



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 10:34 AM UTC

PDB ID : 4KNN / pdb_00004knn
Title : Crystal structure of human carbonic anhydrase isozyme XIII with 2-Chloro-4-
-[(pyrimidin-2-ylsulfanyl)acetyl]benzenesulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2013-05-10
Resolution : 1.40 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

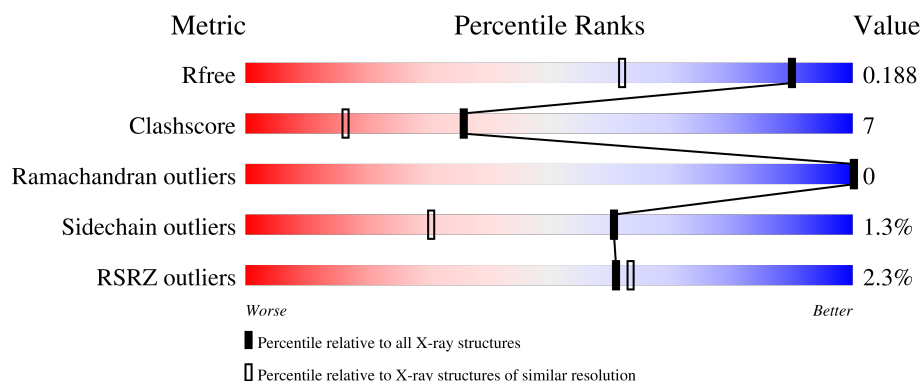
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	2% 74% 23% ..
1	B	263	3% 75% 22% ..

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	E1F	B	302[A]	-	X	-	-
6	ACY	B	306	-	-	X	-
7	PEG	A	304	-	X	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5047 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	11	0
			2143	1364	374	404	1			
1	A	258	Total	C	N	O	S	0	19	0
			2214	1407	387	419	1			

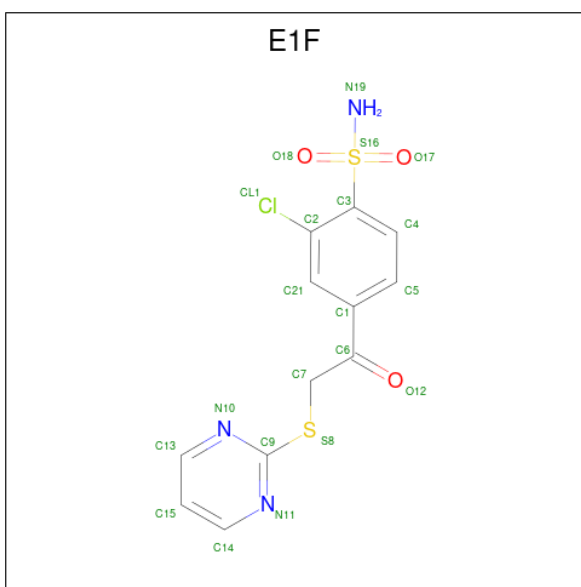
There are 2 discrepancies between the modelled and reference sequences:

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).

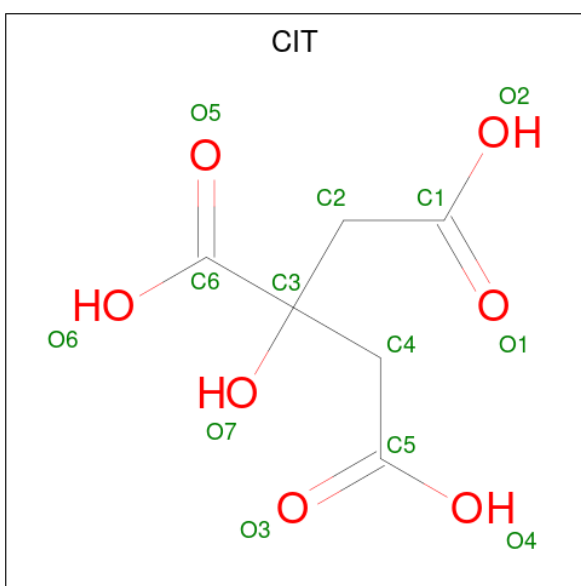
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is 2-chloro-4-[(pyrimidin-2-ylsulfanyl)acetyl]benzenesulfonamide (CCD ID: E1F) (formula: C₁₂H₁₀ClN₃O₃S₂).



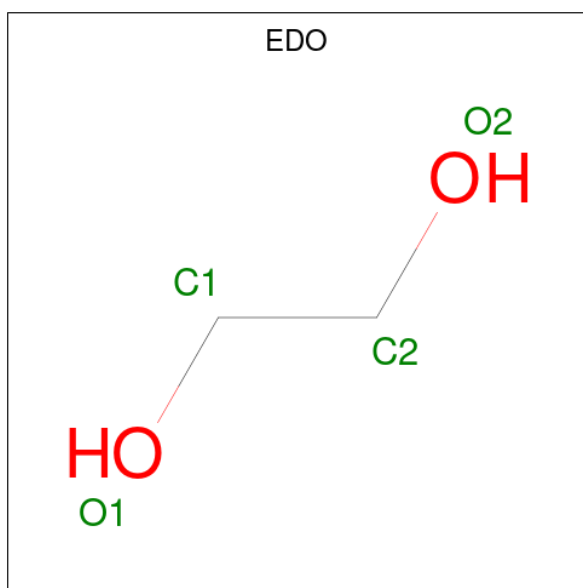
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	B	1	Total	C	Cl	N	O	S	0	1
			42	24	2	6	6	4		
3	A	1	Total	C	Cl	N	O	S	0	0
			21	12	1	3	3	2		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



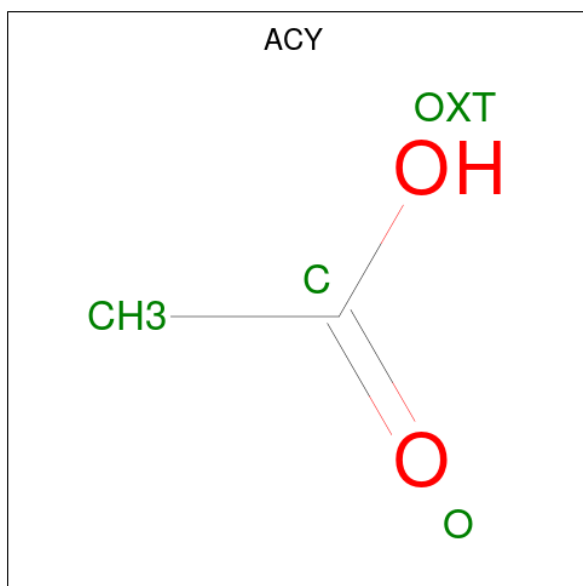
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	C O	0	0
			13	6 7		
4	A	1	Total	C O	0	0
			13	6 7		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



