



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2026 – 10:41 AM UTC

PDB ID : 8DR2 / pdb_00008dr2
Title : Crystal structure of Neisseria gonorrhoeae carbonic anhydrase with 2-cyclohexyl-N-(5-sulfamoyl-1,3,4-thiadiazol-2-yl)acetamide
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Deposited on : 2022-07-20
Resolution : 2.81 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

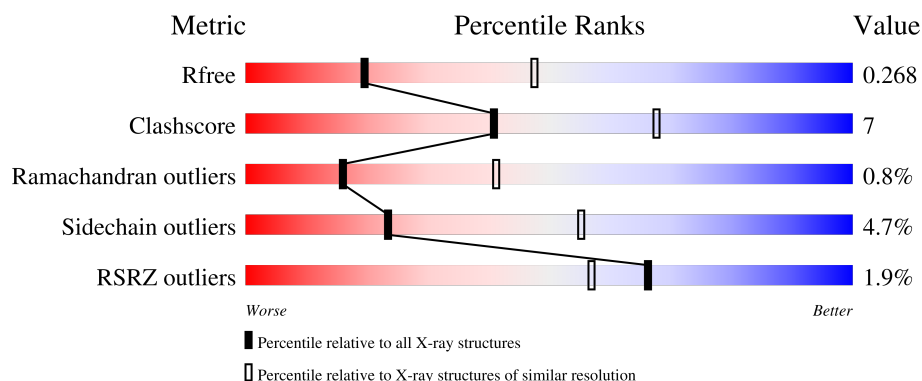
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	243	
1	C	243	
1	E	243	
1	G	243	

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
2	TE3	A	301	-	X	-	-
2	TE3	C	301	-	X	-	-
2	TE3	E	301	-	X	-	-
2	TE3	G	301	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7130 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1743	1103	308	326	6			
1	C	222	Total	C	N	O	S	0	0	0
			1740	1102	306	326	6			
1	E	222	Total	C	N	O	S	0	0	0
			1748	1107	307	328	6			
1	G	222	Total	C	N	O	S	0	0	0
			1751	1107	308	330	6			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	HIS	-	expression tag	UNP Q50940
A	-15	HIS	-	expression tag	UNP Q50940
A	-14	HIS	-	expression tag	UNP Q50940
A	-13	HIS	-	expression tag	UNP Q50940
A	-12	HIS	-	expression tag	UNP Q50940
A	-11	HIS	-	expression tag	UNP Q50940
A	-10	ASP	-	expression tag	UNP Q50940
A	-9	SER	-	expression tag	UNP Q50940
A	-8	GLY	-	expression tag	UNP Q50940
A	-7	LEU	-	expression tag	UNP Q50940
A	-6	VAL	-	expression tag	UNP Q50940
A	-5	PRO	-	expression tag	UNP Q50940
A	-4	ARG	-	expression tag	UNP Q50940
A	-3	GLY	-	expression tag	UNP Q50940
A	-2	SER	-	expression tag	UNP Q50940
A	-1	HIS	-	expression tag	UNP Q50940
A	0	MET	-	expression tag	UNP Q50940
C	-16	HIS	-	expression tag	UNP Q50940
C	-15	HIS	-	expression tag	UNP Q50940
C	-14	HIS	-	expression tag	UNP Q50940
C	-13	HIS	-	expression tag	UNP Q50940

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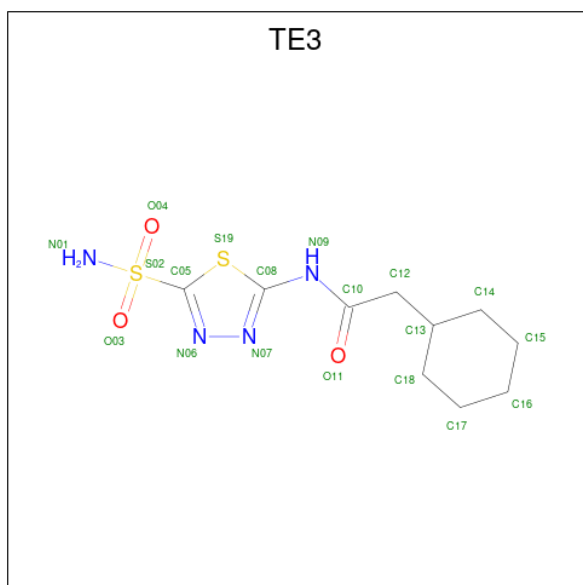
Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q50940
C	-11	HIS	-	expression tag	UNP Q50940
C	-10	ASP	-	expression tag	UNP Q50940
C	-9	SER	-	expression tag	UNP Q50940
C	-8	GLY	-	expression tag	UNP Q50940
C	-7	LEU	-	expression tag	UNP Q50940
C	-6	VAL	-	expression tag	UNP Q50940
C	-5	PRO	-	expression tag	UNP Q50940
C	-4	ARG	-	expression tag	UNP Q50940
C	-3	GLY	-	expression tag	UNP Q50940
C	-2	SER	-	expression tag	UNP Q50940
C	-1	HIS	-	expression tag	UNP Q50940
C	0	MET	-	expression tag	UNP Q50940
E	-16	HIS	-	expression tag	UNP Q50940
E	-15	HIS	-	expression tag	UNP Q50940
E	-14	HIS	-	expression tag	UNP Q50940
E	-13	HIS	-	expression tag	UNP Q50940
E	-12	HIS	-	expression tag	UNP Q50940
E	-11	HIS	-	expression tag	UNP Q50940
E	-10	ASP	-	expression tag	UNP Q50940
E	-9	SER	-	expression tag	UNP Q50940
E	-8	GLY	-	expression tag	UNP Q50940
E	-7	LEU	-	expression tag	UNP Q50940
E	-6	VAL	-	expression tag	UNP Q50940
E	-5	PRO	-	expression tag	UNP Q50940
E	-4	ARG	-	expression tag	UNP Q50940
E	-3	GLY	-	expression tag	UNP Q50940
E	-2	SER	-	expression tag	UNP Q50940
E	-1	HIS	-	expression tag	UNP Q50940
E	0	MET	-	expression tag	UNP Q50940
G	-16	HIS	-	expression tag	UNP Q50940
G	-15	HIS	-	expression tag	UNP Q50940
G	-14	HIS	-	expression tag	UNP Q50940
G	-13	HIS	-	expression tag	UNP Q50940
G	-12	HIS	-	expression tag	UNP Q50940
G	-11	HIS	-	expression tag	UNP Q50940
G	-10	ASP	-	expression tag	UNP Q50940
G	-9	SER	-	expression tag	UNP Q50940
G	-8	GLY	-	expression tag	UNP Q50940
G	-7	LEU	-	expression tag	UNP Q50940
G	-6	VAL	-	expression tag	UNP Q50940
G	-5	PRO	-	expression tag	UNP Q50940

