



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:22 PM UTC

PDB ID : 4Q SJ / pdb_00004qsj
Title : Crystal structure of human carbonic anhydrase isozyme XIII with 2-chloro-4-
{[(4-methyl-6-oxo-1,6-dihydropyrimidin-2-yl)thio]acetyl}benzenesulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2014-07-04
Resolution : 1.70 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

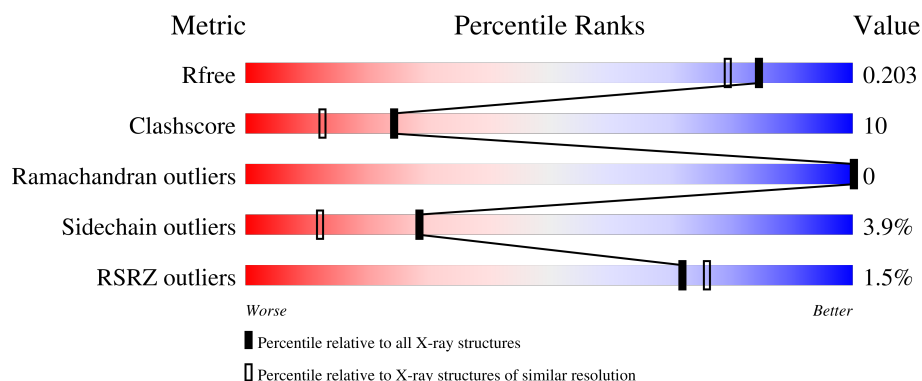
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

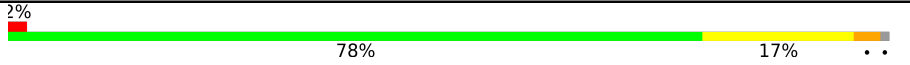
The reported resolution of this entry is 1.70 Å.

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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	263	
1	B	263	

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
3	EWV	A	302	-	-	X	-
3	EWV	B	302[A]	-	-	X	-
4	PEG	B	303	-	-	X	-
4	PEG	B	306	-	-	X	-
6	CIT	B	308	-	X	-	-
7	EDO	B	309	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 4942 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 13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	258	Total	C	N	O	S	0	8	0
			2115	1346	368	400	1			
1	A	260	Total	C	N	O	S	0	10	0
			2160	1375	375	409	1			

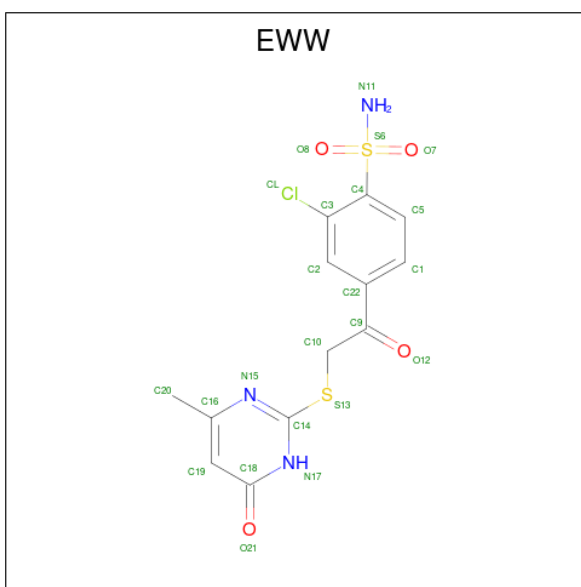
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	MET	-	expression tag	UNP Q8N1Q1
A	-1	MET	-	expression tag	UNP Q8N1Q1

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

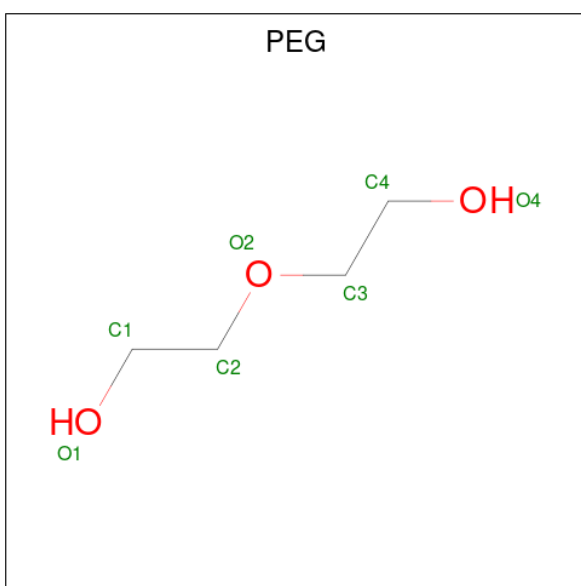
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-chloro-4-[[[4-methyl-6-oxo-1,6-dihydropyrimidin-2-yl)sulfanyl]acetyl]benzenesulfonamide (CCD ID: EWW) (formula: C₁₃H₁₂ClN₃O₄S₂).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	S	0	1
			46	26	2	6	8	4		
3	A	1	Total	C	Cl	N	O	S	0	0
			23	13	1	3	4	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



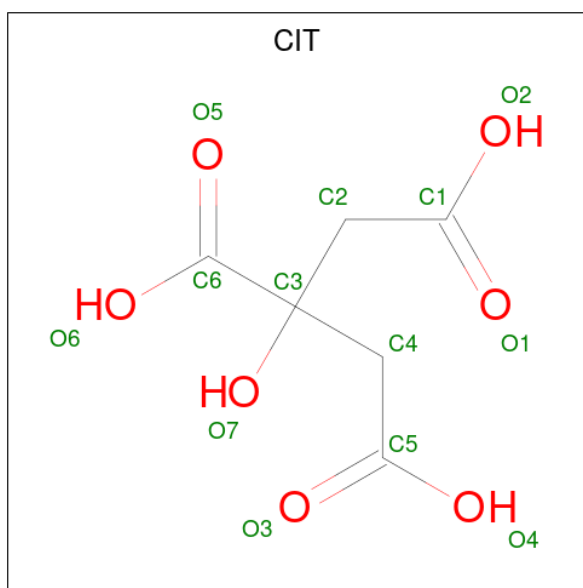
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

