



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2024 – 07:09 am GMT

PDB ID : 5OHH
Title : Crystal structure of human carbonic anhydrase isozyme XIII with 2-[(1S)-2,3-Dihydro-1H-inden-1-ylamino]-3,5,6-trifluoro-4-[(2-hydroxyethyl)thio]benzene sulfonamide
Authors : Smirnov, A.; Manakova, E.; Grazulis, S.
Deposited on : 2017-07-17
Resolution : 1.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

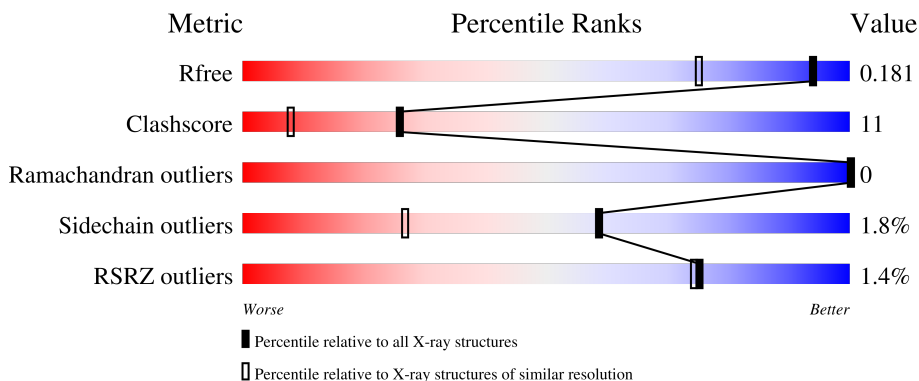
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2579 (1.44-1.40)
Clashscore	141614	2696 (1.44-1.40)
Ramachandran outliers	138981	2632 (1.44-1.40)
Sidechain outliers	138945	2631 (1.44-1.40)
RSRZ outliers	127900	2528 (1.44-1.40)

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	 83% 13% 2% 2%
1	B	263	 84% 14% 2% 2%

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	CIT	B	302	-	X	-	-
3	CIT	B	312	-	X	-	-
5	AZI	B	305	-	-	X	-
6	BCN	B	306	-	-	X	-
7	PEG	A	302	-	X	X	-
7	PEG	B	309	-	-	X	-
8	LCP	B	310	-	X	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5154 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
			Total	C	N	O	S			
1	B	258	2146	1367	371	407	1	0	12	0
1	A	259	2159	1376	370	412	1	0	12	0

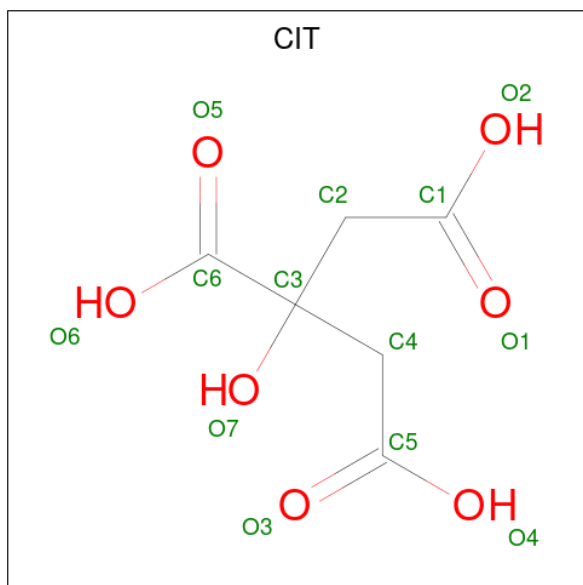
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP Q8N1Q1
A	1	MET	-	initiating methionine	UNP Q8N1Q1

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

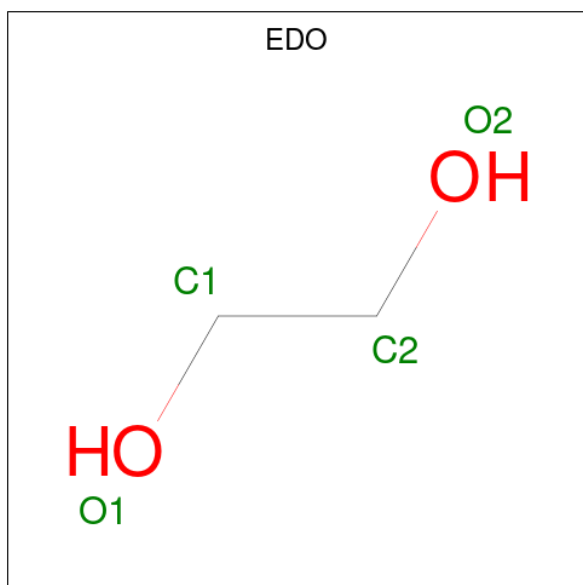
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	B	1	1	1	0	0
2	A	1	1	1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



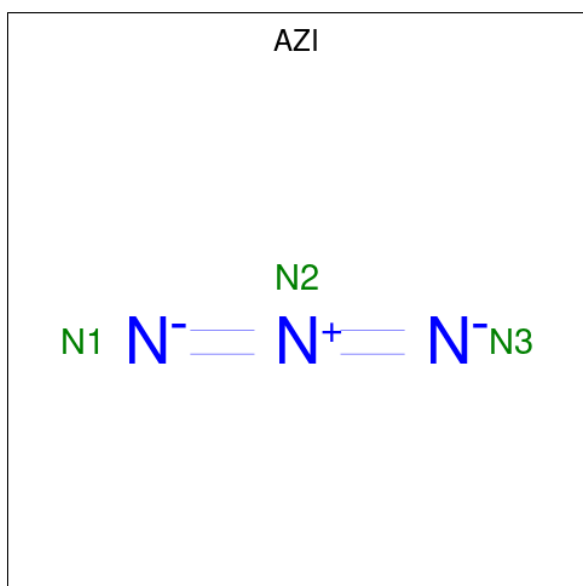
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		
3	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