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	ARG	-	expression tag	UNP Q50940
G	-3	GLY	-	expression tag	UNP Q50940
G	-2	SER	-	expression tag	UNP Q50940
G	-1	HIS	-	expression tag	UNP Q50940
G	0	MET	-	expression tag	UNP Q50940

- Molecule 2 is 2-cyclohexyl-N-(5-sulfamoyl-1,3,4-thiadiazol-2-yl)acetamide (CCD ID: TE3) (formula: C₁₀H₁₆N₄O₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			19	10	4	3	2		
2	C	1	Total	C	N	O	S	0	0
			19	10	4	3	2		
2	E	1	Total	C	N	O	S	0	0
			19	10	4	3	2		
2	G	1	Total	C	N	O	S	0	0
			19	10	4	3	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

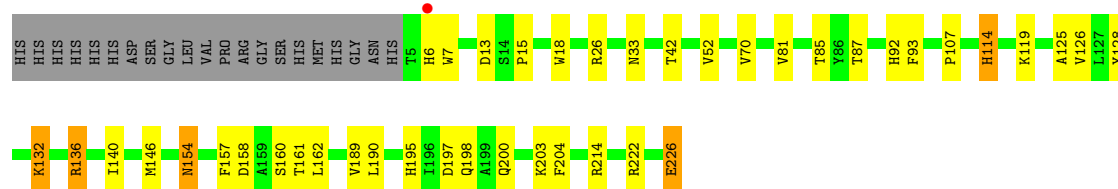
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		
5	C	2	Total	O	0	0
			2	2		
5	E	2	Total	O	0	0
			2	2		
5	G	5	Total	O	0	0
			5	5		

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.

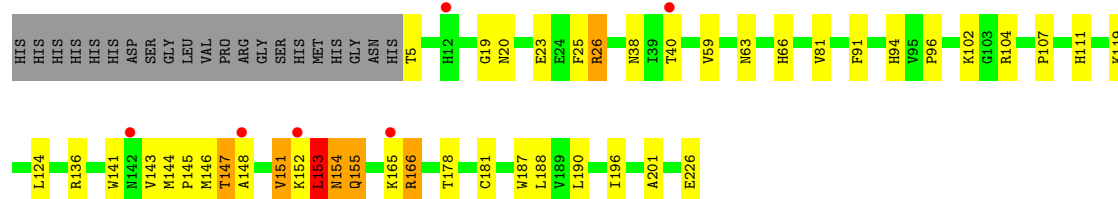
- Molecule 1: Carbonic anhydrase

Chain A: 



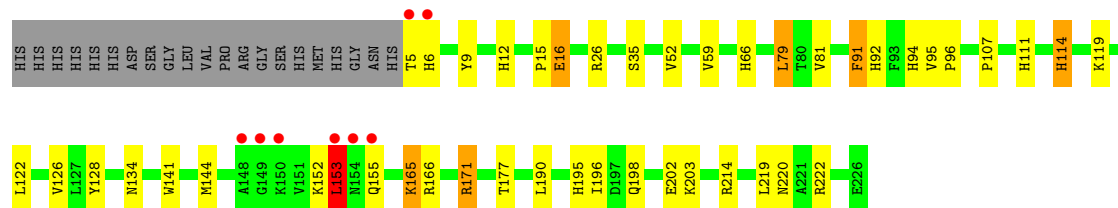
- Molecule 1: Carbonic anhydrase

Chain C: 



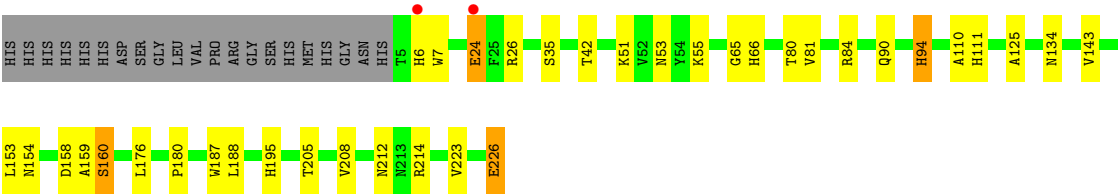
- Molecule 1: Carbonic anhydrase

Chain E: 



- Molecule 1: Carbonic anhydrase

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.67Å 120.58Å 80.42Å 90.00° 116.62° 90.00°	Depositor
Resolution (Å)	46.20 – 2.81 46.20 – 2.81	Depositor EDS
% Data completeness (in resolution range)	91.0 (46.20-2.81) 91.0 (46.20-2.81)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.192 , 0.266 0.197 , 0.268	Depositor DCC
R_{free} test set	1321 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	35.4	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.057 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7130	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: ZN, TE3, SO4

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	0.66	3/1789 (0.2%)	1.02	0/2436
1	C	0.66	2/1786 (0.1%)	1.06	0/2432
1	E	0.67	6/1794 (0.3%)	1.08	1/2441 (0.0%)
1	G	0.65	1/1797 (0.1%)	1.06	1/2446 (0.0%)
All	All	0.66	12/7166 (0.2%)	1.05	2/9755 (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	3
1	C	0	5
1	E	0	3
1	G	0	1
All	All	0	12

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	66	HIS	CE1-NE2	6.08	1.38	1.32
1	A	92	HIS	CE1-NE2	5.86	1.38	1.32
1	C	66	HIS	CE1-NE2	5.70	1.38	1.32
1	E	92	HIS	CE1-NE2	5.63	1.38	1.32
1	E	12	HIS	CE1-NE2	5.55	1.38	1.32
1	E	114	HIS	CE1-NE2	5.50	1.38	1.32
1	A	6	HIS	CE1-NE2	5.48	1.38	1.32
1	C	94	HIS	CE1-NE2	5.22	1.37	1.32
1	G	94	HIS	CE1-NE2	5.13	1.37	1.32
1	E	94	HIS	CE1-NE2	5.12	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	114	HIS	CE1-NE2	5.10	1.37	1.32
1	E	6	HIS	CE1-NE2	5.03	1.37	1.32

