



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:12 AM UTC

PDB ID : 1CNY / pdb_00001cny
Title : SECONDARY INTERACTIONS SIGNIFICANTLY REMOVED FROM THE
SULFONAMIDE BINDING POCKET OF CARBONIC ANHYDRASE II IN-
FLUENCE BINDING CONSTANTS
Authors : Boriack, P.A.; Christianson, D.W.
Deposited on : 1995-07-21
Resolution : 2.30 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

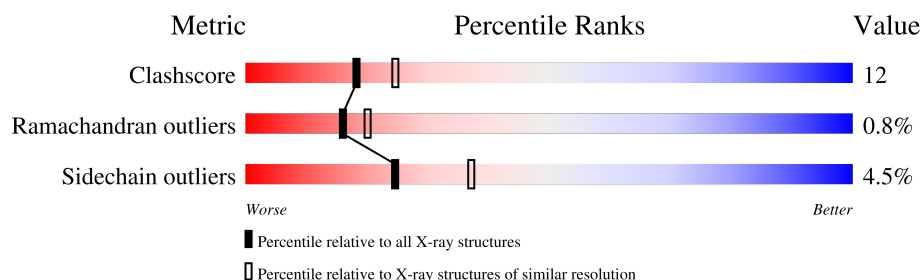
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	260	 47% 41% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2150 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 II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			2039	1309	350	378	2			

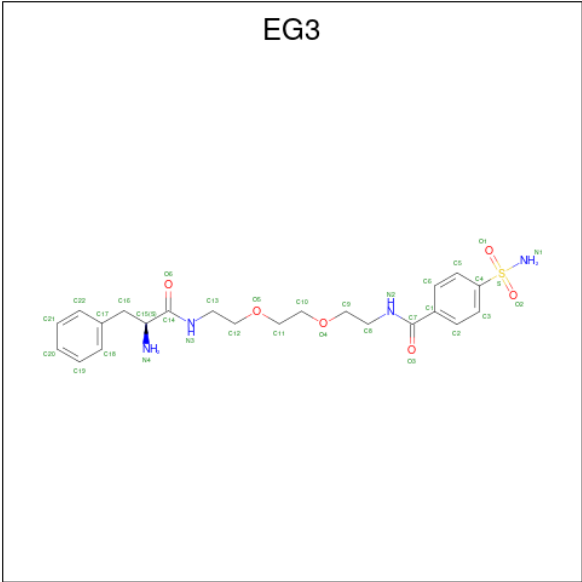
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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

- Molecule 4 is PHENYLALANYLAMINODI(ETHYLOXY)ETHYL BENZENESULFONAMIDEAMINOCARBONYLBENZENESULFONAMIDE (CCD ID: EG3) (formula: C₂₂H₃₀N₄O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	14	0
			33	22	4	6	1		

- Molecule 5 is water.

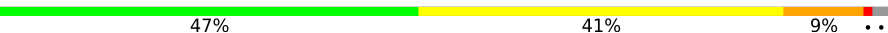
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	76	Total	O	0	0
			76	76		

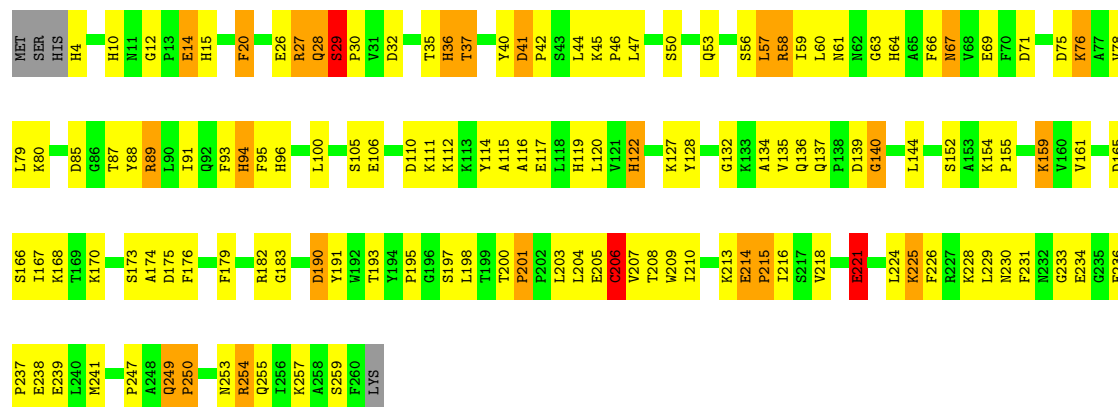
3 Residue-property plots

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. 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. 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.