- Molecule 6 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O		
			13	6	7	0	0
6	B	1	Total	C	O		
			13	6	7	0	0

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Ni	0	0
			1	1		

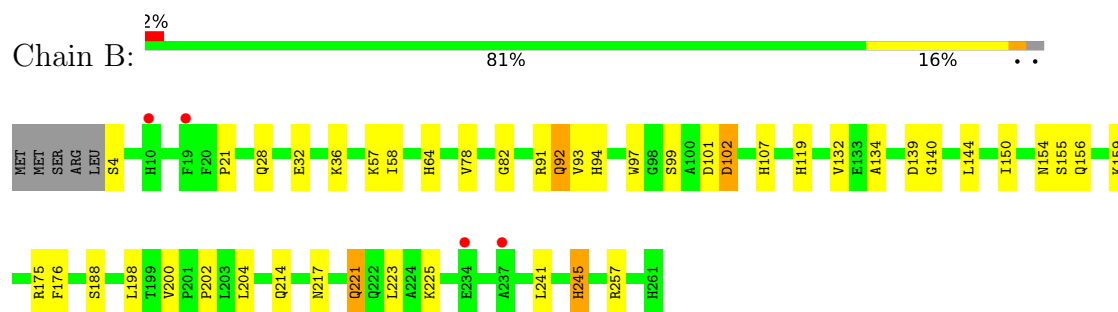
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	290	Total	O	0	0
			290	290		
9	A	253	Total	O	0	0
			253	253		

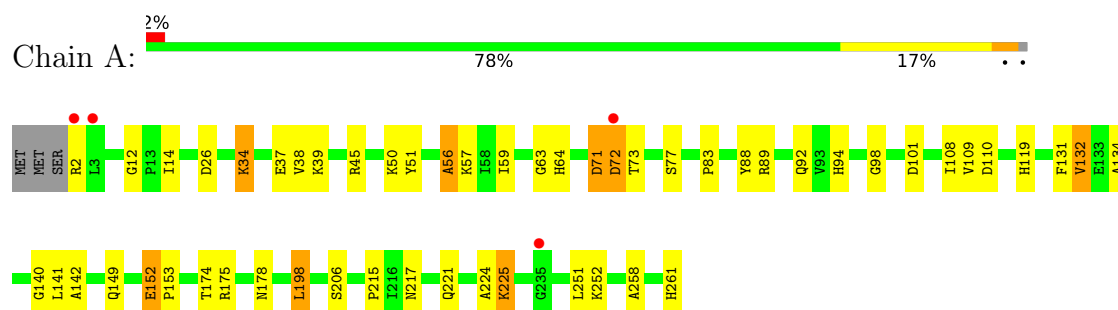
3 Residue-property plots

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 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 13



• Molecule 1: Carbonic anhydrase 13



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.66Å 57.78Å 160.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.87 – 1.70 27.87 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (27.87-1.70) 98.8 (27.87-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.60 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.164 , 0.204 0.162 , 0.203	Depositor DCC
R_{free} test set	5865 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	15.3	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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: EWW, CIT, EDO, DMS, NI, ZN, PEG

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	1.60	15/2223 (0.7%)	1.28	8/3025 (0.3%)
1	B	1.56	13/2178 (0.6%)	1.19	0/2963
All	All	1.58	28/4401 (0.6%)	1.24	8/5988 (0.1%)

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	72	ASP	CA-C	10.35	1.66	1.52
1	A	98	GLY	N-CA	8.39	1.52	1.44
1	A	59	ILE	C-O	8.35	1.32	1.24
1	B	144	LEU	C-N	7.11	1.38	1.33
1	B	245	HIS	ND1-CE1	6.94	1.39	1.32
1	B	78	VAL	C-O	6.69	1.30	1.23
1	A	71	ASP	CA-C	-6.26	1.45	1.52
1	A	215	PRO	C-O	6.22	1.31	1.23
1	A	64	HIS	ND1-CE1	6.13	1.38	1.32
1	A	56	ALA	N-CA	6.10	1.53	1.46
1	A	119	HIS	ND1-CE1	6.10	1.38	1.32
1	A	108	ILE	N-CA	6.02	1.53	1.46
1	A	94	HIS	ND1-CE1	6.00	1.38	1.32
1	A	83	PRO	N-CA	-5.91	1.40	1.47
1	B	64	HIS	ND1-CE1	5.86	1.38	1.32
1	B	107	HIS	ND1-CE1	5.79	1.38	1.32
1	A	88	TYR	C-O	5.78	1.30	1.24
1	B	94	HIS	C-O	-5.70	1.17	1.23
1	B	119	HIS	ND1-CE1	5.51	1.38	1.32
1	B	257	ARG	CZ-NH1	5.45	1.40	1.32
1	A	142	ALA	N-CA	5.40	1.52	1.46
1	B	223	LEU	N-CA	5.25	1.52	1.46
1	A	141	LEU	N-CA	5.18	1.52	1.45
1	B	28	GLN	C-O	-5.17	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLY	N-CA	5.16	1.51	1.44
1	B	32	GLU	C-O	5.14	1.30	1.24
1	A	63	GLY	N-CA	5.12	1.52	1.45
1	B	241	LEU	C-O	5.05	1.30	1.23

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	101	ASP	N-CA-C	6.35	120.13	112.38
1	A	198	LEU	N-CA-C	-5.81	102.44	110.35
1	A	73	THR	N-CA-CB	5.76	119.66	110.73
1	A	224	ALA	N-CA-C	5.66	118.22	111.71
1	A	12	GLY	N-CA-C	5.59	118.70	112.00
1	A	132	VAL	N-CA-C	5.24	115.45	110.42
1	A	206	SER	CA-C-N	-5.12	116.85	123.19
1	A	206	SER	C-N-CA	-5.12	116.85	123.19

There are no chirality outliers.