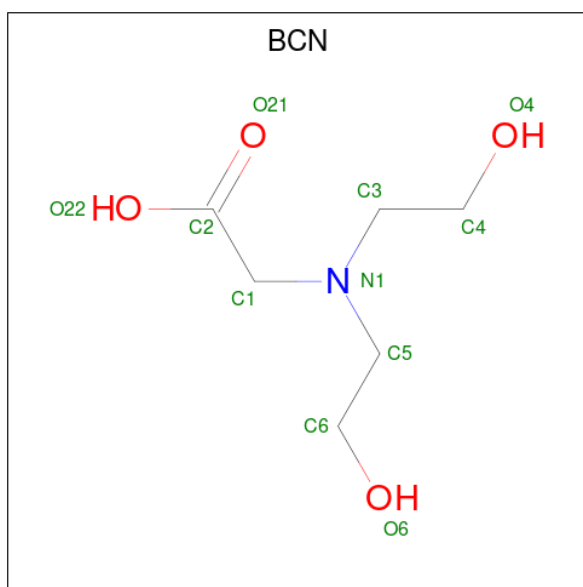
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is AZIDE ION (three-letter code: AZI) (formula: N₃).



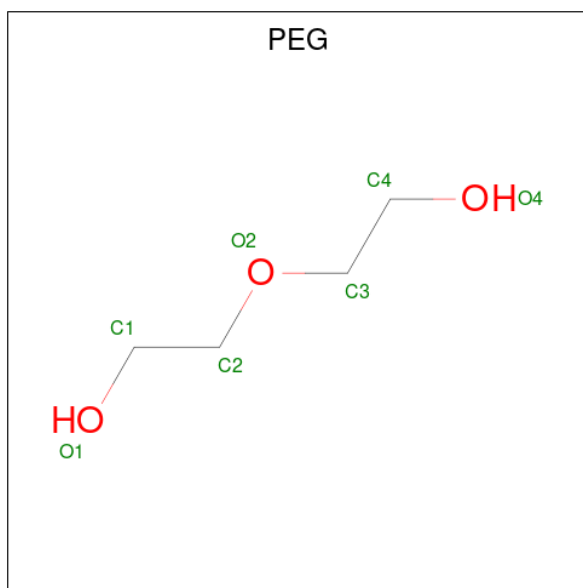
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total N 3 3	0	0

- Molecule 6 is BICINE (three-letter code: BCN) (formula: C₆H₁₃NO₄).



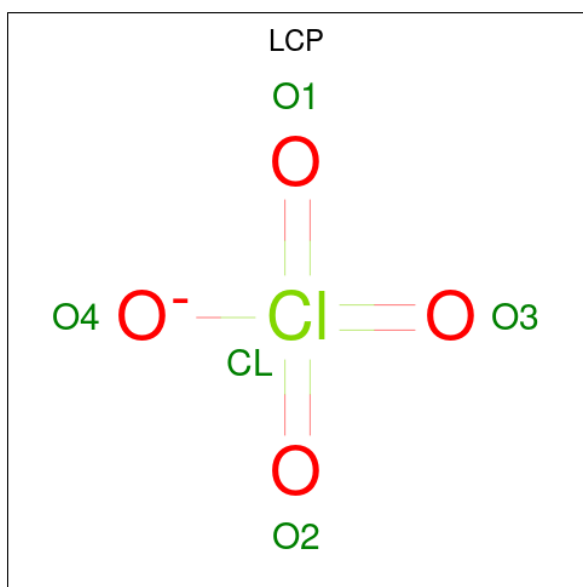
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
6	B	1	11	6	1	4	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



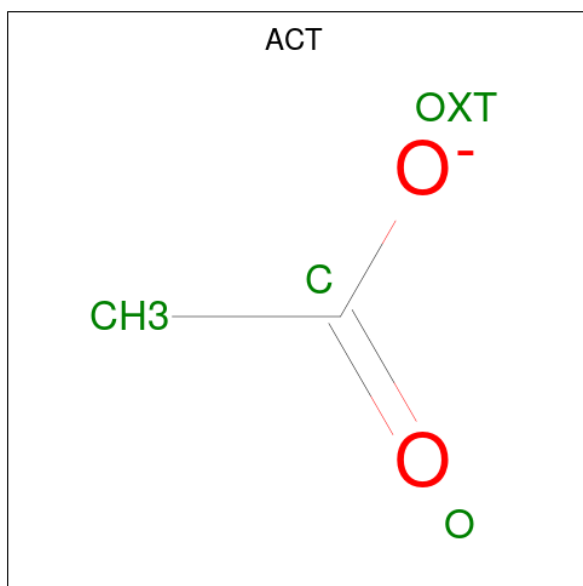
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	B	1	7	4	3	0	0
7	A	1	7	4	3	0	0

- Molecule 8 is PERCHLORATE ION (three-letter code: LCP) (formula: ClO_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Cl	O	0	0
			5	1	4		