Note EDS was not executed.

• Molecule 1: CARBONIC ANHYDRASE II

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.70 Å 41.70 Å 73.00 Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.180 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2150	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EG3, HG, 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	1.83	28/2100 (1.3%)	2.35	96/2851 (3.4%)

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	A	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	HIS	CE1-NE2	10.02	1.42	1.32
1	A	28	GLN	C-N	-8.81	1.21	1.33
1	A	105	SER	C-N	-7.22	1.24	1.33
1	A	139	ASP	C-N	-7.11	1.25	1.33
1	A	214	GLU	CA-C	-6.95	1.45	1.52
1	A	29	SER	C-O	-6.66	1.10	1.23
1	A	26	GLU	C-O	6.58	1.32	1.24
1	A	204	LEU	C-N	-6.31	1.25	1.33
1	A	215	PRO	N-CA	-6.13	1.39	1.46
1	A	176	PHE	CA-C	-5.91	1.46	1.53
1	A	174	ALA	CA-C	5.86	1.59	1.52
1	A	239	GLU	CD-OE2	5.80	1.36	1.25
1	A	247	PRO	C-N	-5.76	1.25	1.33
1	A	29	SER	N-CA	-5.60	1.35	1.46
1	A	253	ASN	C-O	5.52	1.32	1.23
1	A	225	LYS	C-O	5.51	1.31	1.24
1	A	182	ARG	N-CA	5.50	1.53	1.46
1	A	216	ILE	N-CA	5.49	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	159	LYS	C-O	5.39	1.30	1.24
1	A	80	LYS	N-CA	5.37	1.52	1.46
1	A	195	PRO	CA-CB	-5.32	1.47	1.53
1	A	91	ILE	N-CA	5.29	1.51	1.46
1	A	115	ALA	N-CA	5.29	1.53	1.46
1	A	234	GLU	CD-OE1	5.27	1.35	1.25
1	A	231	PHE	C-N	-5.24	1.26	1.33
1	A	32	ASP	CA-C	5.16	1.59	1.52
1	A	56	SER	CA-C	5.13	1.59	1.52
1	A	57	LEU	CA-C	-5.08	1.47	1.52