There are no planarity outliers.

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	2160	0	2086	32	0
1	B	2115	0	2039	49	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	23	0	12	7	0
3	B	46	0	22	16	0
4	B	14	0	20	12	0
5	B	4	0	6	1	0
6	B	26	0	10	2	0
7	B	8	0	12	5	0
8	A	1	0	0	0	0
9	A	253	0	0	4	0
9	B	290	0	0	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4942	0	4207	85	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 (85) 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)
4:B:306:PEG:H41	9:B:536:HOH:O	1.31	1.24
1:A:221:GLN:O	1:A:225:LYS:HD3	1.53	1.08
1:B:175:ARG:HE	4:B:303:PEG:H31	0.93	1.08
1:B:175:ARG:HE	4:B:303:PEG:C3	1.77	0.97
1:B:175:ARG:NE	4:B:303:PEG:H31	1.78	0.96
1:A:252:LYS:HE2	9:A:622:HOH:O	1.69	0.90
1:A:225:LYS:N	1:A:225:LYS:HD2	1.85	0.88
1:A:221:GLN:O	1:A:225:LYS:CD	2.23	0.85
1:B:92[A]:GLN:HE21	3:B:302[A]:EWW:H12	1.40	0.83
1:A:178:ASN:HB3	9:A:639:HOH:O	1.85	0.77
1:B:155:SER:OG	7:B:309:EDO:H21	1.86	0.76
1:B:92[A]:GLN:NE2	3:B:302[A]:EWW:H12	2.00	0.75
1:B:217[B]:ASN:HD22	1:B:217[B]:ASN:H	1.33	0.74
1:A:109[B]:VAL:O	1:A:109[B]:VAL:HG23	1.88	0.73
1:B:92[A]:GLN:HE21	3:B:302[A]:EWW:C20	2.05	0.68
1:B:198:LEU:HD22	3:B:302[A]:EWW:C3	2.24	0.67
1:B:217[A]:ASN:ND2	9:B:682:HOH:O	2.26	0.67
1:A:225:LYS:HD2	1:A:225:LYS:H	1.58	0.66
1:B:217[B]:ASN:H	1:B:217[B]:ASN:ND2	1.95	0.65
1:A:149:GLN:HE21	1:A:217[A]:ASN:HD21	1.48	0.62
1:B:198:LEU:HD22	3:B:302[A]:EWW:C2	2.31	0.60
1:B:92[B]:GLN:HG2	1:B:93:VAL:N	2.18	0.59
1:A:174[B]:THR:HG22	1:A:175[B]:ARG:O	2.02	0.59
1:B:150:ILE:HG21	4:B:306:PEG:H12	1.83	0.59
1:A:149:GLN:HE21	1:A:217[A]:ASN:ND2	2.01	0.58
1:B:156[B]:GLN:HG3	7:B:309:EDO:C2	2.34	0.57
1:A:57:LYS:HE2	1:A:71:ASP:HB2	1.86	0.56
1:A:132:VAL:HG22	3:A:302:EWW:C19	2.36	0.56
1:B:221:GLN:HE21	1:B:221:GLN:H	1.52	0.56
1:B:221:GLN:H	1:B:221:GLN:NE2	2.05	0.55
1:B:175:ARG:NE	4:B:303:PEG:C3	2.54	0.55
6:B:308:CIT:H22	9:B:471:HOH:O	2.06	0.55
1:B:198:LEU:HD22	3:B:302[A]:EWW:CL	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:ARG:HH21	4:B:303:PEG:H32	1.72	0.53
1:A:198:LEU:CD1	3:A:302:EWV:S13	2.97	0.53
1:B:102:ASP:CG	9:B:632:HOH:O	2.52	0.53
1:B:101:ASP:CB	4:B:306:PEG:H21	2.39	0.52
1:B:101:ASP:HB3	4:B:306:PEG:H21	1.91	0.52
1:A:34:LYS:HG2	9:A:623:HOH:O	2.09	0.52
1:A:26:ASP:HA	1:A:252:LYS:HD2	1.90	0.52
1:B:159:LYS:HG2	1:B:176:PHE:CE1	2.45	0.51
3:B:302[A]:EWV:N15	3:B:302[A]:EWV:C9	2.72	0.51
1:A:134:ALA:O	1:A:140:GLY:HA3	2.11	0.51
1:A:198:LEU:HD13	3:A:302:EWV:S13	2.51	0.50
1:B:200:VAL:HG22	3:B:302[B]:EWV:C5	2.42	0.50
1:B:97:TRP:O	1:B:245:HIS:HD2	1.94	0.49
1:B:92[A]:GLN:CB	3:B:302[A]:EWV:H10	2.42	0.49
1:B:134:ALA:O	1:B:140:GLY:HA3	2.13	0.49
1:A:34:LYS:HE2	1:A:37:GLU:HG3	1.93	0.49
1:B:101:ASP:OD2	4:B:306:PEG:O1	2.25	0.49
1:B:154:ASN:OD1	7:B:309:EDO:H12	2.13	0.49
1:B:92[A]:GLN:NE2	3:B:302[A]:EWV:C20	2.69	0.48
1:B:91:ARG:HE	3:B:302[A]:EWV:H8	1.79	0.48
1:B:200:VAL:HG21	3:B:302[B]:EWV:H5	1.96	0.47
1:A:131:PHE:HZ	3:A:302:EWV:H6	1.78	0.47
1:B:92[A]:GLN:CG	3:B:302[A]:EWV:H10	2.44	0.47
1:B:175:ARG:NH2	4:B:303:PEG:H32	2.30	0.46
1:B:92[B]:GLN:CG	1:B:93:VAL:N	2.79	0.46
1:B:188:SER:H	1:B:214:GLN:NE2	2.14	0.46
1:B:156[B]:GLN:HG3	7:B:309:EDO:C1	2.46	0.45
1:B:198:LEU:HA	3:B:302[B]:EWV:O7	2.15	0.45
1:B:139:ASP:HA	5:B:304:DMS:H11	1.99	0.45
3:A:302:EWV:H6	3:A:302:EWV:H4	1.79	0.45
1:A:109[A]:VAL:O	1:A:110:ASP:C	2.59	0.45
1:A:51[B]:TYR:HD2	9:A:505:HOH:O	2.00	0.44
1:A:38:VAL:CG1	1:A:258:ALA:HB2	2.47	0.44
1:A:132:VAL:HG22	3:A:302:EWV:H8	2.00	0.44
1:B:159:LYS:HG2	1:B:176:PHE:HE1	1.80	0.44
1:A:34:LYS:HZ2	1:A:34:LYS:HG3	1.51	0.44
1:B:156[B]:GLN:HG3	7:B:309:EDO:H12	2.00	0.44
1:B:217[B]:ASN:HD22	1:B:217[B]:ASN:N	2.09	0.44
1:B:200:VAL:CG2	3:B:302[B]:EWV:C1	2.97	0.43
1:A:72:ASP:CA	1:A:89:ARG:HD3	2.49	0.43
1:A:109[B]:VAL:O	1:A:109[B]:VAL:CG2	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:LEU:HD22	3:A:302:EWW:CL	2.56	0.42
1:B:57:LYS:C	1:B:58:ILE:HG13	2.43	0.42
1:A:38:VAL:HG11	1:A:258:ALA:HB2	2.01	0.42
1:B:99:SER:OG	6:B:305:CIT:O5	2.37	0.42
1:B:175:ARG:HH21	4:B:303:PEG:C3	2.33	0.42
1:B:200:VAL:CG2	3:B:302[B]:EWW:H5	2.50	0.42
1:A:72:ASP:OD1	1:A:72:ASP:C	2.63	0.41
1:B:202:PRO:HG2	1:B:204:LEU:HG	2.03	0.40
1:A:50:LYS:O	1:A:77:SER:HA	2.21	0.40
1:A:56:ALA:O	1:A:57:LYS:HD3	2.20	0.40
1:A:152[A]:GLU:O	1:A:153:PRO:C	2.63	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	268/263 (102%)	258 (96%)	10 (4%)	0	100	100
1	B	264/263 (100%)	260 (98%)	4 (2%)	0	100	100
All	All	532/526 (101%)	518 (97%)	14 (3%)	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	239/232 (103%)	227 (95%)	12 (5%)	22	8
1	B	235/232 (101%)	225 (96%)	10 (4%)	26	10
All	All	474/464 (102%)	452 (95%)	22 (5%)	28	9