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	53	ASN	CA-CB-CG	5.70	118.30	112.60
1	E	91	PHE	CA-CB-CG	5.30	119.10	113.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	136	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	26	ARG	Sidechain
1	C	104	ARG	Sidechain
1	C	136	ARG	Sidechain
1	C	155	GLN	Peptide
1	C	166	ARG	Sidechain
1	C	26	ARG	Sidechain
1	E	153	LEU	Peptide
1	E	171	ARG	Sidechain
1	E	214	ARG	Sidechain
1	G	26	ARG	Sidechain

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	1743	0	1702	24	0
1	C	1740	0	1696	25	0
1	E	1748	0	1711	20	0
1	G	1751	0	1710	19	0
2	A	19	0	0	1	0
2	C	19	0	0	1	0
2	E	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	19	0	0	2	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	10	0	0	0	0
4	C	10	0	0	0	0
4	E	15	0	0	0	0
4	G	15	0	0	0	0
5	A	9	0	0	0	0
5	C	2	0	0	0	0
5	E	2	0	0	0	0
5	G	5	0	0	0	0
All	All	7130	0	6819	91	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 (91) 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:C:152:LYS:O	1:C:154:ASN:N	2.00	0.94
1:A:154:ASN:H	1:A:154:ASN:HD22	1.22	0.87
1:G:143:VAL:HG11	1:G:153:LEU:HD13	1.60	0.84
1:C:38:ASN:ND2	1:C:40:THR:HG23	1.95	0.82
1:G:158:ASP:OD1	1:G:160:SER:HB2	1.82	0.79
1:E:122:LEU:C	1:E:122:LEU:HD23	2.11	0.76
1:C:153:LEU:O	1:C:155:GLN:N	2.20	0.75
1:C:152:LYS:C	1:C:154:ASN:H	1.96	0.71
1:C:187:TRP:C	1:C:188:LEU:HD12	2.20	0.67
1:G:65:GLY:O	1:G:208:VAL:HG13	1.96	0.65
1:E:79:LEU:HD13	1:E:114:HIS:NE2	2.14	0.63
1:C:196:ILE:HD12	1:C:201:ALA:HB2	1.80	0.63
1:C:63:ASN:O	1:C:148:ALA:HA	1.99	0.61
1:C:38:ASN:HD21	1:C:40:THR:HG23	1.61	0.61
1:E:107:PRO:HB2	1:E:196:ILE:HD11	1.84	0.60
1:C:153:LEU:C	1:C:155:GLN:N	2.56	0.59
1:A:154:ASN:H	1:A:154:ASN:ND2	1.99	0.58
2:G:301:TE3:O11	2:G:301:TE3:N07	2.32	0.58
1:E:35:SER:C	1:E:177:THR:HG22	2.28	0.57
1:C:152:LYS:C	1:C:154:ASN:N	2.54	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:VAL:HG12	1:C:154:ASN:CB	2.34	0.57
1:C:143:VAL:O	1:C:151:VAL:HG21	2.05	0.56
1:A:70:VAL:HG21	1:A:140:ILE:HD13	1.88	0.56
1:A:132:LYS:O	1:A:195:HIS:HD2	1.89	0.56
1:A:146:MET:HE1	1:A:203:LYS:HG3	1.89	0.55
1:A:158:ASP:OD1	1:A:160:SER:HB2	2.06	0.55
1:G:158:ASP:OD1	1:G:160:SER:CB	2.54	0.55
2:A:301:TE3:N07	2:A:301:TE3:O11	2.36	0.54
1:G:143:VAL:HG11	1:G:153:LEU:CD1	2.33	0.54
2:C:301:TE3:O11	2:C:301:TE3:N07	2.37	0.53
1:C:188:LEU:HD12	1:C:188:LEU:N	2.24	0.53
1:E:141:TRP:O	1:E:203:LYS:HE2	2.10	0.52
1:A:7:TRP:HA	1:A:13:ASP:HB3	1.93	0.51
1:C:178:THR:O	1:C:181:CYS:N	2.43	0.51
1:A:126:VAL:HG22	1:A:190:LEU:HD12	1.92	0.51
1:E:107:PRO:HD2	1:E:128:TYR:O	2.11	0.51
1:C:196:ILE:CD1	1:C:201:ALA:HB2	2.42	0.49
1:A:197:ASP:OD1	1:A:200:GLN:HG3	2.12	0.49
1:C:23:GLU:O	1:C:26:ARG:HB2	2.13	0.49
1:G:188:LEU:HD12	1:G:188:LEU:N	2.28	0.49
1:G:7:TRP:O	1:G:66:HIS:HE1	1.96	0.49
1:G:187:TRP:C	1:G:188:LEU:HD12	2.38	0.49
1:A:107:PRO:HD2	1:A:128:TYR:O	2.13	0.48
1:A:87:THR:O	1:A:114:HIS:HA	2.13	0.48
1:G:94:HIS:HA	1:G:212:ASN:HD21	1.79	0.48
1:A:154:ASN:HD22	1:A:154:ASN:N	2.02	0.48
1:E:198:GLN:O	1:E:202:GLU:HG3	2.14	0.48
1:C:38:ASN:HD21	1:C:40:THR:CG2	2.24	0.47
1:C:124:LEU:HD11	1:C:190:LEU:HG	1.97	0.47
1:E:9:TYR:HA	1:E:15:PRO:HD3	1.96	0.47
1:E:141:TRP:CE2	1:E:144:MET:HE1	2.49	0.47
1:C:19:GLY:HA2	1:C:25:PHE:O	2.15	0.47
1:C:96:PRO:HA	1:C:107:PRO:O	2.14	0.47
1:E:153:LEU:HD22	1:E:155:GLN:CB	2.45	0.46
1:A:136:ARG:HD2	1:A:161:THR:O	2.14	0.46
1:E:134:ASN:HB2	1:E:195:HIS:O	2.15	0.46
1:A:158:ASP:OD1	1:A:160:SER:CB	2.63	0.46
1:E:122:LEU:C	1:E:122:LEU:CD2	2.83	0.46
1:A:33:ASN:HA	1:A:222:ARG:CZ	2.45	0.45
1:G:94:HIS:CD2	1:G:111:HIS:CE1	3.06	0.44
1:E:59:VAL:O	1:E:153:LEU:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:LYS:HD2	1:E:166:ARG:HD3	2.00	0.44
1:E:91:PHE:HA	1:E:111:HIS:O	2.18	0.44
1:A:93:PHE:HB2	1:A:204:PHE:CE2	2.53	0.43
1:E:219:LEU:HA	1:E:222:ARG:HH21	1.83	0.43
1:C:91:PHE:HA	1:C:111:HIS:O	2.18	0.43
1:G:176:LEU:HD22	2:G:301:TE3:S19	2.59	0.43
1:G:94:HIS:CD2	1:G:111:HIS:ND1	2.87	0.43
1:E:26:ARG:HH11	1:E:26:ARG:HA	1.84	0.42
1:E:126:VAL:HG22	1:E:190:LEU:HD12	2.02	0.42
1:G:24:GLU:O	1:G:180:PRO:HB3	2.19	0.42
1:A:33:ASN:HD22	1:A:222:ARG:CG	2.33	0.42
1:A:125:ALA:HB3	1:A:189:VAL:HG22	2.02	0.42
1:A:33:ASN:HD22	1:A:222:ARG:HG3	1.85	0.42
1:A:42:THR:OG1	1:A:226:GLU:HG2	2.19	0.42
1:A:126:VAL:CG2	1:A:190:LEU:HD12	2.49	0.42
1:G:134:ASN:HB2	1:G:195:HIS:O	2.20	0.42
1:A:15:PRO:HA	1:A:18:TRP:CD2	2.55	0.42
1:C:146:MET:O	1:C:147:THR:HG23	2.20	0.42
1:G:80:THR:HA	1:G:84:ARG:O	2.19	0.42
1:E:171:ARG:HG3	1:E:171:ARG:HH11	1.85	0.42
1:A:157:PHE:HZ	1:A:162:LEU:HD11	1.85	0.41
1:C:141:TRP:HA	1:C:144:MET:HE3	2.02	0.41
1:C:145:PRO:HG3	1:C:151:VAL:HG23	2.03	0.41
1:C:59:VAL:HG23	1:C:155:GLN:CB	2.50	0.41
1:G:35:SER:O	1:G:214:ARG:NH1	2.53	0.41
1:G:159:ALA:O	1:G:160:SER:C	2.63	0.40
1:E:95:VAL:HA	1:E:96:PRO:HA	1.88	0.40
1:A:33:ASN:HD22	1:A:222:ARG:CD	2.34	0.40
1:G:110:ALA:O	1:G:125:ALA:HA	2.21	0.40
1:G:42:THR:OG1	1:G:226:GLU:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	220/243 (90%)	206 (94%)	14 (6%)	0	100	100
1	C	220/243 (90%)	200 (91%)	18 (8%)	2 (1%)	14	38
1	E	220/243 (90%)	209 (95%)	8 (4%)	3 (1%)	9	27
1	G	220/243 (90%)	207 (94%)	11 (5%)	2 (1%)	14	38
All	All	880/972 (90%)	822 (93%)	51 (6%)	7 (1%)	16	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	LEU
1	C	154	ASN
1	E	153	LEU
1	G	154	ASN
1	G	160	SER
1	E	16	GLU
1	E	220	ASN