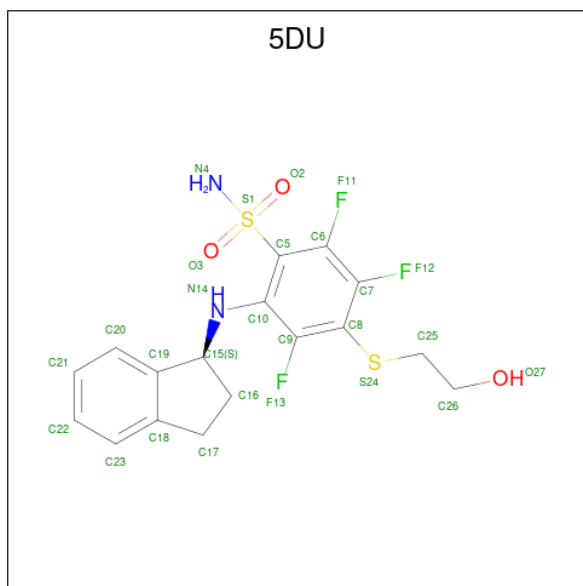
- Molecule 9 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 10 is 2-[(1S)-2,3-dihydro-1H-inden-1-ylamino]-3,5,6-trifluoro-4-[(2-hydroxyethyl)su

lfanyl]benzenesulfonamide (three-letter code: 5DU) (formula: C₁₇H₁₇F₃N₂O₃S₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	N	O			S
10	B	1	27	17	3	2	3	2	0	0

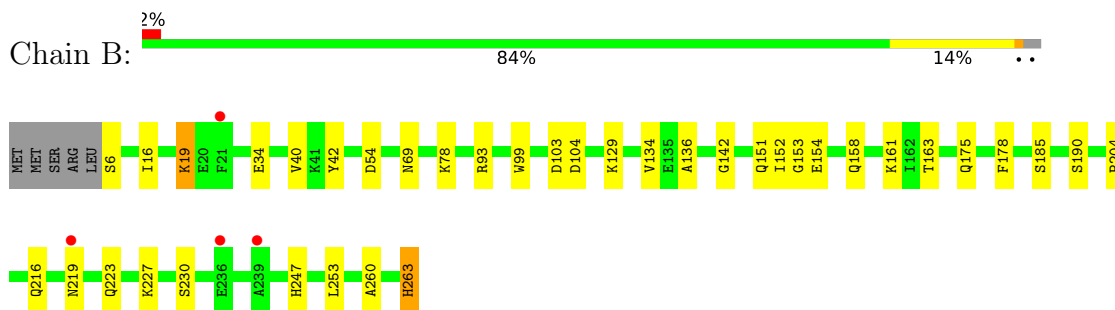
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	355	Total	O	0	0
			355	355		
11	A	344	Total	O	0	0
			344	344		

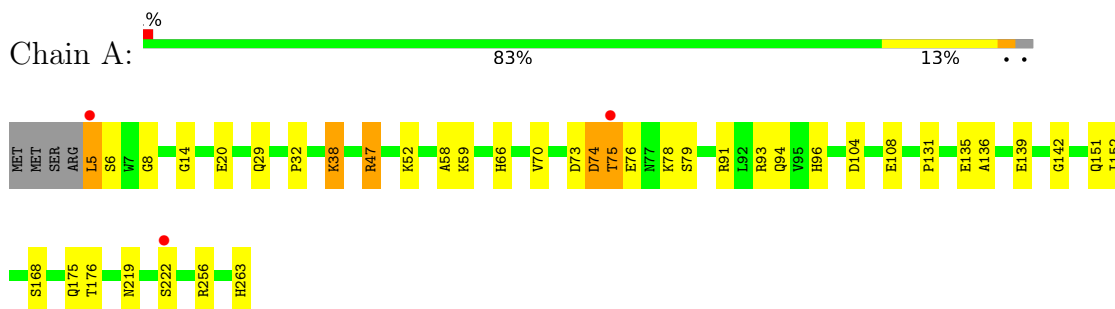
3 Residue-property plots [i](#)

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 i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.50Å 57.42Å 159.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.04 – 1.42 54.04 – 1.42	Depositor EDS
% Data completeness (in resolution range)	100.0 (54.04-1.42) 100.0 (54.04-1.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.27 (at 1.42Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.185 0.154 , 0.181	Depositor DCC
R_{free} test set	9977 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtrriage
Anisotropy	0.419	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.021 for k,h,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5154	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BCN, LCP, ACT, EDO, PEG, 5DU, CIT, AZI, 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	1.26	0/2222	1.22	0/3024
1	B	1.25	0/2209	1.13	1/3002 (0.0%)
All	All	1.26	0/4431	1.17	1/6026 (0.0%)

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

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	175	GLN	CA-CB-CG	5.54	125.60	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	74[B]	ASP	Peptide