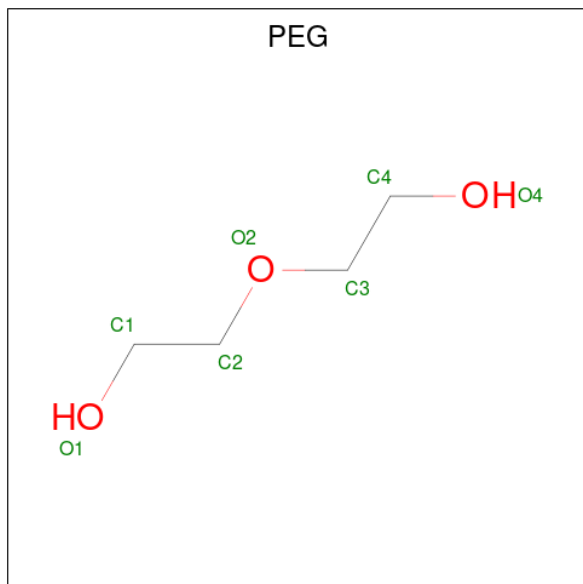
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 7 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



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

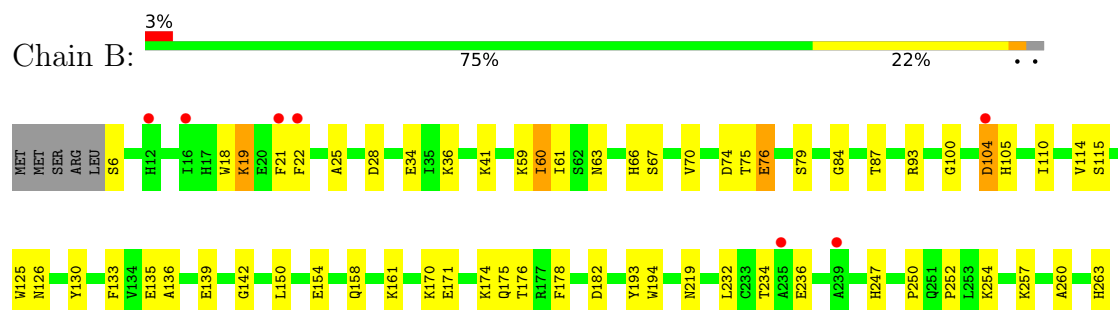
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	299	Total	O	0	0
			299	299		
8	A	269	Total	O	0	0
			269	269		

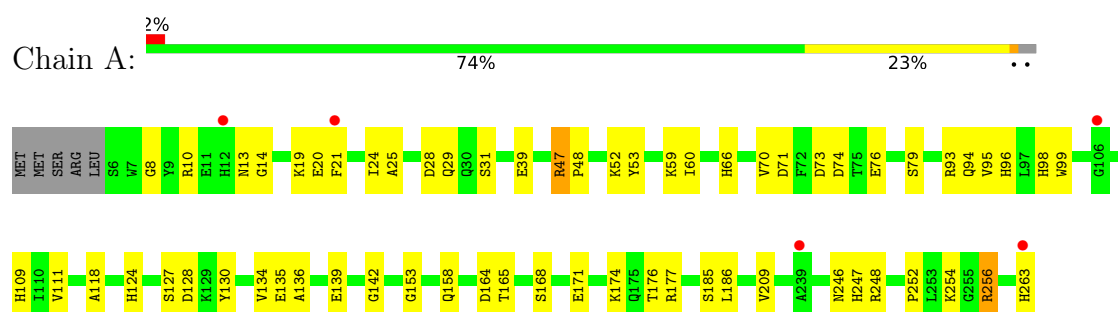
3 Residue-property plots [i](#)

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 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	56.18Å 57.47Å 159.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.07 – 1.40 54.07 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (54.07-1.40) 98.2 (54.07-1.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 1.41Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.166 , 0.191 0.162 , 0.188	Depositor DCC
R_{free} test set	9987 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5047	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 5.13% 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: CIT, PEG, ACY, EDO, E1F, 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	1.72	26/2278 (1.1%)	1.45	9/3095 (0.3%)
1	B	1.76	33/2206 (1.5%)	1.46	9/2997 (0.3%)
All	All	1.74	59/4484 (1.3%)	1.45	18/6092 (0.3%)