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	GLN	CA-C-N	31.61	178.59	121.70
1	A	28	GLN	C-N-CA	31.61	178.59	121.70
1	A	29	SER	O-C-N	14.47	146.15	123.00
1	A	29	SER	CA-C-O	-12.93	98.82	120.80
1	A	30	PRO	N-CA-CB	11.11	114.81	102.60
1	A	30	PRO	CA-N-CD	-10.52	96.77	111.50
1	A	208	THR	CA-C-O	-10.28	108.91	120.43
1	A	30	PRO	N-CD-CG	9.80	115.56	103.80
1	A	218	VAL	CA-C-O	-9.30	111.91	121.67
1	A	231	PHE	CA-CB-CG	8.75	122.55	113.80
1	A	165	ASP	CA-CB-CG	8.66	121.26	112.60
1	A	226	PHE	CA-CB-CG	8.66	122.46	113.80
1	A	214	GLU	CA-C-O	8.37	125.90	119.46
1	A	66	PHE	CA-CB-CG	8.32	122.12	113.80
1	A	214	GLU	CA-C-N	7.99	128.61	120.14
1	A	214	GLU	C-N-CA	7.99	128.61	120.14
1	A	207	VAL	CA-C-O	7.94	128.90	120.48
1	A	116	ALA	O-C-N	7.83	131.48	123.26
1	A	85	ASP	CA-CB-CG	7.70	120.30	112.60
1	A	207	VAL	N-CA-C	7.66	118.90	108.17
1	A	201	PRO	CB-CA-C	7.29	119.81	110.92
1	A	175	ASP	N-CA-C	-7.27	99.69	110.23
1	A	198	LEU	N-CA-C	-6.99	100.13	110.48
1	A	35	THR	CA-C-O	-6.79	112.16	119.97
1	A	12	GLY	CA-C-N	6.79	127.34	119.47
1	A	12	GLY	C-N-CA	6.79	127.34	119.47
1	A	144	LEU	CA-C-O	-6.75	112.87	120.43
1	A	29	SER	N-CA-C	6.75	129.89	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	THR	O-C-N	6.53	130.63	123.13
1	A	208	THR	N-CA-C	-6.48	98.65	108.96
1	A	29	SER	CA-C-N	6.44	142.47	127.00
1	A	29	SER	C-N-CA	6.44	142.47	127.00
1	A	20	PHE	CA-C-N	6.38	126.30	119.28
1	A	20	PHE	C-N-CA	6.38	126.30	119.28
1	A	201	PRO	N-CA-C	-6.33	102.98	110.70
1	A	14	GLU	CB-CG-CD	6.31	123.33	112.60
1	A	41	ASP	CA-C-N	6.17	125.79	119.56
1	A	41	ASP	C-N-CA	6.17	125.79	119.56
1	A	239	GLU	CA-CB-CG	6.13	126.35	114.10
1	A	10	HIS	CA-CB-CG	-6.11	107.69	113.80
1	A	28	GLN	O-C-N	6.06	130.79	123.16
1	A	175	ASP	CA-CB-CG	6.02	118.62	112.60
1	A	254	ARG	N-CA-C	-6.00	102.57	110.43
1	A	87	THR	CA-CB-OG1	-5.99	100.61	109.60
1	A	140	GLY	N-CA-C	5.98	119.44	112.50
1	A	76	LYS	N-CA-C	5.95	118.66	111.40
1	A	27	ARG	CA-C-N	5.94	132.44	122.87
1	A	27	ARG	C-N-CA	5.94	132.44	122.87
1	A	191	TYR	N-CA-C	5.86	117.69	108.96
1	A	221	GLU	CA-CB-CG	5.80	125.70	114.10
1	A	179	PHE	CA-CB-CG	-5.76	108.04	113.80
1	A	206	CYS	O-C-N	5.75	130.14	122.26
1	A	152	SER	CA-CB-OG	-5.75	99.61	111.10
1	A	119	HIS	ND1-CG-CD2	5.74	111.84	106.10
1	A	175	ASP	CB-CA-C	5.72	119.22	109.72
1	A	139	ASP	CA-C-N	5.72	126.28	119.94
1	A	139	ASP	C-N-CA	5.72	126.28	119.94
1	A	200	THR	CA-CB-OG1	-5.71	101.04	109.60
1	A	249	GLN	O-C-N	5.67	126.30	121.20
1	A	36	HIS	CA-CB-CG	-5.60	108.20	113.80
1	A	93	PHE	CA-CB-CG	5.59	119.39	113.80
1	A	136	GLN	N-CA-C	-5.55	105.87	113.30
1	A	26	GLU	CA-C-O	-5.53	112.03	119.11
1	A	61	ASN	N-CA-C	-5.49	100.24	108.96
1	A	27	ARG	NE-CZ-NH1	5.47	126.97	121.50
1	A	36	HIS	ND1-CE1-NE2	5.47	113.87	108.40
1	A	144	LEU	O-C-N	5.46	129.40	123.13
1	A	120	LEU	CB-CA-C	5.45	119.50	110.78
1	A	78	VAL	CA-C-O	5.44	127.22	121.67
1	A	250	PRO	O-C-N	5.44	129.27	123.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	SER	N-CA-C	-5.43	106.43	113.16
1	A	80	LYS	O-C-N	5.35	128.87	123.26
1	A	95	PHE	CA-CB-CG	5.34	119.14	113.80
1	A	166	SER	N-CA-C	5.24	118.94	112.54
1	A	259	SER	N-CA-CB	5.22	118.43	110.44
1	A	233	GLY	N-CA-C	-5.20	104.76	113.02
1	A	122	HIS	ND1-CG-CD2	5.19	111.29	106.10
1	A	94	HIS	ND1-CE1-NE2	5.19	113.59	108.40
1	A	96	HIS	CA-CB-CG	-5.18	108.62	113.80
1	A	91	ILE	CB-CA-C	5.17	115.97	110.91
1	A	96	HIS	O-C-N	5.17	129.35	123.31
1	A	218	VAL	O-C-N	5.08	128.67	123.04
1	A	37	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	106	GLU	CA-C-O	5.07	126.69	120.56
1	A	27	ARG	CD-NE-CZ	5.07	131.49	124.40
1	A	216	ILE	N-CA-CB	5.05	120.34	110.95
1	A	117	GLU	CB-CG-CD	5.05	121.18	112.60
1	A	241	MET	CA-C-O	-5.04	115.76	121.66
1	A	4	HIS	CE1-NE2-CD2	-5.04	103.96	109.00
1	A	67	ASN	CA-CB-CG	5.03	117.63	112.60
1	A	203	LEU	CA-C-N	5.03	127.91	120.82
1	A	203	LEU	C-N-CA	5.03	127.91	120.82
1	A	155	PRO	CA-C-N	5.02	129.38	120.74
1	A	155	PRO	C-N-CA	5.02	129.38	120.74
1	A	190	ASP	CA-C-O	-5.00	115.69	121.19
1	A	198	LEU	O-C-N	5.00	128.61	122.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	ARG	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	2039	0	1988	49	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	33	0	30	0	0
5	A	76	0	0	3	0
All	All	2150	0	2018	49	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 12.

