	C	265	3	20,24,24	2.06	4 (20%)	19,35,35	3.25	11 (57%)
6	TRS	B	1267	-	7,7,7	0.61	0	9,9,9	3.07	6 (66%)
5	SO4	A	1264	-	4,4,4	0.57	0	6,6,6	0.20	0
5	SO4	B	1265	-	4,4,4	0.49	0	6,6,6	0.62	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	82E	B	267	3	-	4/6/16/16	0/3/3/3
2	82E	A	266	3	-	2/6/16/16	0/3/3/3
4	GOL	D	1261	-	-	2/4/4/4	-
4	GOL	B	1261	-	-	2/4/4/4	-
6	TRS	D	1265	-	-	1/9/9/9	-
4	GOL	A	1261	-	-	2/4/4/4	-
2	82E	C	265	3	-	4/6/16/16	0/3/3/3
6	TRS	A	1270	-	-	1/9/9/9	-
6	TRS	B	1267	-	-	4/9/9/9	-
4	GOL	C	1261	-	-	2/4/4/4	-
2	82E	D	269	3	-	2/6/16/16	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	265	82E	C7-S2	-6.58	1.66	1.76
2	B	267	82E	C7-S2	-6.57	1.66	1.76
2	A	266	82E	C7-S2	-6.36	1.66	1.76
2	D	269	82E	C7-S2	-6.00	1.67	1.76
2	B	267	82E	N13-N14	4.93	1.43	1.34
2	C	265	82E	N13-N14	4.18	1.41	1.34
2	D	269	82E	N13-N14	3.91	1.41	1.34
2	A	266	82E	C17-N15	-3.15	1.35	1.44
2	A	266	82E	N13-N14	3.05	1.39	1.34
