



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2WEG / pdb_00002weg
Title : Thermodynamic Optimisation of Carbonic Anhydrase Fragment Inhibitors
Authors : Scott, A.D.; Phillips, C.; Alex, A.; Bent, A.; O'Brien, R.; Damian, L.; Jones, L.H.
Deposited on : 2009-03-31
Resolution : 1.10 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
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

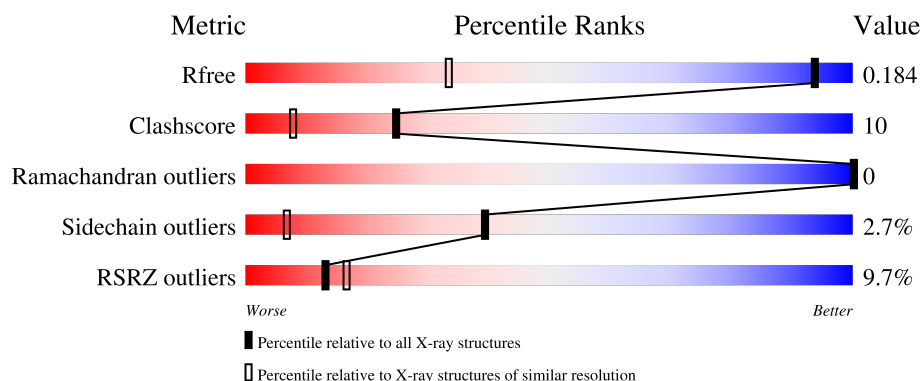
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1625 (1.12-1.08)
Clashscore	190562	1656 (1.12-1.08)
Ramachandran outliers	187476	1616 (1.12-1.08)
Sidechain outliers	187428	1612 (1.12-1.08)
RSRZ outliers	180081	1625 (1.12-1.08)

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	259	10% 74% 22% .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2363 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.

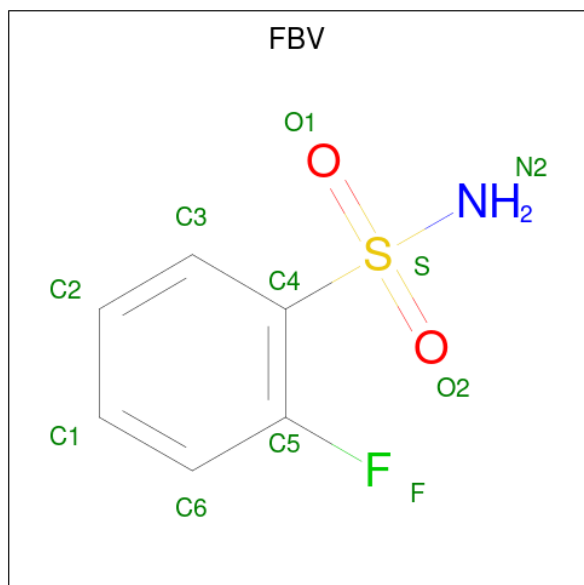
- Molecule 1 is a protein called CARBONIC ANHYDRASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2058	1321	355	380	2			

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

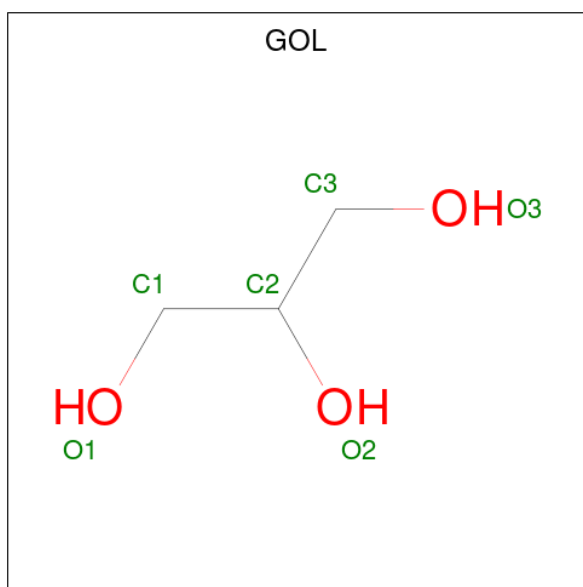
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-fluorobenzenesulfonamide (CCD ID: FBV) (formula: C₆H₆FNO₂S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			11	6	1	1	2	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