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	2159	0	2081	47	1
1	B	2146	0	2078	34	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	26	0	10	1	0
3	B	26	0	10	3	0
4	A	12	0	18	1	0
4	B	16	0	24	4	0
5	B	3	0	0	2	0
6	B	11	0	12	6	0
7	A	7	0	10	7	0
7	B	7	0	10	8	0
8	B	5	0	0	3	0
9	A	4	0	3	0	0
9	B	4	0	3	0	0
10	B	27	0	0	3	0
11	A	344	0	0	14	0
11	B	355	0	0	12	0
All	All	5154	0	4259	92	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (92) 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:76[A]:GLU:HB2	11:A:572:HOH:O	1.31	1.29
7:B:309:PEG:H31	11:B:472:HOH:O	1.43	1.16
1:B:219[B]:ASN:ND2	11:B:402:HOH:O	1.82	1.09
6:B:306:BCN:H31	1:A:263:HIS:HE1	1.06	1.08
1:A:59:LYS:HE2	1:A:73[B]:ASP:OD1	1.52	1.06
6:B:306:BCN:H31	1:A:263:HIS:CE1	1.92	1.04
1:A:59:LYS:HE2	1:A:73[A]:ASP:HB2	1.47	0.97
1:A:74[B]:ASP:OD1	1:A:93:ARG:NH1	1.98	0.97
1:A:29:GLN:HE21	7:A:302:PEG:H31	1.28	0.96
1:A:256:ARG:HG3	7:A:302:PEG:H42	1.53	0.89
1:A:47:ARG:HA	1:A:47:ARG:HE	1.38	0.86
6:B:306:BCN:C3	1:A:263:HIS:HE1	1.89	0.85
1:B:153:GLY:HA3	1:B:219[A]:ASN:HD22	1.41	0.85
6:B:306:BCN:C3	1:A:263:HIS:CE1	2.63	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ARG:NH2	10:B:313:5DU:N4	2.31	0.77
1:A:135[A]:GLU:OE1	1:A:139:GLU:OE2	2.06	0.73
5:B:305:AZI:N1	11:B:406:HOH:O	2.20	0.73
1:A:152:ILE:HG13	4:A:305:EDO:H11	1.70	0.73
1:A:66:HIS:HE1	11:A:686:HOH:O	1.74	0.71
1:A:29:GLN:HG2	7:A:302:PEG:H41	1.72	0.71
1:B:69:ASN:OD1	11:B:404:HOH:O	2.09	0.71
1:A:256:ARG:CG	7:A:302:PEG:H42	2.24	0.68
1:B:16:ILE:O	1:B:19:LYS:HE2	1.93	0.68
1:A:29:GLN:HE21	7:A:302:PEG:C3	2.05	0.67
1:B:230[A]:SER:OG	11:B:403:HOH:O	1.98	0.66
10:B:313:5DU:O27	11:B:405:HOH:O	2.14	0.66
1:B:42:TYR:HE2	6:B:306:BCN:H41	1.62	0.64
1:B:263:HIS:HE1	11:A:630:HOH:O	1.80	0.64
1:B:253:LEU:HB2	7:B:309:PEG:H41	1.79	0.64
1:B:34[A]:GLU:HG3	11:B:700:HOH:O	2.01	0.60
1:A:47:ARG:HA	1:A:47:ARG:NE	2.12	0.60
1:B:204:PRO:HG3	10:B:313:5DU:C23	2.32	0.60
1:A:104:ASP:O	11:A:402:HOH:O	2.17	0.58
1:A:20:GLU:OE2	11:A:403:HOH:O	2.17	0.58
1:A:29:GLN:NE2	7:A:302:PEG:H31	2.09	0.58
1:A:176[B]:THR:HG22	11:A:568:HOH:O	2.04	0.58
1:B:42:TYR:CE2	6:B:306:BCN:H41	2.39	0.57
1:A:151:GLN:HE21	1:A:219:ASN:ND2	2.03	0.57
1:A:176[A]:THR:HG22	11:A:546:HOH:O	2.04	0.56
7:B:309:PEG:H11	8:B:310:LCP:O4	2.05	0.56
1:A:78[A]:LYS:HD2	11:A:406:HOH:O	2.06	0.56
1:A:175:GLN:C	1:A:176[A]:THR:CG2	2.76	0.53
3:B:312:CIT:O4	3:B:312:CIT:O7	2.26	0.52
7:B:309:PEG:H32	11:B:700:HOH:O	2.10	0.52
1:B:253:LEU:HD22	7:B:309:PEG:H21	1.92	0.51
1:A:175:GLN:C	1:A:176[A]:THR:HG23	2.29	0.51
1:B:54:ASP:OD2	1:B:78[B]:LYS:HE2	2.10	0.51
1:A:131:PRO:HG2	1:A:135[B]:GLU:HG3	1.92	0.51
1:A:175:GLN:O	1:A:176[A]:THR:HG22	2.10	0.51
1:B:99:TRP:O	1:B:247:HIS:HD2	1.94	0.49
1:B:154[A]:GLU:HG2	11:B:416:HOH:O	2.12	0.49
1:B:104:ASP:HA	11:B:422:HOH:O	2.12	0.49
7:B:309:PEG:O2	8:B:310:LCP:O2	2.32	0.48
1:A:175:GLN:O	1:A:176[A]:THR:CG2	2.62	0.48
1:B:161:LYS:HG2	1:B:178:PHE:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:SER:H	1:B:216:GLN:NE2	2.13	0.47
5:B:305:AZI:N2	11:B:405:HOH:O	2.35	0.47
1:A:176[B]:THR:CG2	11:A:568:HOH:O	2.60	0.47
1:A:38:LYS:NZ	11:A:401:HOH:O	2.14	0.47
1:A:5:LEU:HD23	1:A:6:SER:H	1.80	0.47
1:B:40:VAL:HG11	1:B:260:ALA:HB2	1.98	0.46
1:B:247:HIS:HE1	3:B:302:CIT:O6	1.98	0.46
1:B:223:GLN:HA	4:B:308:EDO:H12	1.97	0.46
7:B:309:PEG:C2	11:B:472:HOH:O	2.63	0.46
1:B:103:ASP:HB2	4:B:307:EDO:H12	1.96	0.46
1:B:152:ILE:HG21	4:B:307:EDO:H21	1.97	0.45
1:B:103:ASP:CB	4:B:307:EDO:H12	2.47	0.45
1:B:136:ALA:O	1:B:142:GLY:HA3	2.17	0.45
1:A:136:ALA:O	1:A:142:GLY:HA3	2.17	0.45
1:A:52:LYS:O	1:A:79:SER:HA	2.17	0.44
1:B:247:HIS:HE1	3:B:302:CIT:C6	2.30	0.44
1:A:29:GLN:CG	7:A:302:PEG:H41	2.46	0.43
1:A:168:SER:OG	1:A:176[A]:THR:HG21	2.18	0.43
1:B:151:GLN:O	1:B:219[A]:ASN:HA	2.19	0.43
1:A:78[A]:LYS:NZ	11:A:406:HOH:O	2.36	0.42
1:A:32:PRO:HG3	1:A:108:GLU:HB3	2.02	0.42
1:A:74[A]:ASP:C	1:A:91:ARG:HD3	2.40	0.42
1:B:158:GLN:NE2	1:B:185[A]:SER:OG	2.53	0.42
1:B:104:ASP:N	1:B:104:ASP:OD1	2.50	0.41
1:B:163:THR:HB	1:B:227[B]:LYS:HD3	2.01	0.41
1:A:131:PRO:HD2	1:A:135[A]:GLU:HG2	2.01	0.41
1:A:8:GLY:O	1:A:14:GLY:HA2	2.21	0.41
1:B:129:LYS:HE2	1:B:129:LYS:HB3	1.85	0.41
1:A:73[B]:ASP:HB2	11:A:572:HOH:O	2.21	0.41
1:A:94[B]:GLN:CD	1:A:96:HIS:HD1	2.24	0.41
1:B:227[A]:LYS:HE3	1:B:227[A]:LYS:HB3	1.91	0.41
7:B:309:PEG:C1	8:B:310:LCP:O4	2.68	0.41
1:A:58:ALA:O	1:A:59:LYS:HD3	2.20	0.41
1:A:222[B]:SER:HB2	11:A:519:HOH:O	2.21	0.41
1:A:70:VAL:O	1:A:94[B]:GLN:HA	2.21	0.40
3:A:306:CIT:C1	11:A:518:HOH:O	2.70	0.40
1:B:40:VAL:CG1	1:B:260:ALA:HB2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ASP:OD2	1:A:75[B]:THR:CG2[4_545]	1.81	0.39