2	D	269	82E	C17-N15	-2.78	1.36	1.44
2	C	265	82E	C17-N15	-2.66	1.36	1.44
2	B	267	82E	N14-N15	2.48	1.40	1.37
2	D	269	82E	N14-N15	2.45	1.40	1.37
2	B	267	82E	C17-N15	-2.42	1.37	1.44
2	C	265	82E	N14-N15	2.25	1.40	1.37
2	B	267	82E	C18-C17	2.18	1.42	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	265	82E	O6-S2-O5	-6.05	108.81	118.76
2	C	265	82E	C22-C17-N15	5.94	124.34	119.15
2	B	267	82E	O5-S2-N1	5.63	115.71	107.36
2	A	266	82E	O6-S2-O5	-5.61	109.54	118.76
2	B	267	82E	C22-C17-C18	-5.55	113.11	121.33
2	B	267	82E	C22-C17-N15	5.23	123.72	119.15
2	C	265	82E	C22-C17-C18	-5.17	113.67	121.33
6	B	1267	TRS	C3-C-N	-4.90	93.34	107.98
2	B	267	82E	O6-S2-O5	-4.90	110.70	118.76
2	B	267	82E	O6-S2-C7	-4.89	100.12	107.29
2	D	269	82E	C22-C17-N15	4.83	123.37	119.15
2	A	266	82E	C22-C17-N15	4.80	123.35	119.15
2	C	265	82E	O6-S2-N1	4.78	114.45	107.36
2	D	269	82E	C22-C17-C18	-4.68	114.40	121.33