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	SER
1	B	21	PRO
1	B	36	LYS
1	B	92[A]	GLN
1	B	92[B]	GLN
1	B	102	ASP
1	B	132[A]	VAL
1	B	132[B]	VAL
1	B	221	GLN
1	B	225	LYS
1	A	2	ARG
1	A	14	ILE
1	A	34	LYS
1	A	39	LYS
1	A	45	ARG
1	A	92[A]	GLN
1	A	92[B]	GLN
1	A	152[A]	GLU
1	A	152[B]	GLU
1	A	225	LYS
1	A	251	LEU
1	A	261	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	67	ASN
1	B	103	HIS
1	B	173	GLN
1	B	178	ASN
1	B	214	GLN
1	B	221	GLN
1	B	245	HIS
1	A	64	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	67	ASN
1	A	158	GLN
1	A	214	GLN
1	A	221	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	PEG	B	303	-	6,6,6	0.87	0	5,5,5	1.85	2 (40%)
6	CIT	B	308	-	12,12,12	2.04	6 (50%)	17,17,17	3.71	9 (52%)
3	EWB	B	302[A]	2	24,24,24	3.95	8 (33%)	34,35,35	3.17	15 (44%)
6	CIT	B	305	-	12,12,12	2.05	5 (41%)	17,17,17	1.69	4 (23%)
3	EWB	B	302[B]	2	24,24,24	3.93	6 (25%)	34,35,35	2.37	14 (41%)
5	DMS	B	304	-	3,3,3	0.57	0	3,3,3	1.14	0
4	PEG	B	306	-	6,6,6	0.41	0	5,5,5	0.72	0
7	EDO	B	309	-	3,3,3	0.42	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EGW	A	302	2	24,24,24	3.55	7 (29%)	34,35,35	2.31	11 (32%)
7	EDO	B	307	-	3,3,3	0.65	0	2,2,2	0.82	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PEG	B	303	-	-	3/4/4/4	-
6	CIT	B	308	-	-	6/16/16/16	-
3	EGW	B	302[A]	2	-	2/15/15/15	0/2/2/2
6	CIT	B	305	-	-	7/16/16/16	-
3	EGW	B	302[B]	2	-	5/15/15/15	0/2/2/2
4	PEG	B	306	-	-	2/4/4/4	-
7	EDO	B	309	-	-	0/1/1/1	-
3	EGW	A	302	2	-	8/15/15/15	0/2/2/2
7	EDO	B	307	-	-	0/1/1/1	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[B]	EGW	O7-S6	12.97	1.66	1.43
3	B	302[A]	EGW	O7-S6	12.53	1.65	1.43
3	B	302[A]	EGW	S6-N11	12.25	1.84	1.60
3	A	302	EGW	S6-N11	12.18	1.84	1.60
3	B	302[B]	EGW	S6-N11	11.63	1.83	1.60
3	A	302	EGW	O7-S6	10.15	1.61	1.43
3	B	302[B]	EGW	O8-S6	5.25	1.53	1.43
3	A	302	EGW	C14-N15	4.18	1.38	1.31
3	B	302[A]	EGW	O8-S6	3.97	1.50	1.43
3	B	302[A]	EGW	C14-S13	3.94	1.81	1.75
6	B	305	CIT	C4-C3	3.66	1.58	1.54
6	B	305	CIT	C3-C6	-3.50	1.49	1.53
6	B	308	CIT	O1-C1	3.08	1.32	1.22
6	B	308	CIT	C2-C3	3.04	1.57	1.54
3	B	302[B]	EGW	C14-N15	2.92	1.36	1.31
3	B	302[A]	EGW	C14-N15	2.74	1.36	1.31
3	A	302	EGW	C4-S6	2.73	1.81	1.77
6	B	308	CIT	O7-C3	-2.63	1.38	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[B]	EW	C4-S6	2.55	1.80	1.77
3	B	302[B]	EW	C14-S13	2.51	1.79	1.75
6	B	305	CIT	O3-C5	2.45	1.30	1.22
3	A	302	EW	C19-C16	2.43	1.41	1.36
3	A	302	EW	C14-S13	2.43	1.79	1.75
3	B	302[A]	EW	C19-C16	2.42	1.41	1.36
6	B	308	CIT	O3-C5	2.24	1.29	1.22
6	B	308	CIT	C2-C1	2.22	1.57	1.50
6	B	308	CIT	O5-C6	2.14	1.28	1.22
3	A	302	EW	C10-C9	-2.14	1.48	1.51
3	B	302[A]	EW	O21-C18	-2.11	1.20	1.24
6	B	305	CIT	C4-C5	2.02	1.56	1.50
3	B	302[A]	EW	C3-CL	2.02	1.78	1.73
6	B	305	CIT	C2-C3	2.00	1.56	1.54