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	269/263 (102%)	264 (98%)	5 (2%)	0	100	100
1	B	268/263 (102%)	261 (97%)	7 (3%)	0	100	100
All	All	537/526 (102%)	525 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	240/232 (103%)	235 (98%)	5 (2%)	53	20
1	B	239/232 (103%)	235 (98%)	4 (2%)	60	29
All	All	479/464 (103%)	470 (98%)	9 (2%)	59	24

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	6	SER
1	B	19	LYS
1	B	134	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	263	HIS
1	A	5	LEU
1	A	38	LYS
1	A	47	ARG
1	A	75[A]	THR
1	A	75[B]	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	HIS
1	B	151	GLN
1	B	175	GLN
1	B	216	GLN
1	B	247	HIS
1	A	29	GLN
1	A	66	HIS
1	A	219	ASN
1	A	251	GLN
1	A	263	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 2 are monoatomic - leaving 19 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
3	CIT	B	302	-	12,12,12	2.84	3 (25%)	17,17,17	3.76	9 (52%)
4	EDO	B	304	-	3,3,3	1.05	0	2,2,2	0.18	0
3	CIT	A	306	-	12,12,12	2.08	3 (25%)	17,17,17	1.78	3 (17%)
6	BCN	B	306	-	10,10,10	1.07	0	11,11,11	1.50	3 (27%)
8	LCP	B	310	-	4,4,4	4.01	4 (100%)	6,6,6	1.94	2 (33%)
4	EDO	B	307	-	3,3,3	0.60	0	2,2,2	1.51	0
4	EDO	A	305	-	3,3,3	0.58	0	2,2,2	1.10	0
9	ACT	B	311	2	3,3,3	1.03	0	3,3,3	0.36	0
4	EDO	B	308	-	3,3,3	1.10	0	2,2,2	1.04	0
4	EDO	B	303	-	3,3,3	1.19	0	2,2,2	0.76	0
7	PEG	B	309	-	6,6,6	0.68	0	5,5,5	1.53	1 (20%)
3	CIT	A	308	-	12,12,12	1.35	1 (8%)	17,17,17	1.38	3 (17%)
7	PEG	A	302	-	6,6,6	0.72	0	5,5,5	3.84	5 (100%)
10	5DU	B	313	-	28,29,29	2.91	8 (28%)	37,43,43	2.19	8 (21%)
3	CIT	B	312	-	12,12,12	1.53	2 (16%)	17,17,17	2.04	7 (41%)
4	EDO	A	304	-	3,3,3	0.90	0	2,2,2	0.44	0
9	ACT	A	307	2	3,3,3	0.95	0	3,3,3	0.86	0
5	AZI	B	305	-	0,2,2	-	-	0,1,1	-	-
4	EDO	A	303	-	3,3,3	0.78	0	2,2,2	0.36	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	EDO	B	307	-	-	1/1/1/1	-
4	EDO	A	305	-	-	1/1/1/1	-
3	CIT	A	308	-	-	0/16/16/16	-
7	PEG	A	302	-	-	2/4/4/4	-
10	5DU	B	313	-	-	7/14/23/23	0/3/3/3
3	CIT	B	302	-	-	10/16/16/16	-
3	CIT	B	312	-	-	15/16/16/16	-
4	EDO	B	304	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	308	-	-	1/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
3	CIT	A	306	-	-	5/16/16/16	-
6	BCN	B	306	-	-	7/10/10/10	-
4	EDO	A	304	-	-	1/1/1/1	-
7	PEG	B	309	-	-	2/4/4/4	-
4	EDO	A	303	-	-	0/1/1/1	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	313	5DU	S1-N4	8.28	1.76	1.60
3	B	302	CIT	C3-C6	-7.90	1.45	1.53
10	B	313	5DU	O3-S1	7.32	1.57	1.43
10	B	313	5DU	O2-S1	6.92	1.56	1.43
8	B	310	LCP	O2-CL	5.96	1.71	1.41
3	A	306	CIT	C2-C3	4.20	1.59	1.53
10	B	313	5DU	F11-C6	3.95	1.41	1.35
8	B	310	LCP	O3-CL	3.42	1.58	1.41
10	B	313	5DU	C16-C15	3.37	1.58	1.54
3	B	302	CIT	C2-C3	3.30	1.57	1.53
3	A	306	CIT	O7-C3	3.28	1.49	1.43
8	B	310	LCP	O4-CL	2.97	1.58	1.41
3	A	306	CIT	C4-C3	2.90	1.57	1.53
3	B	312	CIT	C3-C6	2.89	1.56	1.53
8	B	310	LCP	O1-CL	2.87	1.56	1.41
3	B	302	CIT	O2-C1	-2.83	1.21	1.30
3	B	312	CIT	O5-C6	2.38	1.29	1.22
10	B	313	5DU	C15-N14	2.21	1.49	1.45
3	A	308	CIT	O7-C3	2.14	1.47	1.43
10	B	313	5DU	C20-C19	2.14	1.42	1.39
10	B	313	5DU	C22-C23	2.04	1.43	1.38