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	192/213 (90%)	184 (96%)	8 (4%)	26	59
1	C	191/213 (90%)	180 (94%)	11 (6%)	18	47
1	E	193/213 (91%)	185 (96%)	8 (4%)	27	60
1	G	194/213 (91%)	185 (95%)	9 (5%)	24	56
All	All	770/852 (90%)	734 (95%)	36 (5%)	23	55

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	VAL

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Mol	Chain	Res	Type
1	A	81	VAL
1	A	85	THR
1	A	119	LYS
1	A	132	LYS
1	A	154	ASN
1	A	198	GLN
1	A	226	GLU
1	C	5	THR
1	C	20	ASN
1	C	81	VAL
1	C	102	LYS
1	C	119	LYS
1	C	147	THR
1	C	151	VAL
1	C	153	LEU
1	C	165	LYS
1	C	166	ARG
1	C	226	GLU
1	E	5	THR
1	E	16	GLU
1	E	52	VAL
1	E	79	LEU
1	E	81	VAL
1	E	119	LYS
1	E	152	LYS
1	E	165	LYS
1	G	6	HIS
1	G	24	GLU
1	G	51	LYS
1	G	55	LYS
1	G	81	VAL
1	G	90	GLN
1	G	205	THR
1	G	223	VAL
1	G	226	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	53	ASN
1	A	69	GLN