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	EW	C18-C19-C16	-9.07	115.11	120.25
6	B	308	CIT	O7-C3-C6	-7.56	98.23	108.96
6	B	308	CIT	C3-C2-C1	7.42	134.20	113.92
6	B	308	CIT	O7-C3-C2	-6.56	94.42	109.38
6	B	308	CIT	C4-C3-C2	6.15	125.08	109.31
3	B	302[A]	EW	C5-C4-C3	5.98	123.33	119.05
3	A	302	EW	C20-C16-N15	5.88	120.95	115.04
3	B	302[A]	EW	C19-C18-N17	5.68	122.31	115.24
3	B	302[A]	EW	O8-S6-N11	-5.65	99.20	107.35
3	B	302[B]	EW	C20-C16-N15	4.98	120.04	115.04
3	A	302	EW	C19-C18-N17	4.82	121.24	115.24
3	A	302	EW	C19-C16-N15	-4.81	117.56	123.19
3	B	302[A]	EW	C2-C3-C4	-4.80	116.71	121.36
3	B	302[B]	EW	O8-S6-N11	-4.79	100.44	107.35
3	B	302[A]	EW	C10-C9-C22	4.54	123.17	117.99
3	B	302[A]	EW	S13-C14-N17	4.45	120.08	113.22
3	B	302[B]	EW	S13-C14-N17	4.36	119.94	113.22
3	B	302[B]	EW	O21-C18-C19	-3.86	120.13	125.46
3	A	302	EW	C5-C4-C3	3.86	121.81	119.05
6	B	305	CIT	C4-C3-C2	3.83	119.13	109.31
3	B	302[A]	EW	O7-S6-O8	3.75	124.56	118.80
3	B	302[B]	EW	C19-C18-N17	3.73	119.88	115.24
3	B	302[B]	EW	C10-S13-C14	-3.58	93.06	100.98
3	B	302[A]	EW	C10-S13-C14	-3.57	93.10	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	EW	O21-C18-N17	-3.55	114.13	119.27
3	A	302	EW	O21-C18-C19	-3.44	120.72	125.46
6	B	308	CIT	O7-C3-C4	-3.33	101.78	109.38
3	A	302	EW	O8-S6-N11	-3.31	102.57	107.35
3	B	302[B]	EW	C5-C4-C3	3.24	121.37	119.05
3	B	302[A]	EW	O7-S6-N11	3.19	111.95	107.35
3	B	302[B]	EW	C18-C19-C16	-3.13	118.48	120.25
3	B	302[B]	EW	O7-S6-N11	3.06	111.76	107.35
3	B	302[A]	EW	O12-C9-C22	-3.06	116.64	120.73
3	A	302	EW	O12-C9-C22	2.89	124.59	120.73
3	A	302	EW	O7-S6-N11	2.84	111.44	107.35
3	A	302	EW	S13-C14-N17	2.83	117.59	113.22
6	B	305	CIT	O2-C1-C2	2.78	123.16	114.35
3	B	302[B]	EW	C10-C9-C22	2.78	121.16	117.99
4	B	303	PEG	O1-C1-C2	2.73	127.87	111.82
3	B	302[A]	EW	C5-C4-S6	-2.69	113.87	117.52
3	B	302[B]	EW	C19-C16-N15	-2.68	120.05	123.19
6	B	308	CIT	C4-C3-C6	2.62	115.83	110.03
6	B	308	CIT	C3-C4-C5	2.57	120.95	113.92
3	B	302[B]	EW	O12-C9-C22	-2.54	117.33	120.73
6	B	305	CIT	O2-C1-O1	-2.37	117.25	123.33
3	B	302[A]	EW	N17-C14-N15	-2.32	119.84	123.84
4	B	303	PEG	O2-C2-C1	2.31	120.30	110.11
6	B	308	CIT	O5-C6-C3	2.25	126.46	122.09
3	B	302[B]	EW	S13-C14-N15	-2.23	120.01	121.98
3	A	302	EW	C14-N17-C18	-2.22	118.63	122.27
6	B	305	CIT	C3-C4-C5	2.22	119.98	113.92
3	B	302[B]	EW	N17-C14-N15	-2.19	120.06	123.84
3	A	302	EW	C10-S13-C14	-2.19	96.14	100.98
3	B	302[A]	EW	S13-C14-N15	-2.14	120.08	121.98
6	B	308	CIT	O4-C5-O3	-2.12	117.88	123.33