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	HIS	ND1-CE1	9.17	1.41	1.32
1	B	100	GLY	N-CA	7.99	1.52	1.45
1	A	109	HIS	ND1-CE1	7.73	1.40	1.32
1	A	76	GLU	N-CA	-7.46	1.36	1.45
1	A	247	HIS	ND1-CE1	7.46	1.40	1.32
1	B	130	TYR	CA-C	-7.38	1.45	1.52
1	A	153	GLY	N-CA	7.38	1.53	1.44
1	B	139	GLU	N-CA	-7.36	1.37	1.45
1	A	130	TYR	CA-CB	7.23	1.64	1.53
1	A	118	ALA	N-CA	6.97	1.54	1.46
1	A	134	VAL	N-CA	-6.96	1.38	1.46
1	A	24	ILE	CA-C	6.76	1.62	1.52
1	B	75	THR	N-CA	6.60	1.54	1.46
1	B	84	GLY	N-CA	6.50	1.53	1.44
1	B	247	HIS	ND1-CE1	6.49	1.39	1.32
1	B	234	THR	C-O	6.47	1.31	1.23
1	A	66	HIS	ND1-CE1	6.35	1.38	1.32
1	A	246	ASN	N-CA	6.29	1.54	1.46
1	A	98	HIS	CD2-NE2	6.21	1.44	1.37
1	B	114	VAL	N-CA	6.14	1.53	1.46
1	B	66	HIS	ND1-CE1	6.12	1.38	1.32
1	A	10	ARG	N-CA	6.11	1.53	1.45
1	A	13	ASN	N-CA	6.11	1.53	1.46
1	A	19	LYS	N-CA	6.05	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	254	LYS	CA-C	5.97	1.60	1.53
1	A	25	ALA	C-N	5.95	1.41	1.33
1	B	125	TRP	NE1-CE2	5.92	1.44	1.37
1	A	31	SER	CA-CB	5.92	1.61	1.54
1	B	150	LEU	N-CA	5.91	1.53	1.46
1	B	74	ASP	CA-C	5.87	1.61	1.52
1	B	130	TYR	CA-CB	5.87	1.62	1.54
1	B	126	ASN	CA-CB	-5.84	1.45	1.52
1	A	247	HIS	CE1-NE2	-5.75	1.26	1.32
1	B	87	THR	N-CA	5.73	1.53	1.46
1	B	67	SER	C-O	5.69	1.29	1.24
1	B	260	ALA	C-O	5.67	1.30	1.24
1	A	124	HIS	CE1-NE2	5.65	1.38	1.32
1	B	176	THR	N-CA	-5.62	1.39	1.45
1	B	260	ALA	CA-C	-5.59	1.46	1.52
1	B	93	ARG	CA-C	5.50	1.57	1.52
1	A	71	ASP	N-CA	5.48	1.52	1.46
1	B	36	LYS	CA-CB	5.47	1.60	1.53
1	B	232	LEU	C-O	5.46	1.30	1.23
1	B	61	ILE	C-O	5.45	1.29	1.24
1	A	95	VAL	N-CA	5.41	1.52	1.46
1	B	28	ASP	N-CA	-5.39	1.38	1.46
1	B	63	ASN	C-O	5.39	1.30	1.24
1	A	247	HIS	C-O	5.36	1.30	1.24
1	B	79	SER	CA-C	-5.35	1.46	1.52
1	B	194	TRP	CA-C	-5.30	1.46	1.52
1	A	164	ASP	N-CA	5.21	1.52	1.46
1	B	175	GLN	C-O	5.19	1.30	1.23
1	B	75	THR	CA-CB	5.18	1.61	1.53
1	A	256	ARG	CZ-NH2	-5.12	1.26	1.33
1	B	19	LYS	N-CA	5.09	1.52	1.46
1	B	60	ILE	C-O	5.09	1.29	1.23
1	A	248	ARG	N-CA	5.09	1.53	1.46
1	B	70	VAL	N-CA	-5.06	1.40	1.46
1	A	247	HIS	CA-C	-5.03	1.46	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	74	ASP	O-C-N	6.41	130.45	122.19
1	B	154	GLU	CA-CB-CG	6.19	126.48	114.10
1	B	18	TRP	CA-C-O	-5.84	114.36	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	N-CA-C	-5.80	105.70	112.89
1	A	186	LEU	CA-C-N	5.59	128.42	120.49
1	A	186	LEU	C-N-CA	5.59	128.42	120.49
1	A	165	THR	CA-C-O	5.56	125.80	119.18
1	A	209	VAL	N-CA-C	5.43	115.77	108.17
1	B	252	PRO	O-C-N	5.40	129.56	123.03
1	B	135	GLU	CA-C-O	5.37	126.12	120.42
1	A	99	TRP	CA-C-O	5.33	127.15	121.45
1	A	39	GLU	N-CA-C	5.30	119.73	113.16
1	A	127	SER	N-CA-C	-5.29	106.77	113.18
1	B	105	HIS	N-CA-CB	-5.25	102.87	111.74
1	A	76	GLU	CA-C-O	-5.21	115.23	121.11
1	B	76	GLU	CA-C-O	-5.03	115.38	121.32
1	B	193	TYR	N-CA-C	5.03	116.83	109.24
1	B	171	GLU	N-CA-C	5.01	118.12	110.20

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	2214	0	2137	39	0
1	B	2143	0	2071	21	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	21	0	9	0	0
3	B	42	0	18	4	0
4	A	13	0	5	0	0
4	B	13	0	5	1	0
5	A	4	0	6	0	0
5	B	8	0	12	1	0
6	B	12	0	9	4	0
7	A	7	0	9	8	0
8	A	269	0	0	6	0
8	B	299	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5047	0	4281	64	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 7.