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Mol	Chain	Res	Type
1	A	82	ASN
1	A	142	ASN
1	A	154	ASN
1	A	195	HIS
1	C	66	HIS
1	C	69	GLN
1	C	134	ASN
1	C	198	GLN
1	E	66	HIS
1	E	82	ASN
1	E	195	HIS
1	G	33	ASN
1	G	53	ASN
1	G	66	HIS
1	G	142	ASN
1	G	195	HIS
1	G	198	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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
2	TE3	C	301	3	20,20,20	2.55	6 (30%)	28,28,28	5.44	17 (60%)
2	TE3	G	301	3	20,20,20	2.40	7 (35%)	28,28,28	5.46	16 (57%)
4	SO4	E	305	-	4,4,4	0.20	0	6,6,6	0.16	0
2	TE3	E	301	3	20,20,20	2.44	6 (30%)	28,28,28	4.83	15 (53%)
4	SO4	G	305	-	4,4,4	0.30	0	6,6,6	0.12	0
4	SO4	C	303	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	C	304	-	4,4,4	0.26	0	6,6,6	0.20	0
4	SO4	G	303	-	4,4,4	0.35	0	6,6,6	0.13	0
4	SO4	G	304	-	4,4,4	0.27	0	6,6,6	0.15	0
2	TE3	A	301	3	20,20,20	2.41	6 (30%)	28,28,28	4.61	15 (53%)
4	SO4	E	304	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	E	303	-	4,4,4	0.30	0	6,6,6	0.18	0
4	SO4	A	304	-	4,4,4	0.28	0	6,6,6	0.13	0
4	SO4	A	303	-	4,4,4	0.32	0	6,6,6	0.17	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
2	TE3	C	301	3	-	8/14/22/22	0/2/2/2
2	TE3	G	301	3	-	7/14/22/22	0/2/2/2
2	TE3	A	301	3	-	8/14/22/22	0/2/2/2
2	TE3	E	301	3	-	9/14/22/22	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	TE3	S02-N01	5.85	1.71	1.58
2	G	301	TE3	S02-N01	5.61	1.71	1.58
2	E	301	TE3	S02-N01	5.51	1.70	1.58
2	E	301	TE3	C10-N09	5.42	1.47	1.37
2	A	301	TE3	S02-N01	5.18	1.70	1.58
2	G	301	TE3	C10-N09	5.04	1.46	1.37
2	A	301	TE3	C10-N09	4.95	1.46	1.37
2	C	301	TE3	O03-S02	4.68	1.50	1.43
2	C	301	TE3	C10-N09	4.64	1.45	1.37
2	E	301	TE3	C08-N09	4.62	1.45	1.38
2	A	301	TE3	C08-N09	4.30	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	TE3	C08-N09	4.16	1.44	1.38
2	C	301	TE3	O04-S02	4.06	1.49	1.43
2	A	301	TE3	O03-S02	4.05	1.49	1.43
2	E	301	TE3	C05-S02	-4.04	1.75	1.78
2	G	301	TE3	O04-S02	3.65	1.49	1.43
2	A	301	TE3	O04-S02	3.39	1.48	1.43
2	G	301	TE3	C08-N09	3.37	1.43	1.38
2	G	301	TE3	C05-N06	3.12	1.32	1.29
2	G	301	TE3	O03-S02	2.52	1.47	1.43
2	E	301	TE3	O03-S02	2.43	1.47	1.43
2	C	301	TE3	N07-N06	-2.40	1.34	1.39
2	A	301	TE3	C05-N06	2.29	1.31	1.29
2	G	301	TE3	C05-S19	2.24	1.75	1.73
2	E	301	TE3	O04-S02	2.22	1.46	1.43

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	TE3	C05-S19-C08	15.20	92.68	85.47
2	G	301	TE3	O04-S02-N01	15.19	129.55	108.39
2	C	301	TE3	S19-C05-N06	-14.79	108.31	116.10
2	E	301	TE3	C05-S19-C08	13.58	91.91	85.47
2	A	301	TE3	C05-S19-C08	12.68	91.49	85.47
2	G	301	TE3	O04-S02-O03	-12.27	102.72	120.27
2	A	301	TE3	S19-C05-N06	-12.09	109.73	116.10
2	G	301	TE3	S19-C05-N06	-11.17	110.22	116.10
2	E	301	TE3	S19-C05-N06	-10.65	110.49	116.10
2	G	301	TE3	C05-S19-C08	10.59	90.50	85.47
2	E	301	TE3	O04-S02-O03	-8.59	107.98	120.27
2	C	301	TE3	S19-C08-N07	-8.12	105.45	114.52
2	C	301	TE3	S19-C08-N09	7.70	134.03	123.72
2	E	301	TE3	S19-C08-N07	-7.69	105.94	114.52
2	A	301	TE3	O04-S02-O03	-7.23	109.94	120.27
2	A	301	TE3	C05-S02-N01	7.11	114.48	107.40
2	E	301	TE3	O03-S02-N01	7.11	118.29	108.39
2	E	301	TE3	S19-C08-N09	6.74	132.75	123.72
2	C	301	TE3	S19-C05-S02	6.52	130.27	121.62
2	G	301	TE3	C10-N09-C08	-6.18	113.12	123.69
2	C	301	TE3	C05-N06-N07	5.91	115.14	111.48
2	G	301	TE3	S19-C05-S02	5.80	129.31	121.62
2	A	301	TE3	C10-N09-C08	-5.79	113.78	123.69
2	A	301	TE3	S19-C08-N07	-5.55	108.32	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	TE3	S19-C05-S02	5.49	128.91	121.62
2	C	301	TE3	O03-S02-C05	-5.18	97.91	105.65
2	A	301	TE3	C05-N06-N07	5.15	114.67	111.48
2	C	301	TE3	C08-N07-N06	4.93	118.30	112.02
2	E	301	TE3	C08-N07-N06	4.93	118.29	112.02
2	G	301	TE3	C05-N06-N07	4.85	114.48	111.48
2	C	301	TE3	C10-N09-C08	-4.75	115.56	123.69
2	G	301	TE3	S19-C08-N07	-4.74	109.23	114.52
2	C	301	TE3	O04-S02-O03	-4.61	113.68	120.27
2	A	301	TE3	S19-C05-S02	4.61	127.73	121.62
2	G	301	TE3	C13-C12-C10	-4.31	107.11	113.22
2	C	301	TE3	C12-C10-N09	3.93	122.42	115.38
2	C	301	TE3	O03-S02-N01	3.89	113.80	108.39
2	C	301	TE3	O04-S02-C05	3.71	111.18	105.65
2	G	301	TE3	O04-S02-C05	-3.65	100.20	105.65
2	A	301	TE3	O03-S02-N01	3.47	113.22	108.39
2	C	301	TE3	C05-S02-N01	3.47	110.85	107.40
2	E	301	TE3	C13-C12-C10	-3.41	108.38	113.22
2	G	301	TE3	O03-S02-N01	3.36	113.07	108.39
2	A	301	TE3	S19-C08-N09	3.23	128.05	123.72
2	G	301	TE3	O03-S02-C05	-3.23	100.83	105.65
2	A	301	TE3	C12-C10-N09	3.22	121.15	115.38
2	A	301	TE3	N09-C08-N07	3.07	123.55	120.81
2	E	301	TE3	C05-S02-N01	3.03	110.42	107.40
2	E	301	TE3	C05-N06-N07	3.00	113.33	111.48
2	E	301	TE3	C10-N09-C08	-2.97	118.61	123.69
2	A	301	TE3	C08-N07-N06	2.96	115.78	112.02
2	G	301	TE3	C12-C10-N09	2.92	120.61	115.38
2	G	301	TE3	S19-C08-N09	2.84	127.52	123.72
2	G	301	TE3	C08-N07-N06	2.77	115.55	112.02
2	C	301	TE3	C18-C13-C12	2.70	115.00	111.48
2	C	301	TE3	O11-C10-C12	-2.63	117.69	121.54
2	E	301	TE3	O11-C10-C12	-2.61	117.72	121.54
2	E	301	TE3	C12-C10-N09	2.49	119.85	115.38
2	C	301	TE3	C14-C13-C12	-2.45	108.29	111.48
2	A	301	TE3	O03-S02-C05	-2.39	102.08	105.65
2	G	301	TE3	N09-C08-N07	2.24	122.81	120.81
2	E	301	TE3	O03-S02-C05	-2.23	102.33	105.65
2	A	301	TE3	C14-C13-C12	-2.10	108.74	111.48