2	B	267	82E	C18-C17-N15	4.50	123.09	119.15
6	B	1267	TRS	C2-C-N	-4.44	94.71	107.98
2	D	269	82E	O6-S2-O5	-4.40	111.52	118.76
2	A	266	82E	C22-C17-C18	-4.16	115.17	121.33
2	A	266	82E	O5-S2-N1	4.01	113.31	107.36
6	B	1267	TRS	C1-C-N	-3.80	96.64	107.98
2	C	265	82E	O5-S2-N1	-3.69	101.90	107.36
2	D	269	82E	O6-S2-C7	-3.59	102.02	107.29
2	D	269	82E	O5-S2-C7	3.57	112.53	107.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	267	82E	C19-C18-C17	3.54	124.22	119.07
6	B	1267	TRS	C2-C-C1	3.49	121.62	110.81
2	B	267	82E	C24-O23-C20	3.45	124.99	117.51
2	C	265	82E	C24-O23-C20	3.38	124.85	117.51
2	B	267	82E	C21-C22-C17	3.36	123.96	119.07
2	D	269	82E	C18-C17-N15	3.33	122.06	119.15
2	C	265	82E	C19-C18-C17	3.29	123.85	119.07
2	D	269	82E	C19-C18-C17	3.27	123.83	119.07
2	B	267	82E	C17-N15-N14	3.26	123.81	117.19
2	C	265	82E	C18-C17-N15	3.24	121.98	119.15
2	A	266	82E	O5-S2-C7	3.22	112.01	107.29
2	C	265	82E	C21-C22-C17	3.05	123.50	119.07