All (64) 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:29:GLN:HE21	7:A:304:PEG:H22	0.97	1.12
1:A:29:GLN:NE2	7:A:304:PEG:H22	1.82	0.95
1:A:47:ARG:HA	1:A:47:ARG:HE	1.33	0.94
1:A:94[B]:GLN:HE22	1:A:96:HIS:HD1	1.06	0.94
1:A:93[A]:ARG:NH1	8:A:607:HOH:O	2.01	0.93
1:B:170:LYS:HE2	8:B:509:HOH:O	1.78	0.82
1:A:94[B]:GLN:NE2	1:A:96:HIS:HD1	1.80	0.79
1:A:29:GLN:HE21	7:A:304:PEG:C2	1.89	0.78
1:A:47:ARG:HE	1:A:47:ARG:CA	1.97	0.78
1:A:59:LYS:HE3	1:A:73[B]:ASP:OD1	1.84	0.78
1:A:74:ASP:OD1	1:A:93[B]:ARG:NH1	2.21	0.74
1:B:257:LYS:NZ	6:B:306:ACY:H1	2.09	0.67
6:B:307:ACY:H3	8:B:498:HOH:O	1.95	0.67
1:A:171:GLU:OE2	1:A:174[A]:LYS:HD2	1.96	0.65
1:A:94[B]:GLN:HE21	1:A:94[B]:GLN:C	2.06	0.64
1:A:111[B]:VAL:O	1:A:111[B]:VAL:HG13	1.97	0.64
5:B:305:EDO:H21	1:A:263:HIS:NE2	2.12	0.64
1:B:161[B]:LYS:HG2	1:B:178:PHE:CE1	2.35	0.61
1:B:110:ILE:HD12	1:B:115[A]:SER:OG	2.02	0.60
1:B:41:LYS:HD2	1:B:257:LYS:HG3	1.87	0.56
1:A:177[B]:ARG:NH2	8:A:659:HOH:O	1.67	0.56
1:B:104:ASP:N	1:B:104:ASP:OD1	2.39	0.55
1:B:257:LYS:HZ2	6:B:306:ACY:H1	1.71	0.55
1:B:133:PHE:CZ	3:B:302[A]:E1F:H8	2.42	0.54
1:B:161[B]:LYS:HG2	1:B:178:PHE:HE1	1.73	0.52
1:A:158:GLN:NE2	1:A:185[B]:SER:OG	2.42	0.52
1:B:158[A]:GLN:NE2	1:B:182:ASP:H	2.08	0.52
1:A:20:GLU:C	1:A:21:PHE:HD1	2.17	0.52
1:A:93[B]:ARG:HG3	1:A:94[B]:GLN:HB2	1.92	0.52
1:B:133:PHE:HZ	3:B:302[A]:E1F:H8	1.76	0.51
1:A:176[B]:THR:HG22	8:A:509:HOH:O	2.10	0.51
4:B:303:CIT:O1	4:B:303:CIT:C6	2.59	0.50
1:A:256:ARG:HG3	7:A:304:PEG:C1	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:ALA:O	1:B:142:GLY:HA3	2.13	0.49
3:B:302[A]:E1F:C15	8:B:644:HOH:O	2.61	0.49
1:A:168:SER:OG	1:A:176[B]:THR:HG21	2.12	0.48
1:A:28:ASP:HB3	7:A:304:PEG:H31	1.95	0.47
1:B:257:LYS:HZ3	6:B:306:ACY:H1	1.80	0.46
1:A:136:ALA:O	1:A:142:GLY:HA3	2.16	0.46
1:B:110:ILE:HD12	1:B:115[B]:SER:HB2	1.97	0.46
1:A:52:LYS:O	1:A:79:SER:HA	2.16	0.45
1:A:256:ARG:HG3	7:A:304:PEG:H12	1.98	0.45
1:B:59:LYS:C	1:B:60:ILE:HG13	2.40	0.45
1:A:53[B]:TYR:HD2	8:A:503:HOH:O	2.00	0.44
1:A:60[B]:ILE:HD13	1:A:60[B]:ILE:HA	1.74	0.44
1:A:70:VAL:O	1:A:94[A]:GLN:HA	2.17	0.44
1:A:252:PRO:HB2	1:A:254[A]:LYS:HG3	2.01	0.43
1:B:76:GLU:HB2	8:B:695:HOH:O	2.17	0.43
1:A:47:ARG:O	1:A:48:PRO:C	2.60	0.43
1:A:60[B]:ILE:HD12	1:A:60[B]:ILE:HG23	1.70	0.43
3:B:302[A]:E1F:C13	8:B:467:HOH:O	2.67	0.43
1:A:47:ARG:HA	1:A:47:ARG:NE	2.15	0.42
1:B:21[B]:PHE:HB3	1:B:22:PHE:CD2	2.54	0.42
1:A:135[B]:GLU:CD	1:A:135[B]:GLU:C	2.87	0.42
1:B:34:GLU:HG3	8:B:600:HOH:O	2.17	0.42
1:A:254[B]:LYS:O	7:A:304:PEG:O1	2.38	0.42
1:A:177[A]:ARG:NH2	8:A:659:HOH:O	2.51	0.42
1:A:8:GLY:O	1:A:14:GLY:HA2	2.20	0.41
1:B:219[B]:ASN:ND2	1:B:219[B]:ASN:H	2.18	0.41
1:A:177[A]:ARG:HD3	8:A:626:HOH:O	2.21	0.41
1:A:256:ARG:HG3	7:A:304:PEG:H11	2.03	0.41
1:B:19:LYS:HA	1:B:25:ALA:HB3	2.03	0.41
1:B:34:GLU:OE2	1:B:250:PRO:HG3	2.21	0.40
1:A:135[B]:GLU:OE2	1:A:139:GLU:OE2	2.40	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	275/263 (105%)	270 (98%)	5 (2%)	0	100	100
1	B	267/263 (102%)	260 (97%)	7 (3%)	0	100	100
All	All	542/526 (103%)	530 (98%)	12 (2%)	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	246/232 (106%)	245 (100%)	1 (0%)	84	67
1	B	238/232 (103%)	233 (98%)	5 (2%)	47	15
All	All	484/464 (104%)	478 (99%)	6 (1%)	61	34

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

Mol	Chain	Res	Type
1	B	6	SER
1	B	104	ASP
1	B	174	LYS
1	B	236	GLU
1	B	263	HIS
1	A	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	12	HIS
1	B	66	HIS
1	B	151	GLN
1	B	175	GLN

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Mol	Chain	Res	Type
1	A	29	GLN
1	A	66	HIS
1	A	69	ASN
1	A	158	GLN
1	A	251	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 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	CIT	B	303	-	12,12,12	1.83	2 (16%)	17,17,17	3.84	9 (52%)
6	ACY	B	307	-	3,3,3	0.75	0	3,3,3	1.36	0
5	EDO	A	305	-	3,3,3	1.16	0	2,2,2	1.63	1 (50%)
5	EDO	B	304	-	3,3,3	1.07	0	2,2,2	0.13	0
3	E1F	A	302	2	22,22,22	2.35	10 (45%)	31,31,31	2.55	10 (32%)
3	E1F	B	302[A]	2	22,22,22	3.07	9 (40%)	31,31,31	4.07	16 (51%)
6	ACY	B	306	-	3,3,3	0.87	0	3,3,3	0.77	0
7	PEG	A	304	-	6,6,6	0.90	0	5,5,5	2.77	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACY	B	308	-	3,3,3	0.86	0	3,3,3	0.69	0
4	CIT	A	303	-	12,12,12	1.71	2 (16%)	17,17,17	1.55	4 (23%)
3	E1F	B	302[B]	2	22,22,22	3.05	7 (31%)	31,31,31	2.70	15 (48%)
5	EDO	B	305	-	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	CIT	B	303	-	-	3/16/16/16	-
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	B	304	-	-	0/1/1/1	-
3	E1F	A	302	2	-	4/15/15/15	0/2/2/2
3	E1F	B	302[A]	2	-	9/15/15/15	0/2/2/2
7	PEG	A	304	-	-	3/4/4/4	-
4	CIT	A	303	-	-	0/16/16/16	-
3	E1F	B	302[B]	2	-	4/15/15/15	0/2/2/2
5	EDO	B	305	-	-	0/1/1/1	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302[B]	E1F	O18-S16	11.11	1.63	1.43
3	B	302[A]	E1F	O18-S16	9.35	1.60	1.43
3	B	302[B]	E1F	S16-N19	5.65	1.71	1.60
3	B	302[A]	E1F	C21-C2	5.05	1.46	1.38
3	A	302	E1F	S16-N19	4.93	1.70	1.60
3	B	302[A]	E1F	S16-N19	4.62	1.69	1.60
3	A	302	E1F	C9-S8	3.92	1.83	1.75
3	A	302	E1F	O18-S16	3.82	1.50	1.43
3	B	302[A]	E1F	O12-C6	3.66	1.28	1.22
3	B	302[B]	E1F	C1-C6	-3.59	1.44	1.49
3	A	302	E1F	C7-C6	-3.45	1.46	1.51
3	B	302[A]	E1F	C9-N11	3.44	1.39	1.33
3	B	302[B]	E1F	O17-S16	3.41	1.49	1.43
3	A	302	E1F	C9-N11	3.35	1.39	1.33
4	B	303	CIT	C4-C3	-3.15	1.50	1.54
4	A	303	CIT	C2-C3	3.13	1.57	1.54
4	A	303	CIT	C4-C3	2.94	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	303	CIT	O4-C5	-2.89	1.21	1.30
3	A	302	E1F	O12-C6	2.69	1.27	1.22
3	A	302	E1F	C7-S8	2.67	1.86	1.80
3	B	302[A]	E1F	C2-CL1	2.56	1.79	1.73
3	B	302[B]	E1F	C4-C3	-2.53	1.36	1.39
3	B	302[A]	E1F	C7-S8	2.47	1.86	1.80
3	A	302	E1F	C9-N10	2.40	1.38	1.33
3	B	302[B]	E1F	C21-C1	-2.37	1.35	1.39
3	B	302[A]	E1F	C21-C1	2.32	1.43	1.39
3	B	302[A]	E1F	C4-C5	2.30	1.42	1.38
3	A	302	E1F	C21-C2	2.28	1.42	1.38
3	A	302	E1F	C14-N11	2.23	1.39	1.34
3	B	302[B]	E1F	C9-S8	2.11	1.79	1.75