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TE3	C10-C12-C13-C14
2	A	301	TE3	C10-C12-C13-C18
2	A	301	TE3	N06-C05-S02-N01
2	A	301	TE3	S19-C05-S02-N01
2	A	301	TE3	N07-C08-N09-C10
2	A	301	TE3	S19-C08-N09-C10
2	C	301	TE3	C10-C12-C13-C14
2	C	301	TE3	C10-C12-C13-C18
2	C	301	TE3	N07-C08-N09-C10
2	C	301	TE3	S19-C08-N09-C10
2	E	301	TE3	C10-C12-C13-C18
2	E	301	TE3	N07-C08-N09-C10
2	E	301	TE3	S19-C08-N09-C10
2	G	301	TE3	C10-C12-C13-C18
2	G	301	TE3	N07-C08-N09-C10
2	G	301	TE3	S19-C08-N09-C10
2	E	301	TE3	N06-C05-S02-N01
2	E	301	TE3	S19-C05-S02-N01
2	G	301	TE3	S19-C05-S02-N01
2	C	301	TE3	S19-C05-S02-O03
2	A	301	TE3	N06-C05-S02-O03
2	C	301	TE3	N06-C05-S02-N01
2	C	301	TE3	S19-C05-S02-N01
2	C	301	TE3	N06-C05-S02-O03
2	E	301	TE3	N06-C05-S02-O03
2	E	301	TE3	S19-C05-S02-O03
2	G	301	TE3	N06-C05-S02-N01
2	A	301	TE3	S19-C05-S02-O03
2	G	301	TE3	N06-C05-S02-O03
2	G	301	TE3	S19-C05-S02-O03
2	E	301	TE3	O11-C10-C12-C13
2	E	301	TE3	N09-C10-C12-C13

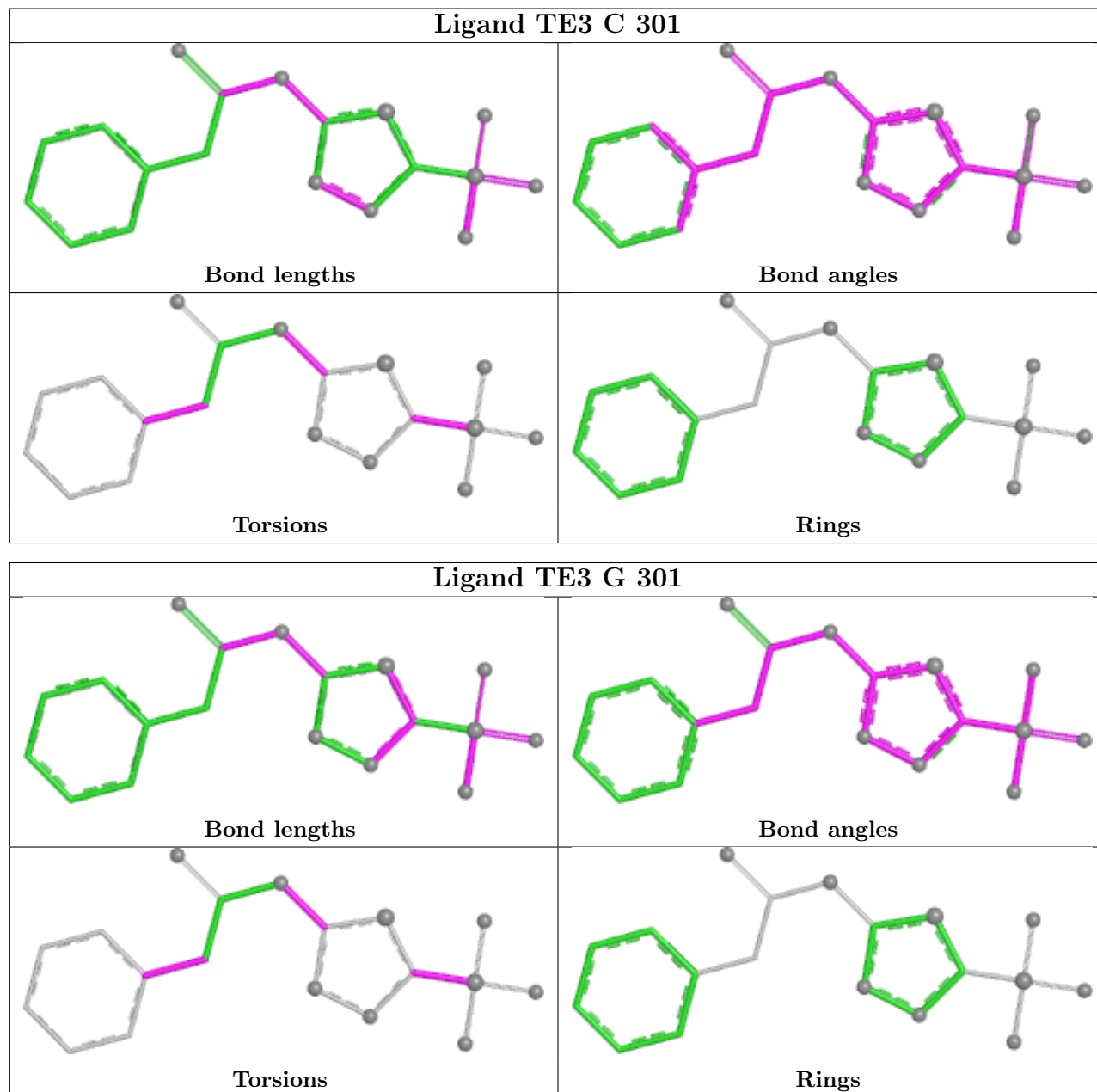
There are no ring outliers.