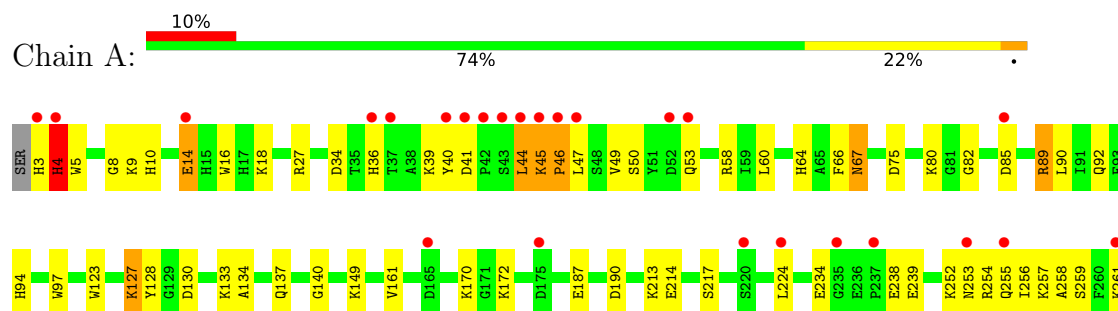
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	287	Total	O	0	0
			287	287		

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	42.43Å 41.22Å 72.04Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	26.64 – 1.10 26.64 – 1.10	Depositor EDS
% Data completeness (in resolution range)	95.2 (26.64-1.10) 95.1 (26.64-1.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.183 0.166 , 0.184	Depositor DCC
R_{free} test set	4651 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	8.0	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	2363	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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: FBV, GOL, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.98	42/2120 (2.0%)	1.44	17/2877 (0.6%)

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	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	161	VAL	CA-CB	11.88	1.68	1.54
1	A	40	TYR	C-O	9.56	1.35	1.23
1	A	44	LEU	N-CA	8.76	1.56	1.46
1	A	214	GLU	CD-OE1	-7.46	1.11	1.25
1	A	49	VAL	C-O	7.11	1.31	1.24
1	A	8	GLY	N-CA	7.01	1.54	1.45
1	A	256	ILE	CA-CB	-7.00	1.45	1.54
1	A	80	LYS	CB-CG	-6.72	1.32	1.52
1	A	90	LEU	C-O	6.69	1.31	1.23
1	A	58	ARG	CZ-NH2	-6.62	1.24	1.33
1	A	27	ARG	CZ-NH2	-6.56	1.25	1.33
1	A	9	LYS	CA-C	-6.47	1.44	1.52
1	A	187	GLU	CG-CD	6.43	1.68	1.52
1	A	170	LYS	CA-C	-6.41	1.44	1.52
1	A	137	GLN	CG-CD	-6.34	1.36	1.52
1	A	190	ASP	CG-OD1	-6.08	1.13	1.25
1	A	238	GLU	N-CA	5.86	1.53	1.46
1	A	41	ASP	N-CA	-5.84	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	213	LYS	CG-CD	5.76	1.69	1.52
1	A	40	TYR	CB-CG	-5.68	1.39	1.51
1	A	34	ASP	CG-OD1	-5.62	1.14	1.25
1	A	80	LYS	CG-CD	5.56	1.69	1.52
1	A	4	HIS	N-CA	5.54	1.52	1.45
1	A	234	GLU	C-O	-5.48	1.17	1.23
1	A	123	TRP	N-CA	5.44	1.52	1.45
1	A	34	ASP	C-N	-5.39	1.26	1.34
1	A	5	TRP	CZ2-CH2	-5.34	1.27	1.37
1	A	217	SER	CB-OG	-5.34	1.31	1.42
1	A	259	SER	C-N	-5.33	1.26	1.33
1	A	47	LEU	C-O	5.28	1.30	1.23
1	A	187	GLU	CB-CG	-5.26	1.36	1.52
1	A	258	ALA	C-O	5.22	1.30	1.24
1	A	47	LEU	CB-CG	-5.19	1.43	1.53
1	A	36	HIS	C-O	5.15	1.30	1.24
1	A	67	ASN	CG-ND2	-5.11	1.22	1.33
1	A	50	SER	C-O	-5.11	1.18	1.23
1	A	127	LYS	CB-CG	-5.09	1.37	1.52
1	A	18	LYS	CA-C	-5.09	1.45	1.52
1	A	16	TRP	C-O	-5.09	1.17	1.24
1	A	252	LYS	C-N	-5.04	1.27	1.33
1	A	127	LYS	C-O	5.03	1.30	1.24
1	A	85	ASP	CA-CB	5.01	1.61	1.53