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302[A]	E1F	C7-S8-C9	-16.47	80.50	101.65
4	B	303	CIT	O7-C3-C6	-8.35	97.12	108.96
3	A	302	E1F	N10-C9-N11	-6.95	115.72	126.86
3	B	302[A]	E1F	C14-N11-C9	6.34	124.32	114.96
3	A	302	E1F	C14-N11-C9	6.20	124.10	114.96
4	B	303	CIT	C2-C3-C6	-6.18	96.37	110.03
4	B	303	CIT	C3-C4-C5	-6.12	97.18	113.92
3	A	302	E1F	C7-S8-C9	-5.73	94.29	101.65
3	B	302[B]	E1F	C7-S8-C9	-5.56	94.51	101.65
3	B	302[A]	E1F	C1-C21-C2	5.22	124.82	120.26
3	B	302[B]	E1F	C14-N11-C9	5.03	122.39	114.96
3	B	302[A]	E1F	C6-C7-S8	4.87	127.33	111.36
3	B	302[A]	E1F	N10-C9-N11	-4.85	119.09	126.86
4	B	303	CIT	C4-C3-C6	-4.84	99.33	110.03
4	B	303	CIT	O6-C6-C3	4.61	121.97	113.14
3	B	302[B]	E1F	O12-C6-C7	4.42	127.31	120.41
3	B	302[B]	E1F	C3-C2-CL1	4.28	124.61	121.52
3	B	302[B]	E1F	N10-C9-N11	-4.21	120.11	126.86
3	B	302[A]	E1F	C21-C2-C3	-4.21	117.29	121.36
7	A	304	PEG	O2-C2-C1	4.08	128.11	110.11
4	B	303	CIT	C4-C3-C2	3.99	119.56	109.31
3	A	302	E1F	C13-N10-C9	3.94	120.78	114.96
3	B	302[A]	E1F	C15-C14-N11	-3.94	117.19	123.42
3	B	302[A]	E1F	C5-C1-C21	-3.91	114.72	119.25
4	B	303	CIT	O7-C3-C2	3.68	117.76	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	303	CIT	O7-C3-C4	3.56	117.50	109.38
3	B	302[B]	E1F	C15-C14-N11	-3.56	117.78	123.42
3	B	302[B]	E1F	O17-S16-N19	3.53	112.44	107.35
7	A	304	PEG	O1-C1-C2	3.52	132.55	111.82
3	A	302	E1F	O17-S16-C3	-3.51	102.16	107.26
3	B	302[B]	E1F	C7-C6-C1	-3.41	114.10	117.99
3	B	302[A]	E1F	O18-S16-C3	3.23	111.95	107.26
3	B	302[A]	E1F	C21-C1-C6	3.21	127.18	120.18
3	B	302[B]	E1F	C21-C2-CL1	-3.12	113.34	118.45
3	B	302[B]	E1F	C13-N10-C9	3.12	119.56	114.96
3	A	302	E1F	C6-C7-S8	-3.11	101.18	111.36
3	B	302[B]	E1F	O18-S16-C3	-2.95	102.97	107.26
3	B	302[A]	E1F	C4-C3-S16	2.94	121.52	117.52
3	B	302[B]	E1F	C1-C21-C2	-2.92	117.71	120.26
3	B	302[A]	E1F	C2-C3-S16	-2.86	120.04	123.47
4	B	303	CIT	O6-C6-O5	-2.84	114.76	123.86
3	B	302[A]	E1F	O17-S16-N19	2.83	111.43	107.35
3	A	302	E1F	C3-C2-CL1	-2.65	119.60	121.52
3	B	302[B]	E1F	C4-C3-C2	2.59	120.91	119.05
3	A	302	E1F	C15-C14-N11	-2.54	119.40	123.42
4	A	303	CIT	O6-C6-C3	2.52	117.97	113.14
4	A	303	CIT	O4-C5-C4	2.47	122.18	114.35
4	A	303	CIT	C3-C2-C1	2.44	120.60	113.92
3	A	302	E1F	C7-C6-C1	2.38	120.71	117.99
3	B	302[B]	E1F	C2-C3-S16	-2.36	120.64	123.47
3	B	302[B]	E1F	S8-C9-N10	2.32	124.51	115.69
3	B	302[A]	E1F	O17-S16-C3	-2.30	103.91	107.26
3	A	302	E1F	O18-S16-C3	2.27	110.56	107.26
3	B	302[A]	E1F	C5-C4-C3	2.27	123.36	119.97
3	B	302[A]	E1F	C13-N10-C9	2.25	118.28	114.96
5	A	305	EDO	O2-C2-C1	2.15	128.80	112.39
7	A	304	PEG	C3-O2-C2	2.12	122.55	113.26
4	A	303	CIT	O4-C5-O3	-2.05	118.06	123.33