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[B]	EW	N17-C14-S13-C10
3	B	302[B]	EW	N15-C14-S13-C10
3	A	302	EW	C9-C10-S13-C14
3	A	302	EW	N17-C14-S13-C10
3	A	302	EW	N15-C14-S13-C10
6	B	305	CIT	O7-C3-C4-C5

Continued on next page...

Continued from previous page...

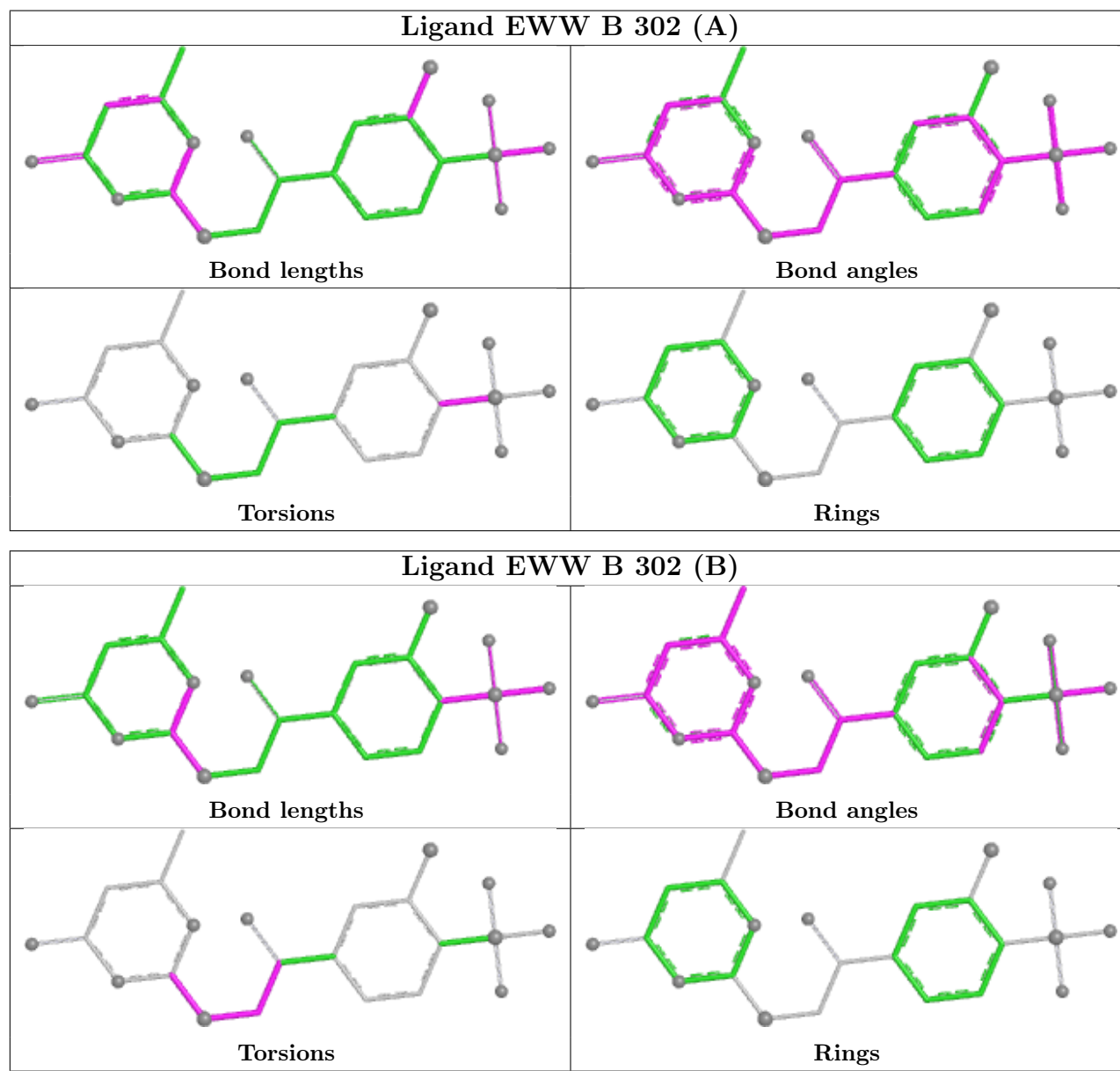
Mol	Chain	Res	Type	Atoms
6	B	308	CIT	O7-C3-C6-O5
6	B	308	CIT	O7-C3-C6-O6
6	B	308	CIT	C4-C3-C6-O5
6	B	308	CIT	C4-C3-C6-O6
4	B	306	PEG	O2-C3-C4-O4
4	B	303	PEG	O2-C3-C4-O4
6	B	305	CIT	C6-C3-C4-C5
6	B	308	CIT	C1-C2-C3-C6
6	B	305	CIT	C2-C3-C4-C5
3	A	302	EWV	S13-C10-C9-C22
4	B	303	PEG	C1-C2-O2-C3
3	B	302[B]	EWV	C9-C10-S13-C14
3	A	302	EWV	S13-C10-C9-O12
6	B	308	CIT	C1-C2-C3-O7
6	B	305	CIT	C2-C3-C6-O6
3	B	302[B]	EWV	S13-C10-C9-C22
3	B	302[A]	EWV	C5-C4-S6-N11
6	B	305	CIT	C2-C3-C6-O5
3	A	302	EWV	C1-C22-C9-C10
3	A	302	EWV	C3-C4-S6-N11
4	B	303	PEG	C4-C3-O2-C2
4	B	306	PEG	O1-C1-C2-O2
3	B	302[A]	EWV	C3-C4-S6-N11
3	B	302[B]	EWV	S13-C10-C9-O12
6	B	305	CIT	C3-C4-C5-O3
6	B	305	CIT	C3-C4-C5-O4
3	A	302	EWV	C1-C22-C9-O12