All (49) 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:137:GLN:O	1:A:206:CYS:HB3	1.68	0.93
1:A:58:ARG:HD2	1:A:69:GLU:OE1	1.80	0.82
1:A:29:SER:HB2	1:A:197:SER:OG	1.86	0.76
1:A:159:LYS:HG3	5:A:372:HOH:O	1.90	0.70
1:A:190:ASP:OD2	1:A:213:LYS:NZ	2.17	0.70
1:A:137:GLN:O	1:A:206:CYS:CB	2.43	0.66
1:A:221:GLU:HA	1:A:224:LEU:HD12	1.81	0.63
1:A:190:ASP:HB2	1:A:213:LYS:HE2	1.80	0.62
1:A:36:HIS:HD2	5:A:282:HOH:O	1.83	0.62
1:A:58:ARG:HD2	1:A:69:GLU:CD	2.27	0.59
1:A:59:ILE:HG12	1:A:167:ILE:HD13	1.83	0.59
1:A:168:LYS:NZ	1:A:228:LYS:O	2.33	0.59
1:A:40:TYR:CE2	1:A:42:PRO:HG3	2.37	0.58
1:A:89:ARG:O	1:A:122:HIS:HA	2.05	0.56
1:A:161:VAL:HG13	1:A:225:LYS:HD2	1.88	0.55
1:A:14:GLU:HG2	1:A:15:HIS:CD2	2.42	0.54
1:A:236:GLU:HB3	1:A:237:PRO:CD	2.38	0.54
1:A:63:GLY:HA3	1:A:170:LYS:NZ	2.23	0.54
1:A:28:GLN:O	1:A:254:ARG:NH2	2.26	0.54
1:A:67:ASN:ND2	1:A:94:HIS:HB3	2.24	0.52
1:A:64:HIS:ND1	5:A:332:HOH:O	2.17	0.52
1:A:154:LYS:HE3	1:A:183:GLY:O	2.12	0.49
1:A:161:VAL:CG1	1:A:225:LYS:HD2	2.43	0.49
1:A:29:SER:CB	1:A:197:SER:H	2.26	0.49
1:A:230:ASN:OD1	1:A:238:GLU:HG3	2.13	0.48
1:A:29:SER:HB2	1:A:197:SER:H	1.79	0.48
1:A:45:LYS:HB3	1:A:46:PRO:CD	2.44	0.48
1:A:110:ASP:O	1:A:111:LYS:HB2	2.14	0.47
1:A:193:THR:HA	1:A:209:TRP:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:ARG:HG3	1:A:205:GLU:HB3	1.97	0.46
1:A:88:TYR:HB3	1:A:122:HIS:HB3	1.97	0.46
1:A:45:LYS:HB3	1:A:46:PRO:HD2	1.97	0.46
1:A:214:GLU:HA	1:A:215:PRO:HD3	1.66	0.46
1:A:60:LEU:CD1	1:A:173:SER:HB3	2.47	0.45
1:A:112:LYS:HE3	1:A:114:TYR:CZ	2.52	0.45
1:A:255:GLN:OE1	1:A:257:LYS:NZ	2.40	0.44
1:A:63:GLY:HA3	1:A:170:LYS:HZ2	1.83	0.44
1:A:132:GLY:O	1:A:135:VAL:HG22	2.18	0.44
1:A:53:GLN:HB3	1:A:76:LYS:O	2.18	0.43
1:A:128:TYR:CE1	1:A:137:GLN:HG3	2.53	0.43
1:A:47:LEU:HD21	1:A:210:ILE:HG21	1.99	0.43
1:A:57:LEU:HD11	1:A:71:ASP:HB2	1.99	0.42
1:A:20:PHE:CD2	1:A:201:PRO:HB3	2.54	0.42
1:A:249:GLN:HB3	1:A:250:PRO:HD2	2.02	0.41
1:A:41:ASP:C	1:A:41:ASP:OD1	2.63	0.41
1:A:134:ALA:O	1:A:140:GLY:HA3	2.21	0.41
1:A:112:LYS:HE3	1:A:114:TYR:CE1	2.56	0.41
1:A:60:LEU:HD12	1:A:173:SER:HB3	2.03	0.41
1:A:20:PHE:CE2	1:A:201:PRO:HB3	2.56	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	254/260 (98%)	241 (95%)	11 (4%)	2 (1%)	16 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	75	ASP