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302[A]	E1F	C1-C6-C7-S8
3	B	302[A]	E1F	O12-C6-C7-S8
3	B	302[A]	E1F	N11-C9-S8-C7
3	B	302[A]	E1F	N10-C9-S8-C7

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Mol	Chain	Res	Type	Atoms
3	A	302	E1F	C21-C1-C6-C7
3	A	302	E1F	C5-C1-C6-C7
3	A	302	E1F	C5-C1-C6-O12
3	A	302	E1F	C21-C1-C6-O12
7	A	304	PEG	C1-C2-O2-C3
7	A	304	PEG	O2-C3-C4-O4
3	B	302[A]	E1F	C5-C1-C6-O12
7	A	304	PEG	O1-C1-C2-O2
3	B	302[A]	E1F	C21-C1-C6-O12
3	B	302[A]	E1F	C5-C1-C6-C7
3	B	302[A]	E1F	C6-C7-S8-C9
3	B	302[B]	E1F	C21-C1-C6-O12
4	B	303	CIT	C2-C3-C4-C5
3	B	302[B]	E1F	C5-C1-C6-O12
3	B	302[A]	E1F	C21-C1-C6-C7
3	B	302[B]	E1F	C21-C1-C6-C7
3	B	302[B]	E1F	C5-C1-C6-C7
4	B	303	CIT	C4-C3-C6-O5
4	B	303	CIT	C2-C3-C6-O5

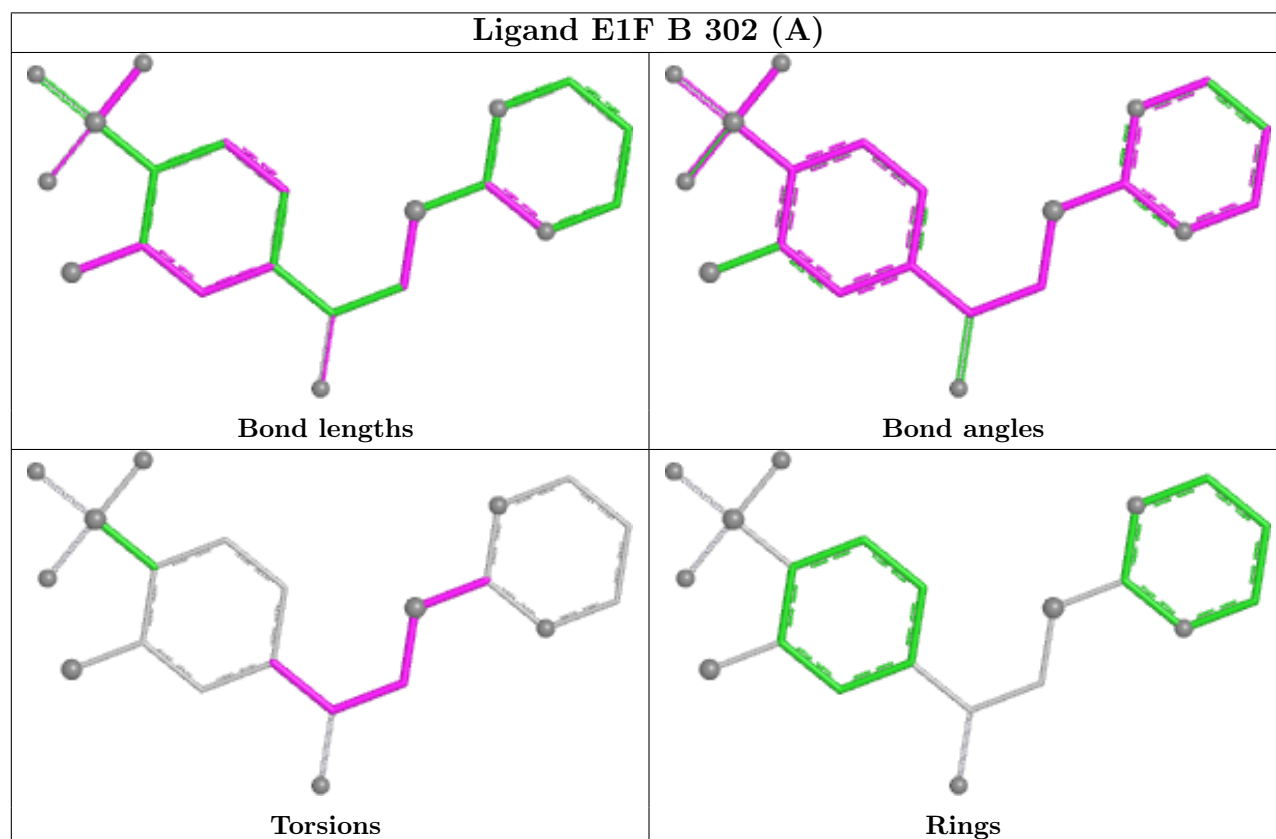
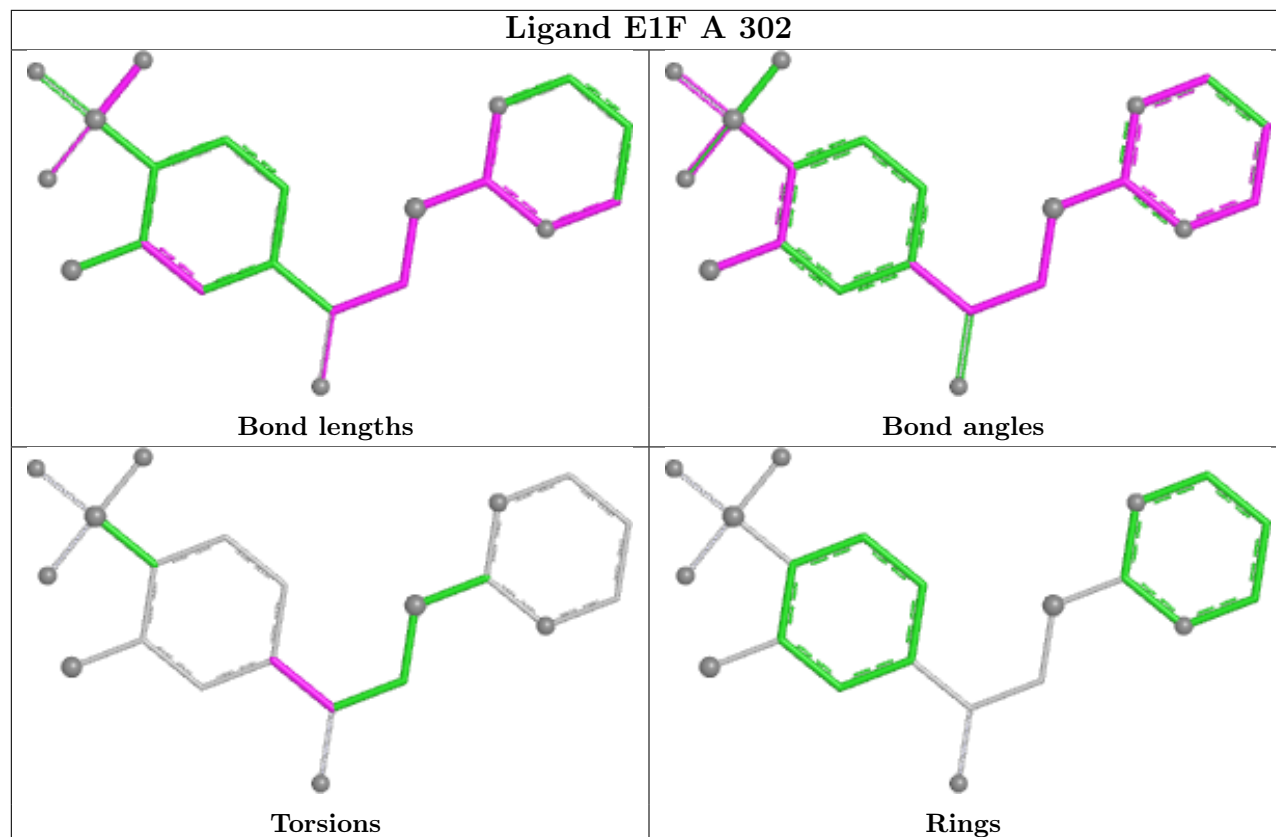
There are no ring outliers.