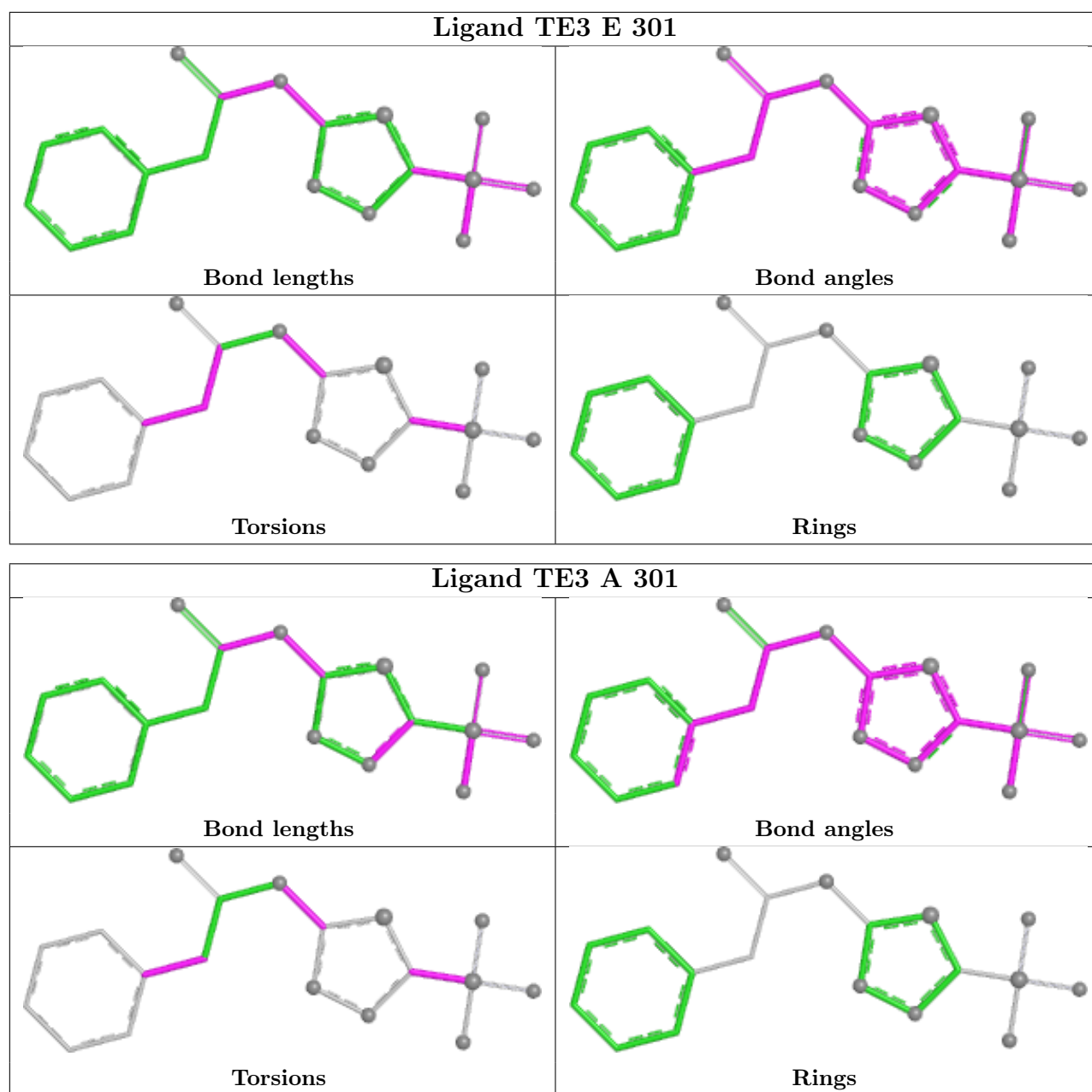
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	301	TE3	1	0
2	G	301	TE3	2	0
2	A	301	TE3	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	222/243 (91%)	-0.26	1 (0%) 87 82	24, 37, 55, 77	0
1	C	222/243 (91%)	-0.22	6 (2%) 56 46	24, 36, 55, 88	0
1	E	222/243 (91%)	-0.13	8 (3%) 46 37	23, 36, 60, 105	0
1	G	222/243 (91%)	-0.18	2 (0%) 81 74	24, 37, 55, 75	0
All	All	888/972 (91%)	-0.20	17 (1%) 66 57	23, 37, 56, 105	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	154	ASN	6.4
1	E	155	GLN	4.1
1	C	12	HIS	3.5
1	E	153	LEU	3.5
1	E	149	GLY	3.0
1	C	148	ALA	2.7
1	E	6	HIS	2.7
1	C	142	ASN	2.7
1	C	40	THR	2.4
1	A	6	HIS	2.3
1	E	148	ALA	2.2
1	C	152	LYS	2.2
1	E	150	LYS	2.2
1	G	6	HIS	2.1
1	G	24	GLU	2.1
1	C	165	LYS	2.0
1	E	5	THR	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](#)