2	A	266	82E	C19-C18-C17	2.90	123.28	119.07
2	D	269	82E	C24-O23-C20	2.72	123.42	117.51
2	A	266	82E	C18-C17-N15	2.59	121.42	119.15
2	C	265	82E	O6-S2-C7	2.55	111.02	107.29
2	A	266	82E	C24-O23-C20	2.52	122.98	117.51
2	A	266	82E	C21-C22-C17	2.46	122.64	119.07
6	B	1267	TRS	C3-C-C1	2.44	118.37	110.81
2	D	269	82E	C21-C22-C17	2.41	122.57	119.07
2	B	267	82E	C7-S2-N1	2.36	112.63	108.28
6	B	1267	TRS	C3-C-C2	2.26	117.83	110.81
2	A	266	82E	O6-S2-C7	-2.23	104.01	107.29
2	B	267	82E	C10-C12-N13	2.21	124.54	120.88
2	C	265	82E	C17-N15-N14	2.14	121.53	117.19

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	266	82E	C22-C17-N15-C16
4	B	1261	GOL	C1-C2-C3-O3
4	C	1261	GOL	C1-C2-C3-O3
4	D	1261	GOL	C1-C2-C3-O3
4	D	1261	GOL	O2-C2-C3-O3
2	A	266	82E	C18-C17-N15-C16
2	D	269	82E	C18-C17-N15-C16
4	B	1261	GOL	O2-C2-C3-O3
4	C	1261	GOL	O2-C2-C3-O3
6	B	1267	TRS	C1-C-C2-O2
6	B	1267	TRS	C1-C-C3-O3
2	B	267	82E	C18-C17-N15-N14