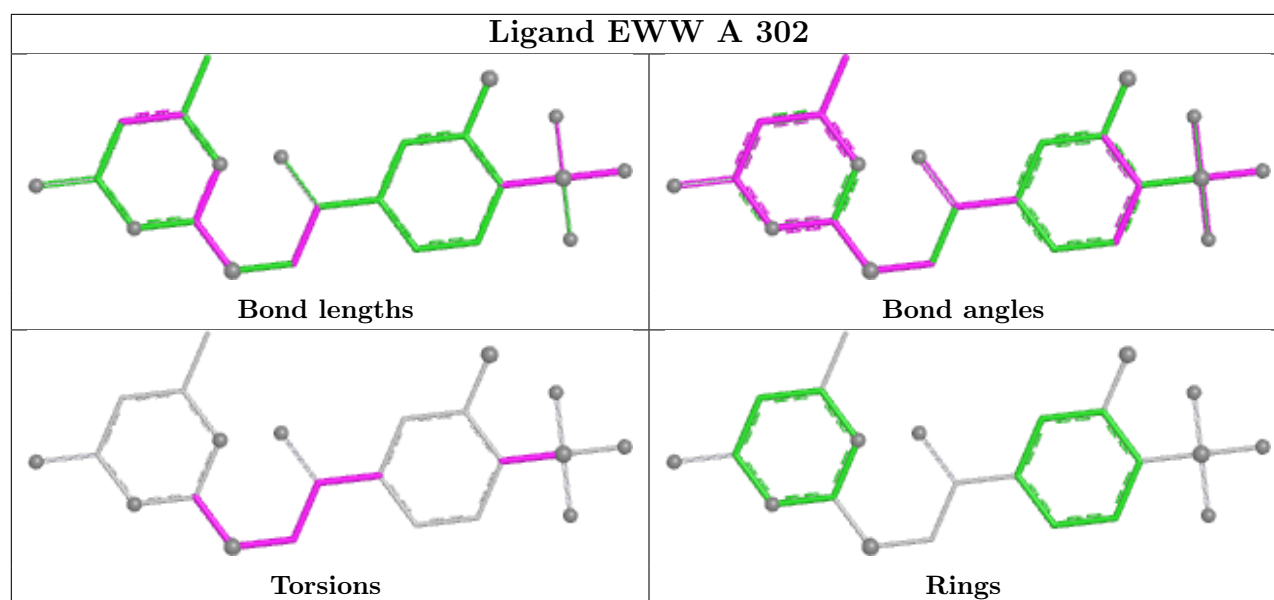
There are no ring outliers.

9 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	PEG	7	0
6	B	308	CIT	1	0
3	B	302[A]	EWV	11	0
6	B	305	CIT	1	0
3	B	302[B]	EWV	5	0
5	B	304	DMS	1	0
4	B	306	PEG	5	0
7	B	309	EDO	5	0
3	A	302	EWV	7	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 [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	260/263 (98%)	-0.34	4 (1%) 72 76	4, 14, 29, 48	12 (4%)
1	B	258/263 (98%)	-0.45	4 (1%) 70 75	6, 13, 27, 47	10 (3%)
All	All	518/526 (98%)	-0.40	8 (1%) 72 76	4, 13, 28, 48	22 (4%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	LEU	9.3
1	B	19	PHE	7.3
1	B	234	GLU	4.2
1	A	2	ARG	4.0
1	B	237	ALA	3.7
1	B	10[A]	HIS	3.0
1	A	72	ASP	2.1
1	A	235	GLY	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,