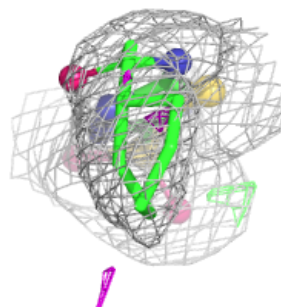
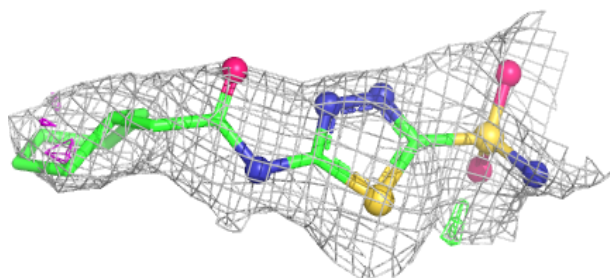
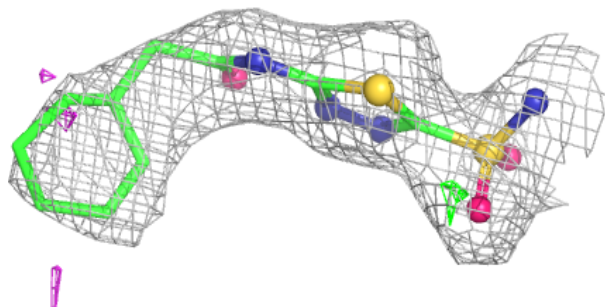
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	G	305	5/5	0.71	0.21	149,152,159,165	0
4	SO4	C	304	5/5	0.87	0.15	77,80,90,97	0
4	SO4	G	304	5/5	0.89	0.16	70,80,84,85	0
4	SO4	E	305	5/5	0.89	0.12	59,65,73,74	0
4	SO4	A	304	5/5	0.90	0.13	64,68,73,79	0
4	SO4	E	304	5/5	0.93	0.12	66,67,74,76	0
2	TE3	C	301	19/19	0.96	0.09	30,34,45,45	0
2	TE3	E	301	19/19	0.96	0.11	34,39,71,73	0
2	TE3	G	301	19/19	0.97	0.08	29,34,41,41	0
4	SO4	A	303	5/5	0.97	0.07	43,43,44,53	0
4	SO4	G	303	5/5	0.98	0.06	34,34,37,38	0
4	SO4	C	303	5/5	0.98	0.07	36,42,44,47	0
2	TE3	A	301	19/19	0.98	0.07	28,38,50,50	0
3	ZN	G	302	1/1	0.99	0.02	30,30,30,30	0
3	ZN	A	302	1/1	0.99	0.03	34,34,34,34	0
4	SO4	E	303	5/5	0.99	0.05	31,32,36,36	0
3	ZN	E	302	1/1	0.99	0.03	30,30,30,30	0
3	ZN	C	302	1/1	1.00	0.02	29,29,29,29	0

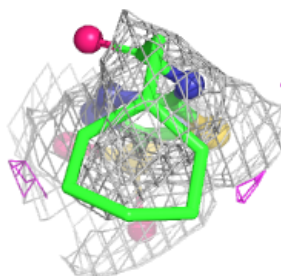
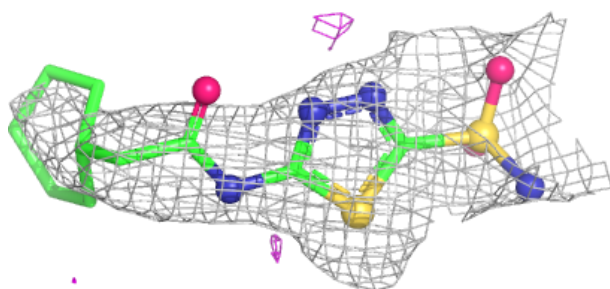
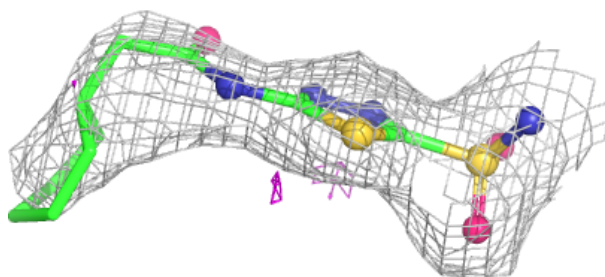
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TE3 C 301:

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

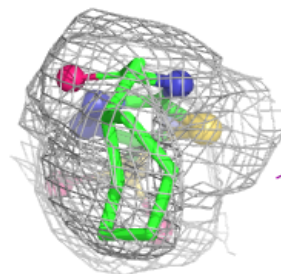
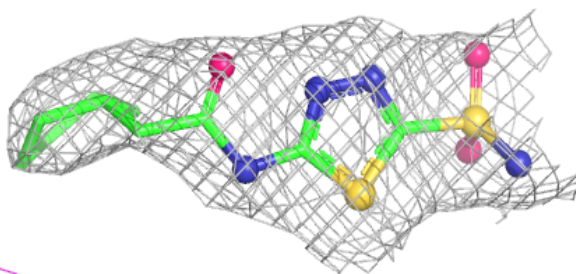
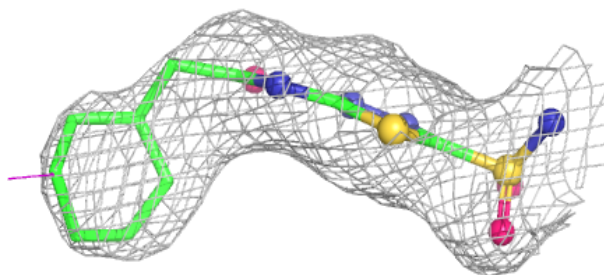
**Electron density around TE3 E 301:**

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

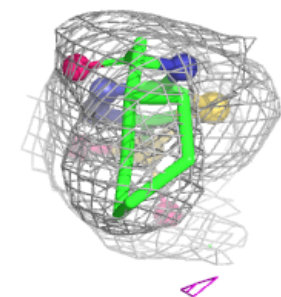
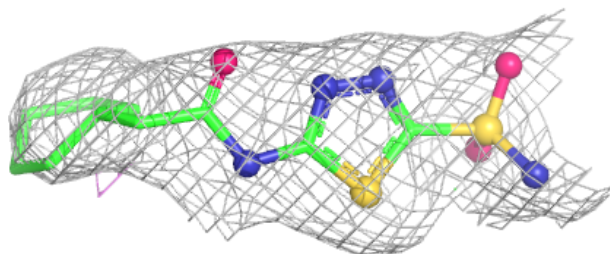
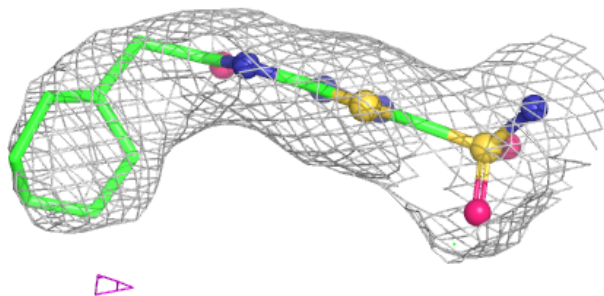


Electron density around TE3 G 301:

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

**Electron density around TE3 A 301:**

$2mF_o-DF_c$ (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.