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	CIT	O5-C6-C3	-9.10	109.37	122.25
7	A	302	PEG	C3-O2-C2	6.37	140.90	113.29
3	B	302	CIT	C4-C3-C6	-5.96	97.30	110.11
3	B	302	CIT	C4-C3-C2	5.63	123.85	109.16
10	B	313	5DU	O2-S1-O3	-5.42	109.85	118.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	313	5DU	C16-C17-C18	-5.42	98.04	103.31
10	B	313	5DU	C5-S1-N4	4.98	117.46	108.26
10	B	313	5DU	O3-S1-N4	-4.67	100.44	107.36
3	B	302	CIT	C3-C4-C5	-4.66	102.53	113.81
3	B	302	CIT	O7-C3-C6	-4.51	102.53	108.86
10	B	313	5DU	C7-C6-C5	-4.09	116.55	121.74
3	B	312	CIT	O7-C3-C6	4.05	114.56	108.86
3	A	306	CIT	O6-C6-C3	3.98	119.97	113.05
3	B	302	CIT	O6-C6-C3	3.92	119.86	113.05
3	B	312	CIT	C4-C3-C6	-3.89	101.74	110.11
7	A	302	PEG	O1-C1-C2	3.65	132.97	111.81
10	B	313	5DU	C7-C8-C9	3.56	122.29	116.18
3	A	306	CIT	O7-C3-C4	3.38	117.31	109.40
3	B	312	CIT	O6-C6-C3	3.25	118.70	113.05
8	B	310	LCP	O3-CL-O2	-3.15	94.18	109.43
7	A	302	PEG	O2-C3-C4	3.13	123.81	110.07
8	B	310	LCP	O4-CL-O3	2.99	125.74	109.03
6	B	306	BCN	C1-N1-C5	2.93	119.06	111.94
3	B	302	CIT	O2-C1-O1	-2.85	116.20	123.30
3	A	306	CIT	C4-C3-C6	-2.83	104.03	110.11
3	B	302	CIT	C3-C2-C1	-2.69	107.30	113.81
3	B	312	CIT	C3-C2-C1	2.59	120.07	113.81
3	A	308	CIT	O6-C6-C3	2.55	117.47	113.05
3	A	308	CIT	C4-C3-C6	-2.51	104.72	110.11
3	B	312	CIT	O5-C6-C3	-2.46	118.77	122.25
7	A	302	PEG	O4-C4-C3	2.44	125.97	111.81
3	B	312	CIT	O2-C1-C2	2.32	121.79	114.35
6	B	306	BCN	C1-N1-C3	-2.30	106.34	111.94
7	B	309	PEG	O2-C2-C1	2.28	120.07	110.07
3	B	312	CIT	O1-C1-C2	-2.24	116.40	122.94
6	B	306	BCN	O4-C4-C3	2.23	120.42	111.19
3	B	302	CIT	O6-C6-O5	2.18	130.74	123.82
10	B	313	5DU	F11-C6-C5	2.15	124.72	120.70
3	A	308	CIT	O4-C5-C4	2.08	121.03	114.35
7	A	302	PEG	O2-C2-C1	2.05	119.09	110.07
10	B	313	5DU	C9-C10-N14	-2.04	113.61	123.45

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	CIT	O7-C3-C6-O5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	302	CIT	O7-C3-C6-O6
3	B	302	CIT	C4-C3-C6-O6
3	B	312	CIT	C2-C3-C4-C5
3	B	312	CIT	O7-C3-C4-C5
3	B	312	CIT	C6-C3-C4-C5
3	B	312	CIT	C2-C3-C6-O5
3	B	312	CIT	C2-C3-C6-O6
3	B	312	CIT	O7-C3-C6-O5
3	B	312	CIT	O7-C3-C6-O6
4	A	305	EDO	O1-C1-C2-O2
6	B	306	BCN	C2-C1-N1-C5
6	B	306	BCN	N1-C1-C2-O21
10	B	313	5DU	C9-C10-N14-C15
10	B	313	5DU	C5-C10-N14-C15
10	B	313	5DU	C6-C5-S1-O2
10	B	313	5DU	C16-C15-N14-C10
6	B	306	BCN	N1-C1-C2-O22
3	B	302	CIT	O7-C3-C4-C5
6	B	306	BCN	N1-C3-C4-O4
4	A	304	EDO	O1-C1-C2-O2
3	B	312	CIT	C1-C2-C3-C6
3	B	312	CIT	O2-C1-C2-C3
3	B	312	CIT	O1-C1-C2-C3
3	B	302	CIT	C1-C2-C3-O7
4	B	308	EDO	O1-C1-C2-O2
3	B	302	CIT	C2-C3-C6-O5
3	B	302	CIT	C2-C3-C6-O6
3	B	312	CIT	C4-C3-C6-O5
3	B	312	CIT	C4-C3-C6-O6
3	A	306	CIT	C2-C3-C6-O5
3	A	306	CIT	C2-C3-C6-O6
4	B	307	EDO	O1-C1-C2-O2
6	B	306	BCN	N1-C5-C6-O6
3	B	302	CIT	C1-C2-C3-C6
7	A	302	PEG	C4-C3-O2-C2
10	B	313	5DU	C19-C15-N14-C10
3	B	312	CIT	C1-C2-C3-O7
10	B	313	5DU	C10-C5-S1-O2
7	B	309	PEG	O1-C1-C2-O2
7	A	302	PEG	C1-C2-O2-C3
3	B	302	CIT	C4-C3-C6-O5
3	A	306	CIT	C4-C3-C6-O6

Continued on next page...