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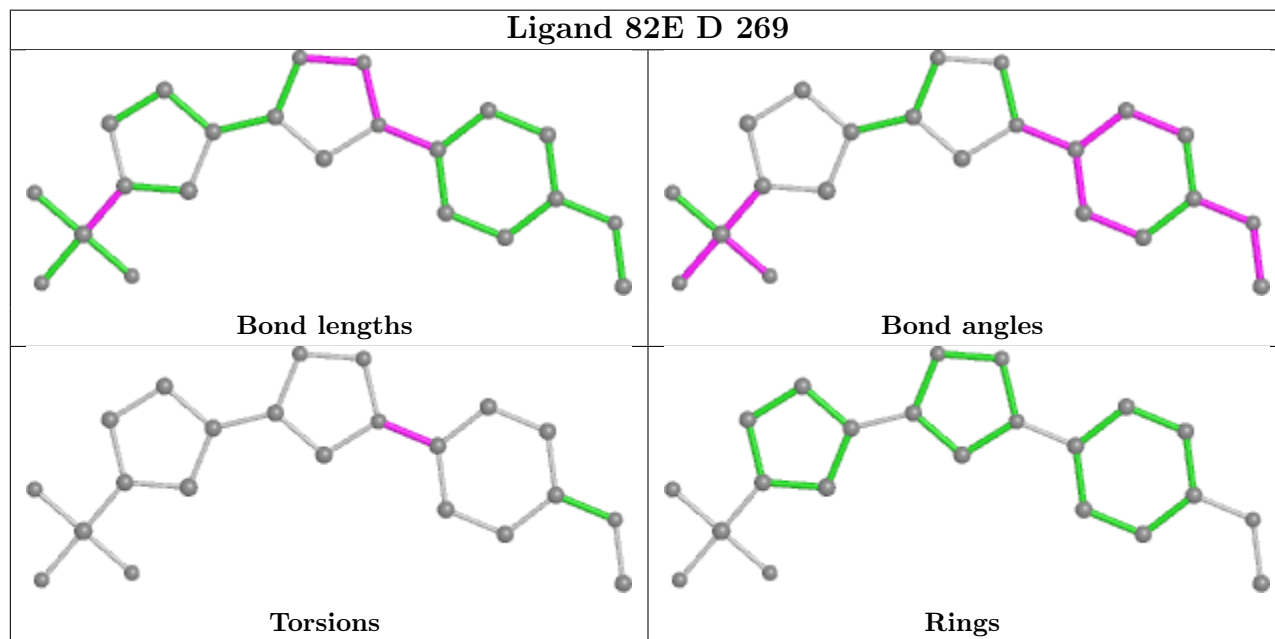
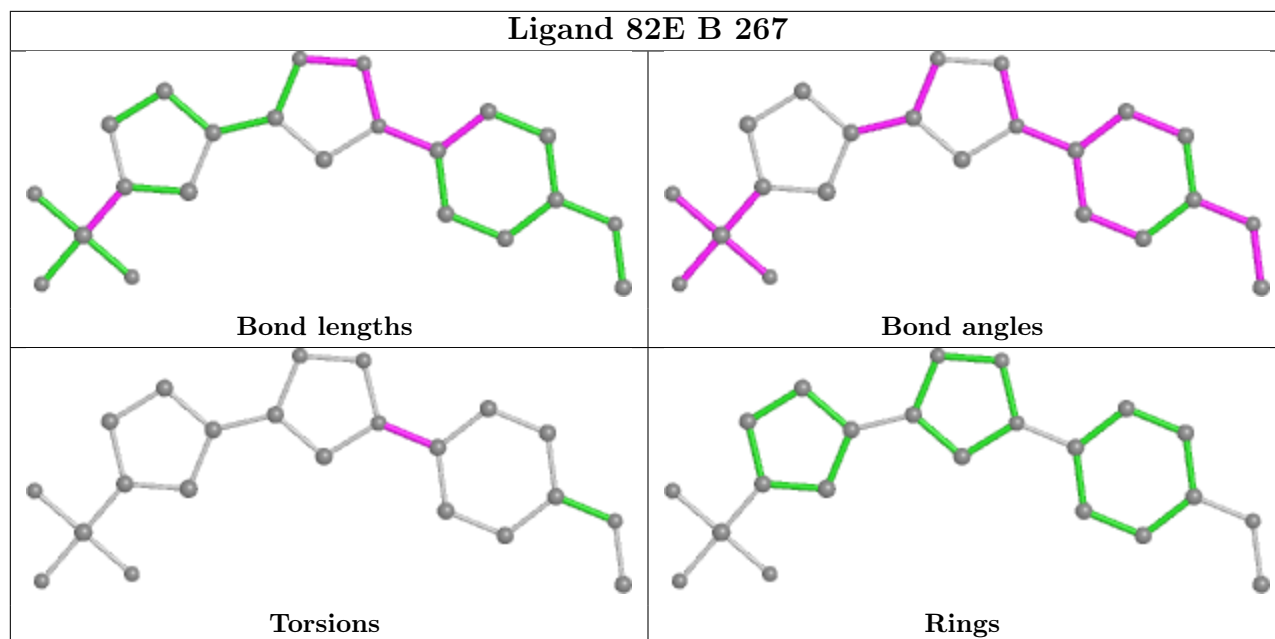
Mol	Chain	Res	Type	Atoms
2	B	267	82E	C22-C17-N15-N14
2	C	265	82E	C18-C17-N15-N14
2	C	265	82E	C22-C17-N15-N14
2	D	269	82E	C22-C17-N15-C16
2	B	267	82E	C22-C17-N15-C16
6	B	1267	TRS	C2-C-C1-O1
6	B	1267	TRS	C3-C-C1-O1
4	A	1261	GOL	O2-C2-C3-O3
4	A	1261	GOL	C1-C2-C3-O3
6	A	1270	TRS	C2-C-C1-O1
6	D	1265	TRS	C2-C-C1-O1
2	B	267	82E	C18-C17-N15-C16
2	C	265	82E	C18-C17-N15-C16
2	C	265	82E	C22-C17-N15-C16

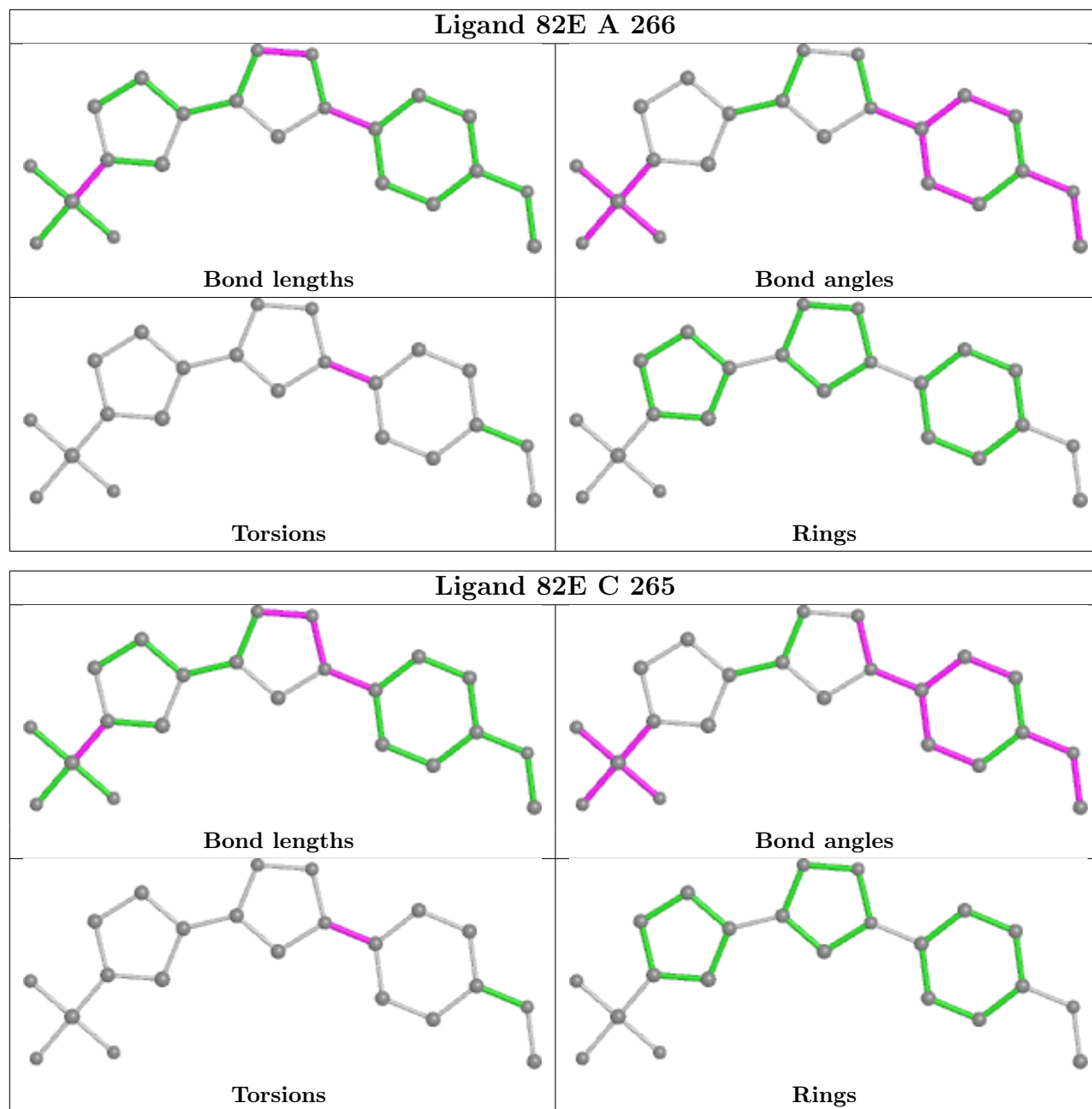
There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1264	SO4	1	0
2	C	265	82E	1	0
6	B	1267	TRS	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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	251/257 (97%)	-0.69	2 (0%) 86 88	13, 19, 39, 55	0
1	B	251/257 (97%)	-0.59	2 (0%) 86 88	14, 22, 41, 54	0