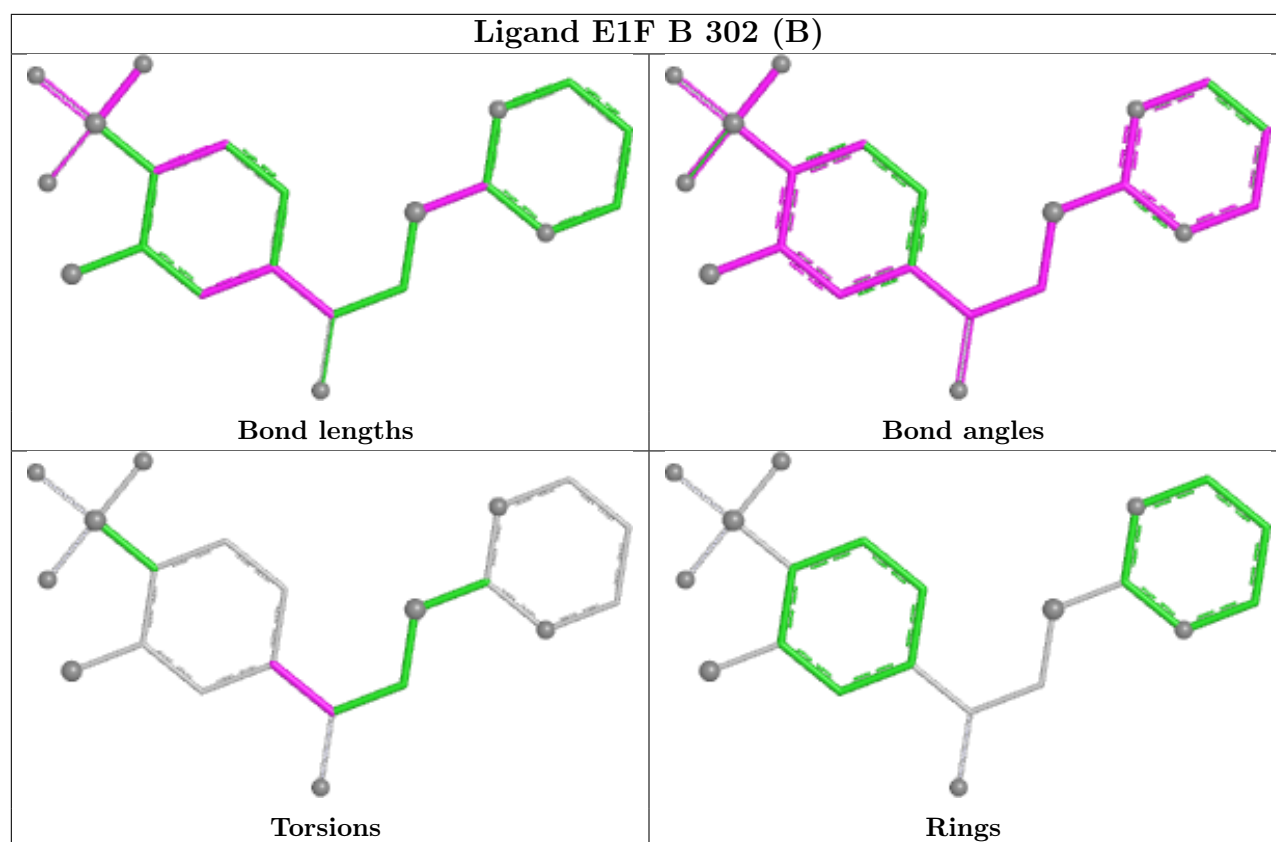
6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	CIT	1	0
6	B	307	ACY	1	0
3	B	302[A]	E1F	4	0
6	B	306	ACY	3	0
7	A	304	PEG	8	0
5	B	305	EDO	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/263 (98%)	-0.13	5 (1%) 66 69	5, 13, 27, 44	19 (7%)
1	B	258/263 (98%)	-0.12	7 (2%) 56 58	6, 14, 30, 57	11 (4%)
All	All	516/526 (98%)	-0.12	12 (2%) 61 63	5, 14, 30, 57	30 (5%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21[A]	PHE	7.1
1	A	12[A]	HIS	3.3
1	B	239	ALA	3.2
1	B	104	ASP	3.1
1	A	21	PHE	3.0
1	B	12	HIS	2.8
1	B	22	PHE	2.7
1	A	239	ALA	2.5
1	A	263	HIS	2.5
1	B	235	ALA	2.2
1	B	16	ILE	2.1
1	A	106	GLY	2.1