Continued from previous page...

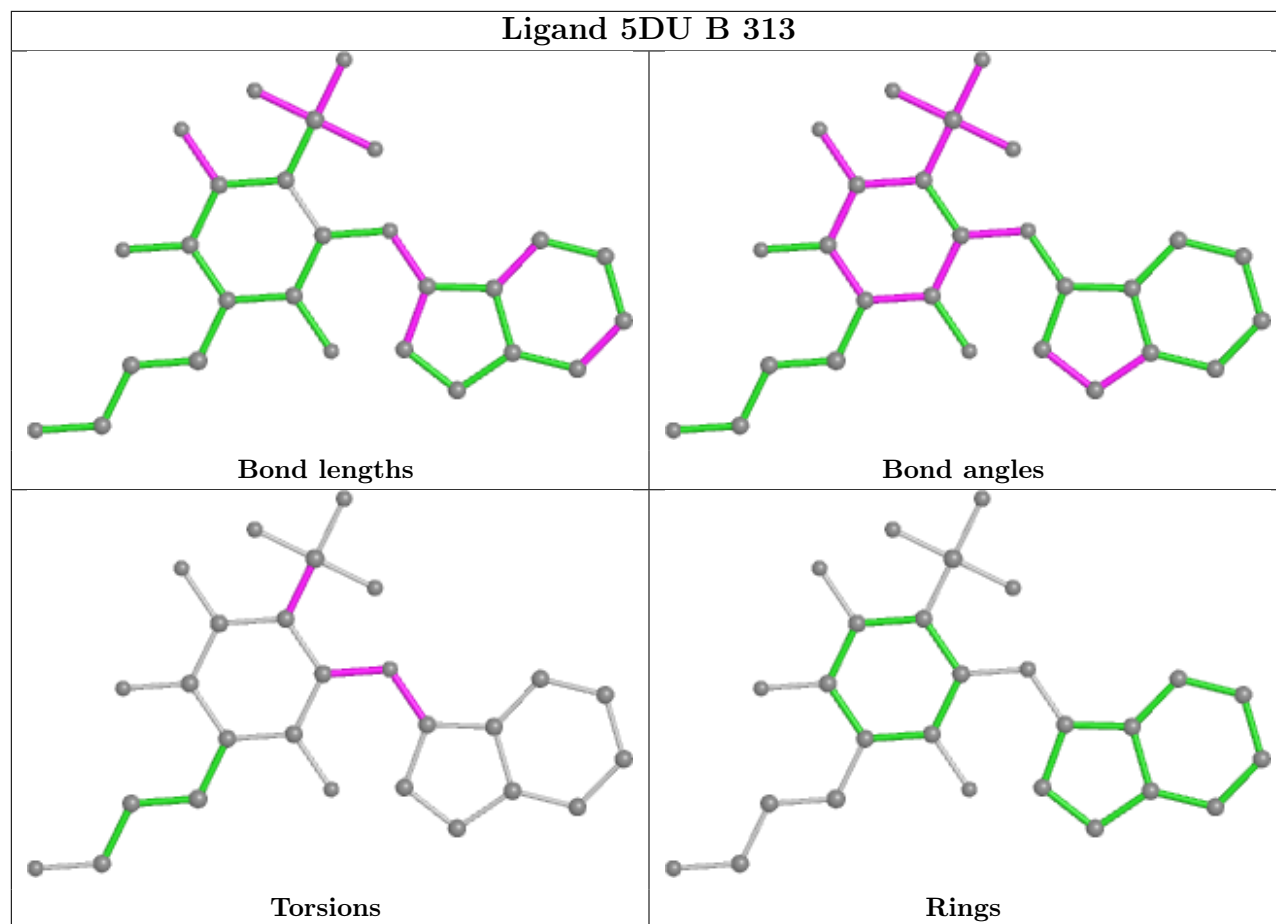
Mol	Chain	Res	Type	Atoms
10	B	313	5DU	C10-C5-S1-N4
3	B	302	CIT	C6-C3-C4-C5
3	A	306	CIT	O2-C1-C2-C3
6	B	306	BCN	C6-C5-N1-C1
3	A	306	CIT	O1-C1-C2-C3
3	B	312	CIT	C3-C4-C5-O4
6	B	306	BCN	C6-C5-N1-C3
3	B	312	CIT	C3-C4-C5-O3
7	B	309	PEG	C4-C3-O2-C2

There are no ring outliers.