1	C	251/257 (97%)	-0.28	12 (4%) 30 33	16, 26, 50, 68	0
1	D	251/257 (97%)	-0.47	5 (1%) 65 69	16, 27, 46, 64	0
All	All	1004/1028 (97%)	-0.51	21 (2%) 63 67	13, 23, 44, 68	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	235	GLY	4.3
1	C	235	GLY	4.2
1	A	235	GLY	4.0
1	C	15	PRO	3.9
1	C	16	PRO	3.8
1	C	20	VAL	3.6
1	C	14	ASP	3.5
1	C	236	ASP	3.3
1	A	236	ASP	3.1
1	D	101	GLY	2.8
1	C	101	GLY	2.8
1	C	37	GLN	2.8
1	C	13	GLY	2.7
1	C	12	GLY	2.7
1	B	101	GLY	2.6
1	D	151	PRO	2.6
1	D	236	ASP	2.4
1	B	235	GLY	2.3
1	C	237	SER	2.2
1	C	232	TRP	2.2
1	D	14	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

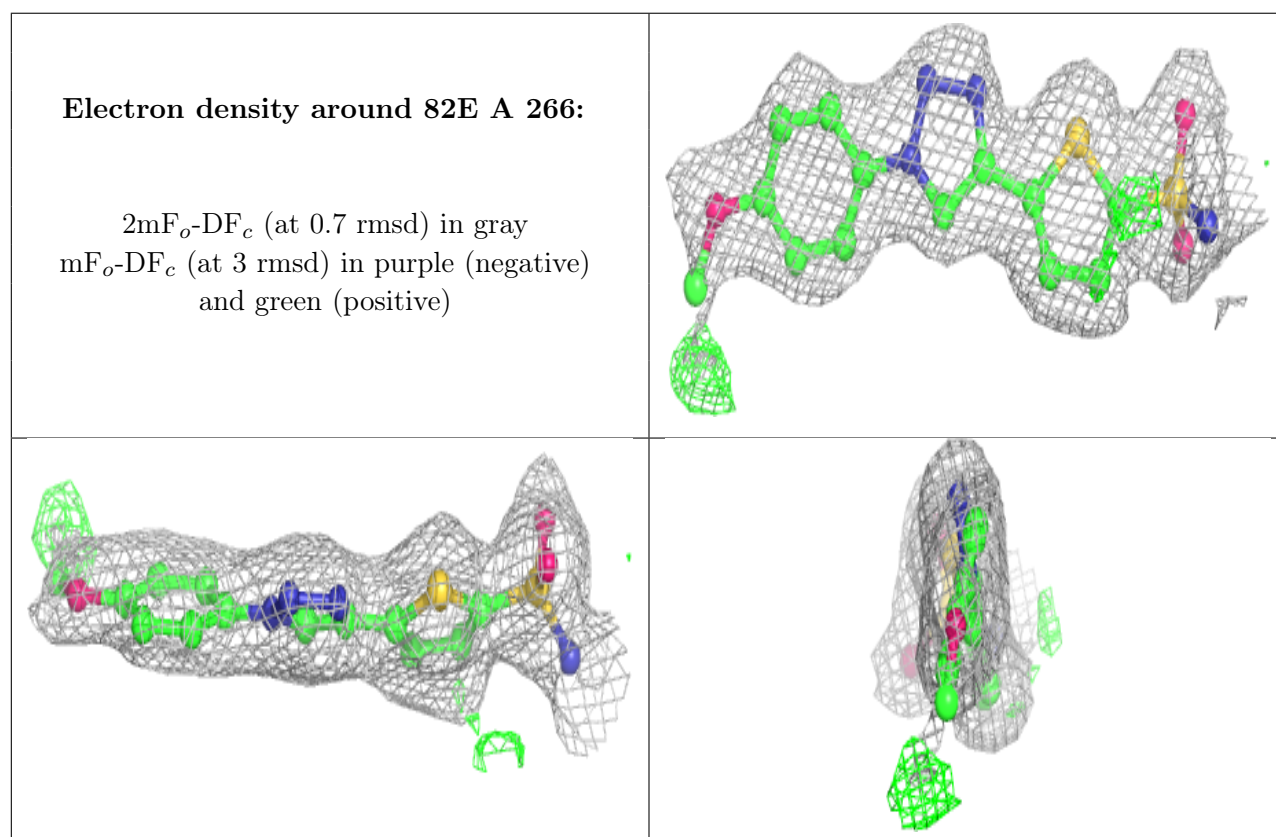
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	C	1264	5/5	0.67	0.30	63,80,88,88	0
5	SO4	A	1266	5/5	0.69	0.27	56,58,74,76	0
5	SO4	A	1265	5/5	0.78	0.19	80,82,91,93	0
5	SO4	C	1263	5/5	0.79	0.17	57,61,69,70	0
5	SO4	B	1265	5/5	0.80	0.25	47,64,65,74	0
5	SO4	A	1267	5/5	0.80	0.21	61,69,82,88	0