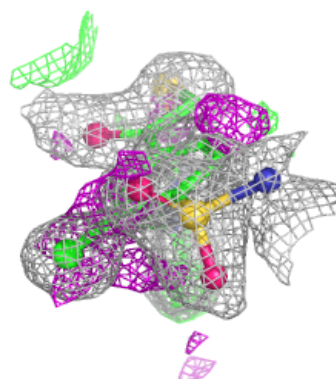
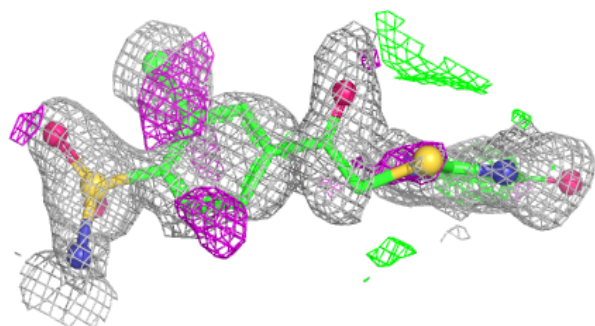
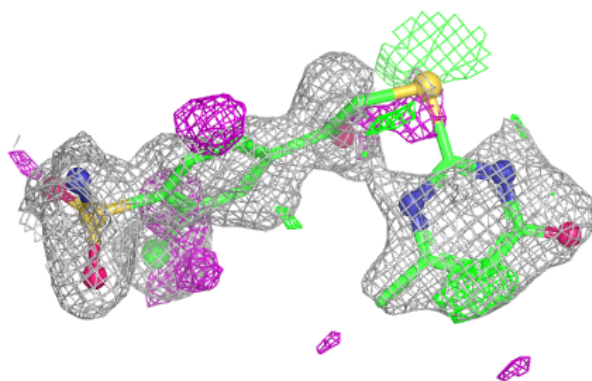
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	B	304	4/4	0.75	0.15	40,51,59,62	0
6	CIT	B	308	13/13	0.79	0.17	29,39,55,63	0
3	EWB	B	302[A]	23/23	0.82	0.17	17,26,32,36	23
6	CIT	B	305	13/13	0.82	0.14	23,36,53,59	0
3	EWB	B	302[B]	23/23	0.82	0.17	22,31,36,40	23
8	NI	A	303	1/1	0.85	0.17	67,67,67,67	0
4	PEG	B	306	7/7	0.87	0.10	28,34,47,47	0
7	EDO	B	309	4/4	0.88	0.18	31,32,35,39	0
7	EDO	B	307	4/4	0.89	0.10	28,29,29,29	0
4	PEG	B	303	7/7	0.90	0.10	22,27,31,35	0
3	EWB	A	302	23/23	0.93	0.16	13,36,84,90	0
2	ZN	A	301	1/1	1.00	0.02	8,8,8,8	0
2	ZN	B	301	1/1	1.00	0.01	10,10,10,10	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.

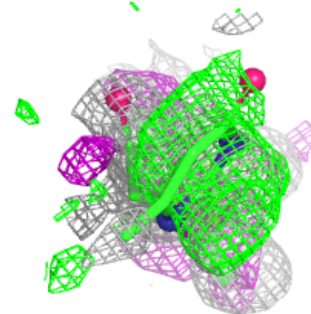
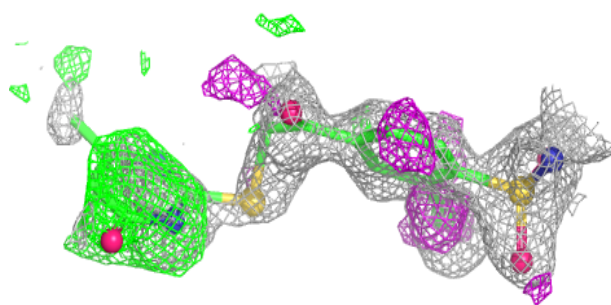
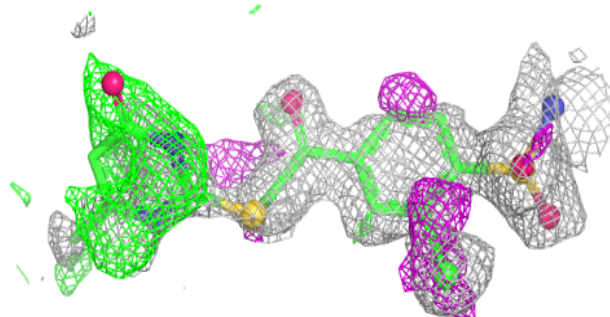
Electron density around EWB B 302 (A):

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

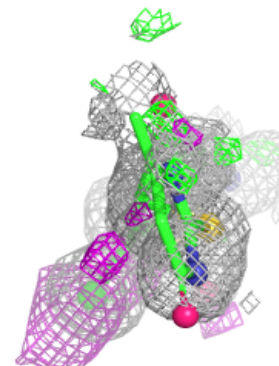
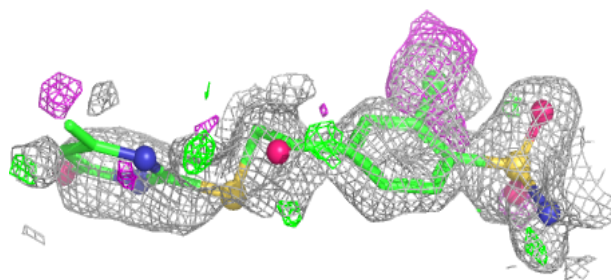
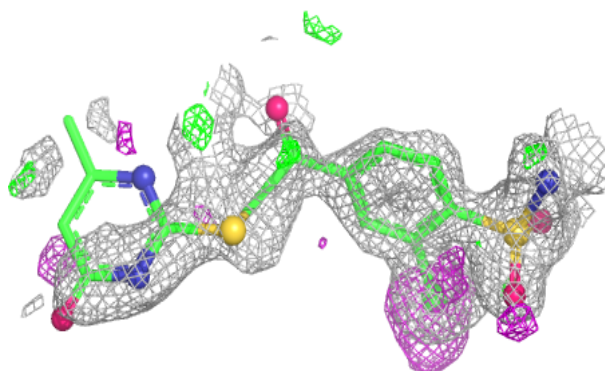


Electron density around EWW B 302 (B):

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

**Electron density around EWW A 302:**

$2mF_o-DF_c$ (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.