12 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	302	CIT	2	0
3	A	306	CIT	1	0
6	B	306	BCN	6	0
8	B	310	LCP	3	0
4	B	307	EDO	3	0
4	A	305	EDO	1	0
4	B	308	EDO	1	0
7	B	309	PEG	8	0
7	A	302	PEG	7	0
10	B	313	5DU	3	0
3	B	312	CIT	1	0
5	B	305	AZI	2	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	259/263 (98%)	-0.55	3 (1%) 79 77	7, 12, 22, 41	0
1	B	258/263 (98%)	-0.56	4 (1%) 72 71	7, 12, 26, 55	0
All	All	517/526 (98%)	-0.55	7 (1%) 75 74	7, 12, 25, 55	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75[A]	THR	3.1
1	A	5	LEU	2.9
1	A	222[A]	SER	2.7
1	B	219[A]	ASN	2.5
1	B	21	PHE	2.4
1	B	239	ALA	2.1
1	B	236	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

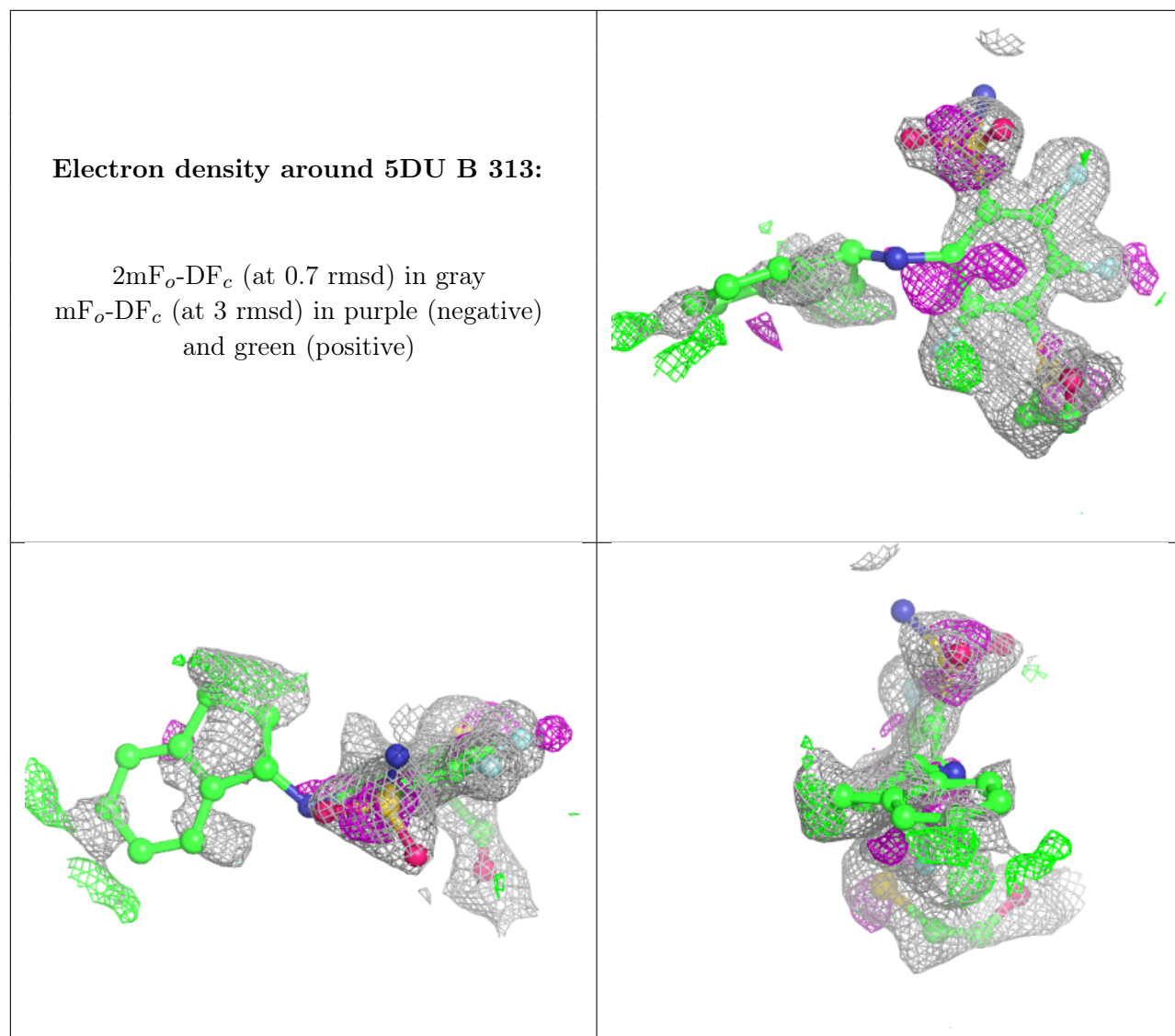
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	LCP	B	310	5/5	0.59	0.29	39,42,54,70	0
3	CIT	B	312	13/13	0.70	0.24	33,52,72,78	0
6	BCN	B	306	11/11	0.76	0.19	30,38,58,58	0
3	CIT	A	308	13/13	0.79	0.24	30,35,44,46	0
4	EDO	A	304	4/4	0.80	0.15	32,32,33,36	0
3	CIT	B	302	13/13	0.82	0.19	19,29,51,52	0
10	5DU	B	313	27/27	0.84	0.28	23,43,65,66	0
3	CIT	A	306	13/13	0.85	0.26	22,41,50,53	0
7	PEG	B	309	7/7	0.85	0.32	21,27,32,40	0
4	EDO	A	305	4/4	0.86	0.19	30,35,35,45	0
4	EDO	B	308	4/4	0.88	0.19	27,27,28,29	0
4	EDO	B	307	4/4	0.92	0.22	23,23,25,34	0
7	PEG	A	302	7/7	0.92	0.20	19,19,25,27	0
4	EDO	B	303	4/4	0.93	0.11	19,20,21,22	0
4	EDO	A	303	4/4	0.94	0.19	26,27,27,29	0
4	EDO	B	304	4/4	0.94	0.14	15,18,20,23	0
9	ACT	A	307	4/4	0.96	0.07	9,10,10,11	0
5	AZI	B	305	3/3	0.96	0.19	22,22,34,35	0
9	ACT	B	311	4/4	0.97	0.06	9,9,10,11	0
2	ZN	A	301	1/1	1.00	0.04	7,7,7,7	0
2	ZN	B	301	1/1	1.00	0.04	7,7,7,7	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.