5	SO4	A	1269	5/5	0.80	0.24	60,71,82,83	0
5	SO4	B	1266	5/5	0.84	0.25	65,73,83,84	0
5	SO4	A	1268	5/5	0.85	0.18	70,74,79,83	0
4	GOL	D	1261	6/6	0.87	0.15	48,53,56,59	0
4	GOL	C	1261	6/6	0.88	0.20	41,47,50,55	0
5	SO4	D	1264	5/5	0.88	0.21	63,77,81,83	0
5	SO4	D	1263	5/5	0.91	0.19	48,53,61,61	0
4	GOL	A	1261	6/6	0.91	0.13	40,42,46,52	0
6	TRS	A	1270	8/8	0.91	0.14	28,32,35,35	0
4	GOL	B	1261	6/6	0.93	0.11	41,47,50,53	0
6	TRS	B	1267	8/8	0.95	0.09	22,23,23,24	0
6	TRS	D	1265	8/8	0.95	0.12	33,37,38,40	0
5	SO4	C	1262	5/5	0.96	0.12	42,43,44,49	0
2	82E	A	266	22/22	0.98	0.09	19,29,43,50	0
2	82E	B	267	22/22	0.98	0.11	17,35,50,55	0
2	82E	C	265	22/22	0.98	0.09	22,40,51,56	0
5	SO4	B	1262	5/5	0.98	0.12	41,42,44,45	0
5	SO4	B	1264	5/5	0.98	0.21	38,52,52,54	0
5	SO4	B	1263	5/5	0.99	0.06	22,24,24,25	0
5	SO4	D	1262	5/5	0.99	0.06	27,28,29,29	0
3	ZN	C	1260	1/1	0.99	0.08	20,20,20,20	0