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	CA-CB-CG	9.48	133.06	114.10
1	A	130	ASP	OD1-CG-OD2	-7.63	104.58	122.90
1	A	46	PRO	O-C-N	7.18	131.92	123.01
1	A	45	LYS	CA-CB-CG	6.20	126.51	114.10
1	A	39	LYS	CG-CD-CE	6.12	125.39	111.30
1	A	214	GLU	OE1-CD-OE2	-5.94	108.64	122.90
1	A	4	HIS	N-CA-CB	5.78	119.21	110.42
1	A	85	ASP	O-C-N	-5.69	116.57	123.29
1	A	80	LYS	CA-CB-CG	5.63	125.35	114.10
1	A	10	HIS	CA-C-O	5.51	125.44	119.15
1	A	239	GLU	CA-CB-CG	5.39	124.89	114.10
1	A	46	PRO	CA-C-O	-5.28	115.43	121.56
1	A	89	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	39	LYS	N-CA-CB	-5.09	102.58	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	89	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
1	A	97	TRP	CA-C-O	5.01	126.81	121.45

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	75	ASP	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	2058	0	2009	40	0
2	A	1	0	0	0	0
3	A	11	0	6	0	0
4	A	6	0	8	0	0
5	A	287	0	0	31	0
All	All	2363	0	2023	40	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 (40) 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:46:PRO:HD2	5:A:2075:HOH:O	1.18	1.33
1:A:253:ASN:HB3	5:A:2274:HOH:O	1.50	1.06
1:A:257:LYS:HE2	5:A:2070:HOH:O	1.61	1.01
1:A:224:LEU:HD22	5:A:2240:HOH:O	1.63	0.99
1:A:89:ARG:HG3	5:A:2112:HOH:O	1.62	0.98
1:A:4:HIS:CE1	5:A:2004:HOH:O	2.17	0.97
1:A:4:HIS:ND1	5:A:2004:HOH:O	1.97	0.96
1:A:14:GLU:H	1:A:14:GLU:CD	1.90	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LYS:HB3	5:A:2075:HOH:O	1.83	0.78
1:A:253:ASN:CB	5:A:2274:HOH:O	2.18	0.77
1:A:44:LEU:O	5:A:2072:HOH:O	2.05	0.74
1:A:255:GLN:CG	5:A:2060:HOH:O	2.37	0.71
1:A:3:HIS:O	5:A:2002:HOH:O	2.10	0.70
1:A:254:ARG:N	5:A:2277:HOH:O	2.28	0.66
1:A:255:GLN:HG2	5:A:2060:HOH:O	1.97	0.64
1:A:89:ARG:CG	5:A:2112:HOH:O	2.33	0.60
1:A:224:LEU:HB2	5:A:2240:HOH:O	2.02	0.59
1:A:172:LYS:HE3	5:A:2200:HOH:O	2.02	0.59
1:A:64:HIS:HE1	5:A:2098:HOH:O	1.88	0.57
1:A:172:LYS:HD3	5:A:2200:HOH:O	2.04	0.57
1:A:224:LEU:CD2	5:A:2240:HOH:O	2.37	0.55
1:A:224:LEU:CG	5:A:2240:HOH:O	2.56	0.54
1:A:255:GLN:HG3	5:A:2060:HOH:O	2.06	0.54
1:A:224:LEU:HG	5:A:2244:HOH:O	2.10	0.51
1:A:14:GLU:CD	1:A:14:GLU:N	2.67	0.50
1:A:224:LEU:CB	5:A:2240:HOH:O	2.59	0.49
1:A:64:HIS:HD2	5:A:2097:HOH:O	1.96	0.48
1:A:172:LYS:CD	5:A:2200:HOH:O	2.59	0.47
1:A:67:ASN:HD22	1:A:94:HIS:HB3	1.79	0.47
1:A:14:GLU:CG	5:A:2022:HOH:O	2.62	0.47
1:A:127:LYS:HE3	1:A:128:TYR:CZ	2.50	0.46
1:A:45:LYS:O	1:A:82:GLY:HA2	2.16	0.45
1:A:134:ALA:O	1:A:140:GLY:HA3	2.16	0.45
1:A:67:ASN:ND2	1:A:94:HIS:HB3	2.32	0.45
1:A:224:LEU:HD13	5:A:2240:HOH:O	2.18	0.44
1:A:14:GLU:CD	5:A:2022:HOH:O	2.61	0.43
1:A:133:LYS:HZ2	1:A:133:LYS:HG2	1.49	0.43
1:A:253:ASN:C	5:A:2277:HOH:O	2.61	0.42
1:A:60:LEU:O	1:A:66:PHE:HA	2.20	0.41
1:A:253:ASN:CG	5:A:2274:HOH:O	2.56	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	256/259 (99%)	247 (96%)	9 (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	223/224 (100%)	217 (97%)	6 (3%)	39	7