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	221/225 (98%)	211 (96%)	10 (4%)	24	37

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

Mol	Chain	Res	Type
1	A	37	THR
1	A	44	LEU
1	A	50	SER
1	A	58	ARG
1	A	79	LEU
1	A	100	LEU
1	A	127	LYS
1	A	206	CYS
1	A	221	GLU
1	A	229	LEU

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	36	HIS
1	A	53	GLN
1	A	67	ASN
1	A	136	GLN
1	A	178	ASN
1	A	230	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, 2 are monoatomic - leaving 1 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	EG3	A	555	2	34,34,34	2.92	11 (32%)	44,44,44	2.85	13 (29%)

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	EG3	A	555	2	-	13/31/31/31	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	555	EG3	C14-N3	8.16	1.52	1.33
4	A	555	EG3	C7-N2	7.78	1.50	1.33
4	A	555	EG3	C1-C7	-6.78	1.35	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	555	EG3	S-N1	-6.43	1.48	1.60
4	A	555	EG3	O4-C10	3.69	1.58	1.42
4	A	555	EG3	C4-S	-3.00	1.72	1.77
4	A	555	EG3	O4-C9	-2.55	1.31	1.42
4	A	555	EG3	C8-N2	2.40	1.51	1.46
4	A	555	EG3	C22-C17	-2.36	1.34	1.38
4	A	555	EG3	O5-C12	2.27	1.51	1.42
4	A	555	EG3	O1-S	2.06	1.47	1.43

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	555	EG3	O3-C7-N2	-9.22	104.62	122.59
4	A	555	EG3	O1-S-C4	7.94	116.32	107.35
4	A	555	EG3	C13-N3-C14	-7.28	109.46	122.55
4	A	555	EG3	O2-S-O1	-4.85	111.34	118.80
4	A	555	EG3	O3-C7-C1	4.72	130.25	120.90
4	A	555	EG3	C1-C7-N2	3.83	125.08	117.12
4	A	555	EG3	O2-S-N1	3.80	112.84	107.35
4	A	555	EG3	O1-S-N1	-3.38	102.48	107.35
4	A	555	EG3	C5-C6-C1	-3.35	117.22	120.80
4	A	555	EG3	C4-S-N1	-2.87	104.41	108.40
4	A	555	EG3	C6-C5-C4	2.48	121.85	119.44
4	A	555	EG3	C8-N2-C7	-2.43	116.62	122.11
4	A	555	EG3	C16-C15-C14	2.10	113.90	108.97