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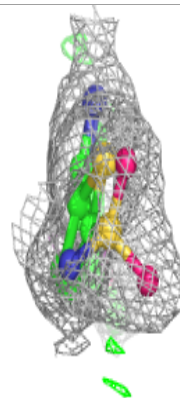
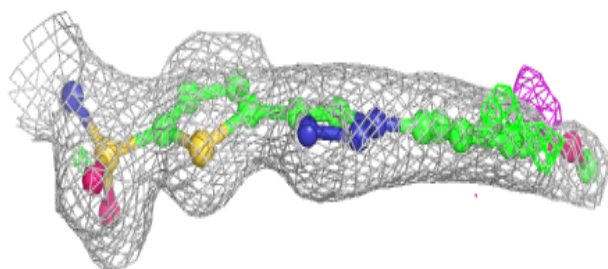
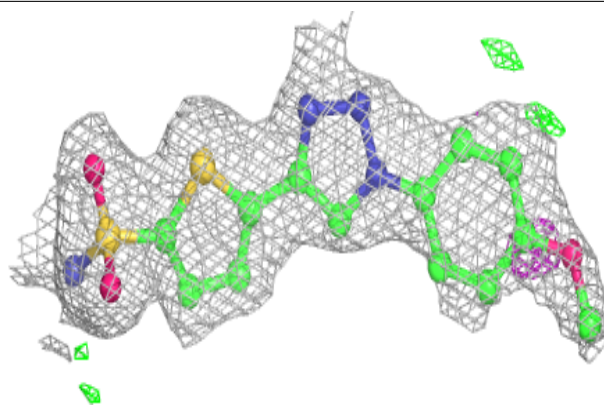
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	SO4	A	1262	5/5	0.99	0.07	34,36,40,42	0
5	SO4	A	1263	5/5	0.99	0.07	28,28,30,30	0
5	SO4	A	1264	5/5	0.99	0.07	20,20,23,23	0
2	82E	D	269	22/22	0.99	0.08	18,31,43,50	0
3	ZN	D	1260	1/1	1.00	0.08	19,19,19,19	0
3	ZN	B	1260	1/1	1.00	0.09	16,16,16,16	0
3	ZN	A	1260	1/1	1.00	0.07	15,15,15,15	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.

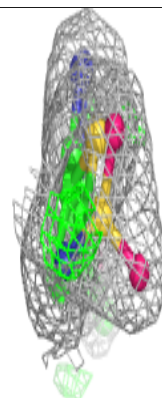
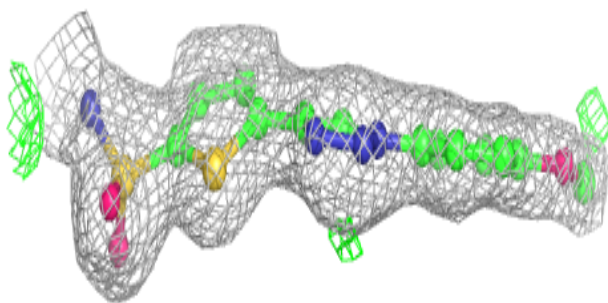
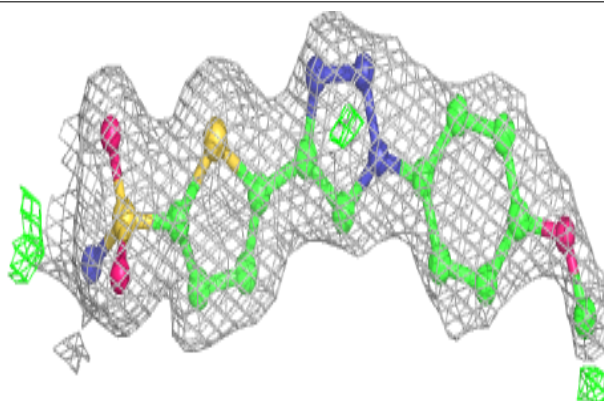


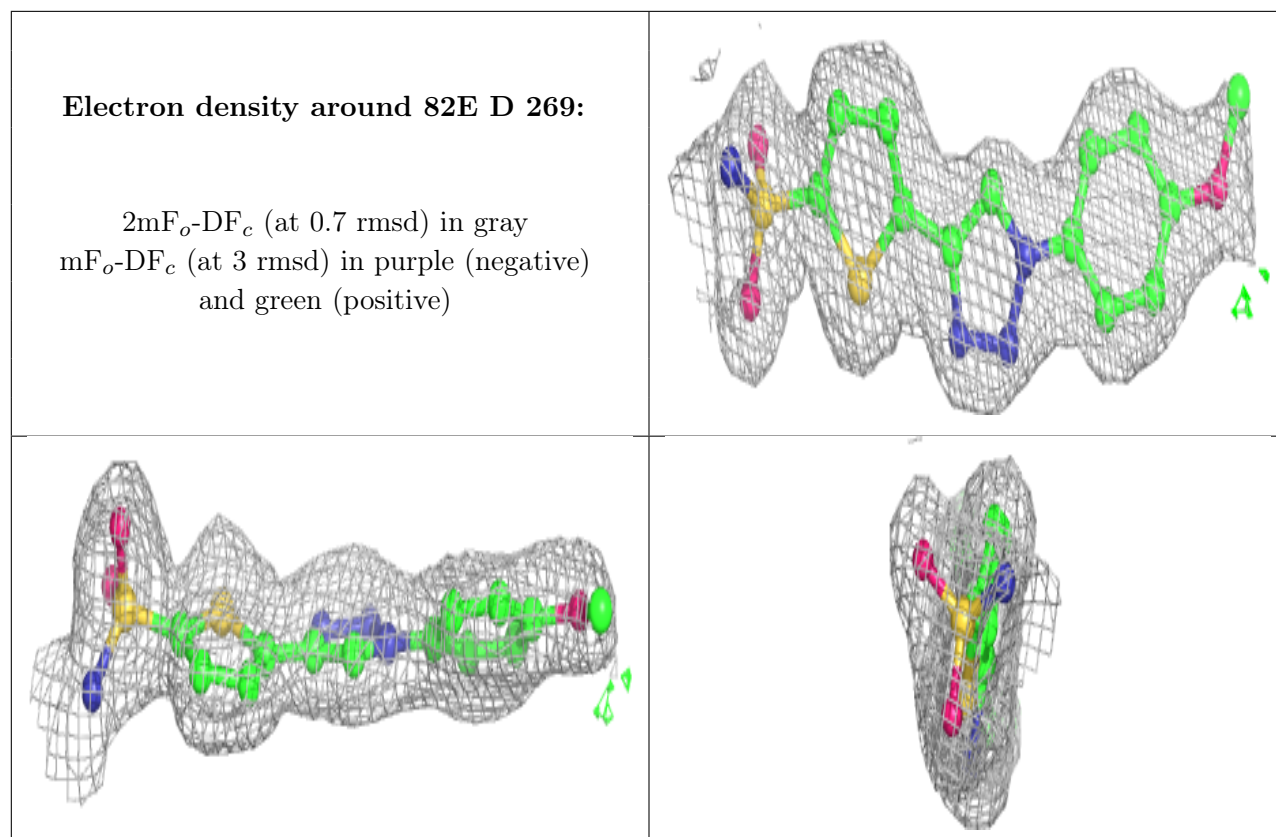
Electron density around 82E B 267:

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

**Electron density around 82E C 265:**

$2mF_o-DF_c$ (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.