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	HIS
1	A	14	GLU
1	A	53	GLN
1	A	92	GLN
1	A	149	LYS
1	A	261	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	53	GLN
1	A	64	HIS
1	A	67	ASN
1	A	253	ASN

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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	GOL	A	1264	-	5,5,5	0.75	0	5,5,5	0.33	0
3	FBV	A	1263	2	11,11,11	2.65	3 (27%)	16,16,16	2.68	6 (37%)

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	GOL	A	1264	-	-	0/4/4/4	-
3	FBV	A	1263	2	-	0/6/6/6	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1263	FBV	C5-C4	7.46	1.44	1.39
3	A	1263	FBV	C3-C4	3.24	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1263	FBV	O1-S	2.40	1.48	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1263	FBV	C6-C5-C4	5.45	124.87	122.22
3	A	1263	FBV	C3-C4-C5	-5.17	115.15	118.53
3	A	1263	FBV	F-C5-C4	-5.07	114.97	118.91
3	A	1263	FBV	C3-C4-S	3.43	122.19	117.52
3	A	1263	FBV	O1-S-N2	2.35	110.73	107.35
3	A	1263	FBV	C5-C4-S	2.23	122.63	121.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	258/259 (99%)	0.51	25 (9%)	13 16	4, 9, 20, 35	2 (0%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	HIS	6.7
1	A	253	ASN	5.2
1	A	261	LYS	4.6
1	A	42	PRO	4.5
1	A	4	HIS	4.4
1	A	235	GLY	4.3
1	A	44	LEU	3.7
1	A	165	ASP	3.7
1	A	43	SER	3.4
1	A	14	GLU	3.4
1	A	52	ASP	3.2
1	A	47	LEU	3.1
1	A	40	TYR	3.0
1	A	224	LEU	2.8
1	A	85	ASP	2.6
1	A	53	GLN	2.6
1	A	37	THR	2.5
1	A	45	LYS	2.4
1	A	255	GLN	2.4
1	A	36	HIS	2.3
1	A	46	PRO	2.3
1	A	220	SER	2.3
1	A	237	PRO	2.3
1	A	41	ASP	2.1
1	A	175	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FBV	A	1263	11/11	0.99	0.04	4,6,8,8	0
4	GOL	A	1264	6/6	0.99	0.04	7,7,9,9	0
2	ZN	A	1262	1/1	1.00	0.01	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.