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	555	EG3	N3-C14-C15-N4
4	A	555	EG3	O6-C14-C15-N4
4	A	555	EG3	O4-C10-C11-O5
4	A	555	EG3	C10-C11-O5-C12
4	A	555	EG3	C3-C4-S-O1
4	A	555	EG3	C5-C4-S-O1
4	A	555	EG3	C8-C9-O4-C10
4	A	555	EG3	C3-C4-S-N1
4	A	555	EG3	C11-C10-O4-C9
4	A	555	EG3	C5-C4-S-N1
4	A	555	EG3	O6-C14-C15-C16
4	A	555	EG3	N3-C14-C15-C16

Continued on next page...

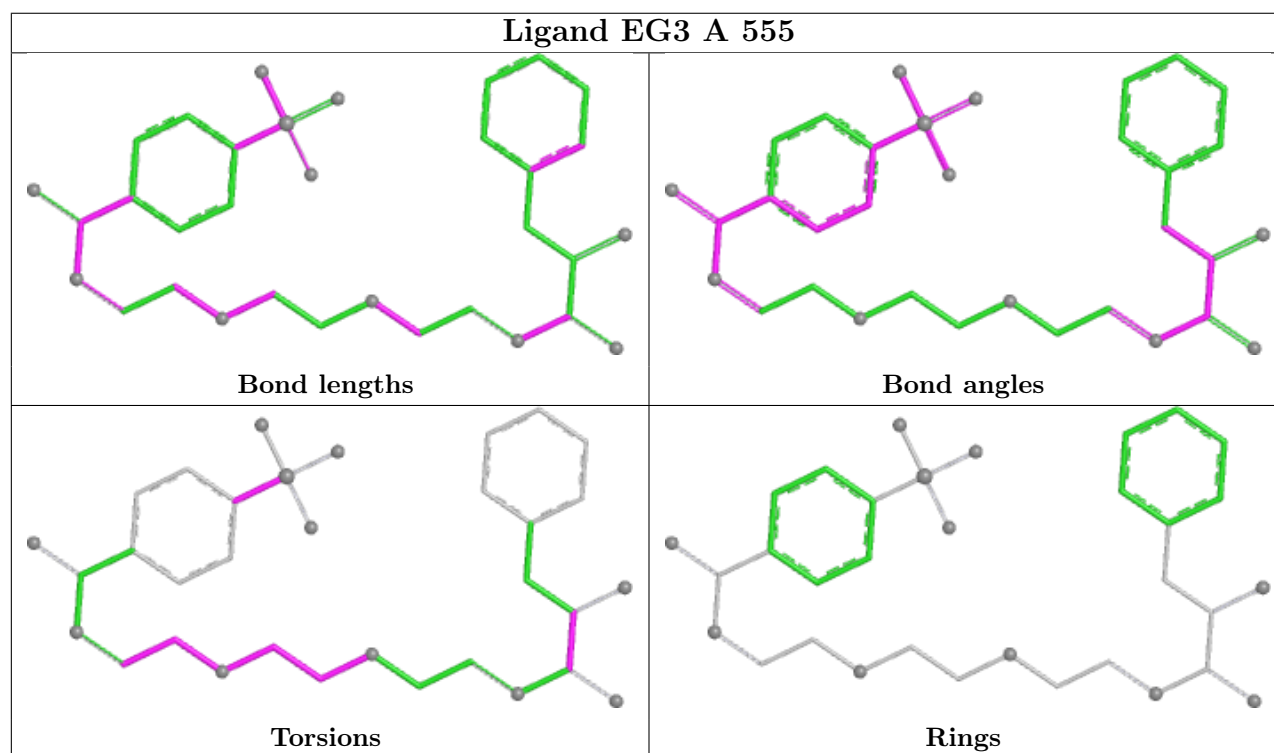
Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	555	EG3	N2-C8-C9-O4

There are no ring outliers.

No monomer is involved in short contacts.

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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.