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

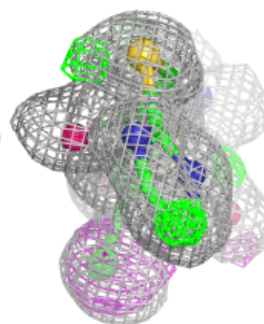
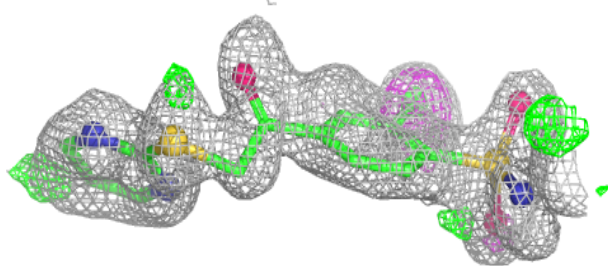
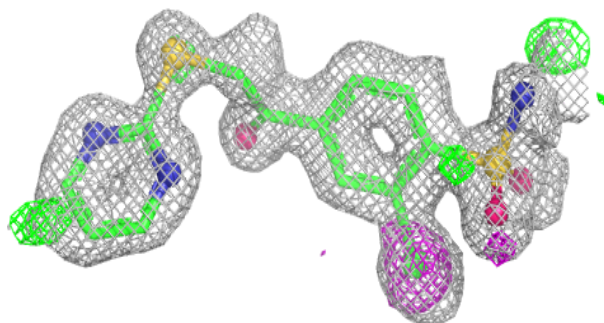
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	EDO	B	305	4/4	0.73	0.21	45,46,47,54	0
6	ACY	B	307	4/4	0.83	0.13	36,38,40,44	0
6	ACY	B	306	4/4	0.84	0.12	27,41,42,43	0
6	ACY	B	308	4/4	0.84	0.14	35,42,43,43	0
4	CIT	A	303	13/13	0.87	0.11	23,34,50,56	0
5	EDO	B	304	4/4	0.88	0.10	21,23,25,29	0
4	CIT	B	303	13/13	0.91	0.10	19,27,49,51	0
7	PEG	A	304	7/7	0.91	0.11	18,23,32,35	0
3	E1F	B	302[B]	21/21	0.92	0.15	10,16,18,19	21
5	EDO	A	305	4/4	0.92	0.10	20,23,29,29	0
3	E1F	B	302[A]	21/21	0.92	0.15	8,13,28,32	21
3	E1F	A	302	21/21	0.97	0.10	11,22,41,48	0
2	ZN	B	301	1/1	1.00	0.01	9,9,9,9	0
2	ZN	A	301	1/1	1.00	0.01	8,8,8,8	0

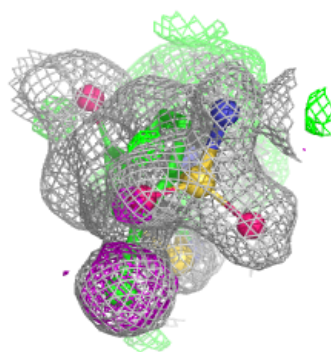
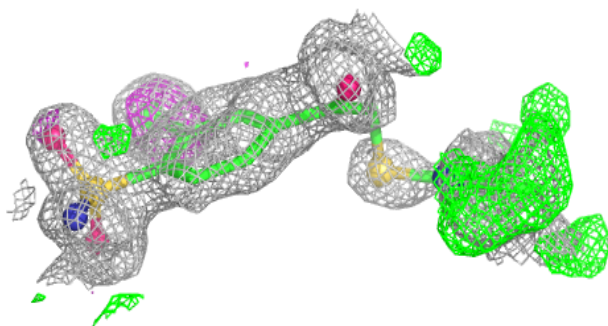
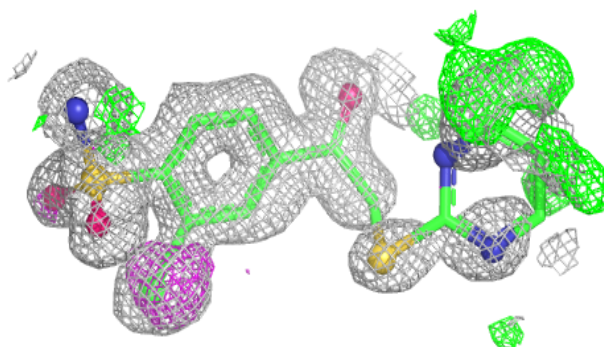
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around E1F 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)

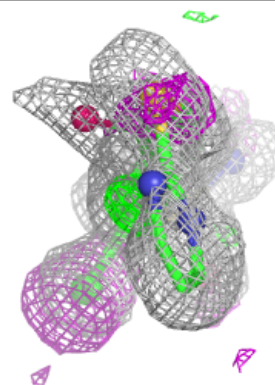
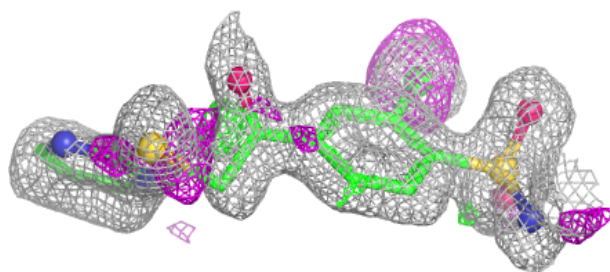
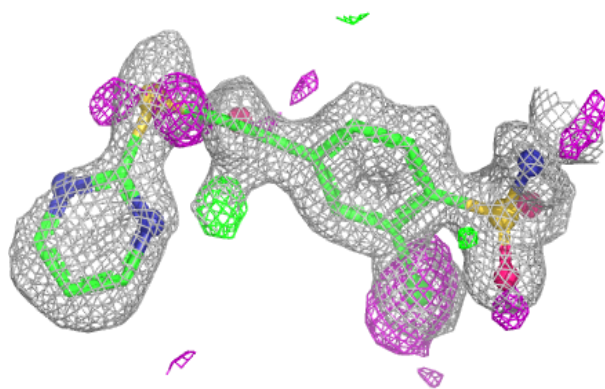
**Electron density around E1F B 302 (A):**

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



Electron density around E1F 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.