



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:14 AM UTC

PDB ID : 5C8C / pdb_00005c8c
Title : Crystal structure of recombinant coxsackievirus A16 capsid
Authors : Ren, J.; Wang, X.; Zhu, L.; Hu, Z.; Gao, Q.; Yang, P.; Li, X.; Wang, J.; Shen, X.; Fry, E.E.; Rao, Z.; Stuart, D.I.
Deposited on : 2015-06-25
Resolution : 2.50 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

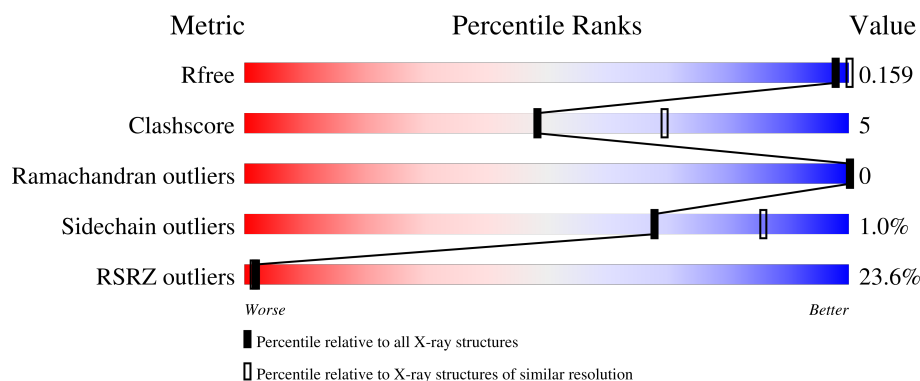
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	297	25% 71% 14% • 13%
2	B	323	25% 77% 11% 11%
3	C	242	13% 85% 15%

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
6	K	A	303	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6642 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 VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2055	1306	350	385	14			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	240	THR	ILE	conflict	UNP I3W9E1

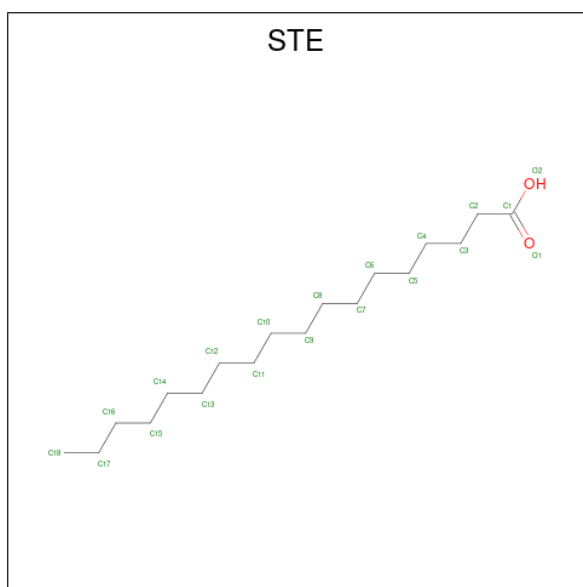
- Molecule 2 is a protein called VP0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	0	0
			2182	1389	363	420	10			

- Molecule 3 is a protein called VP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	242	Total	C	N	O	S	0	0	0
			1876	1203	310	352	11			

- Molecule 4 is STEARIC ACID (CCD ID: STE) (formula: C₁₈H₃₆O₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C O	0	0
			20	18 2		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Cl	0	0
			1	1		
5	B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	K	0	0
			1	1		

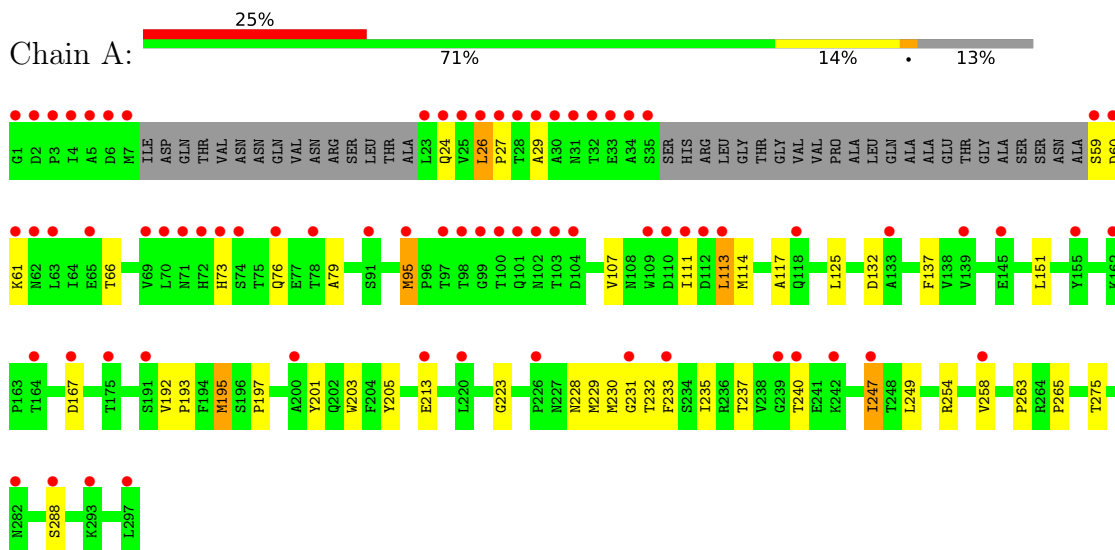
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	155	Total	O	0	0
			155	155		
7	B	187	Total	O	0	0
			187	187		
7	C	164	Total	O	0	0
			164	164		

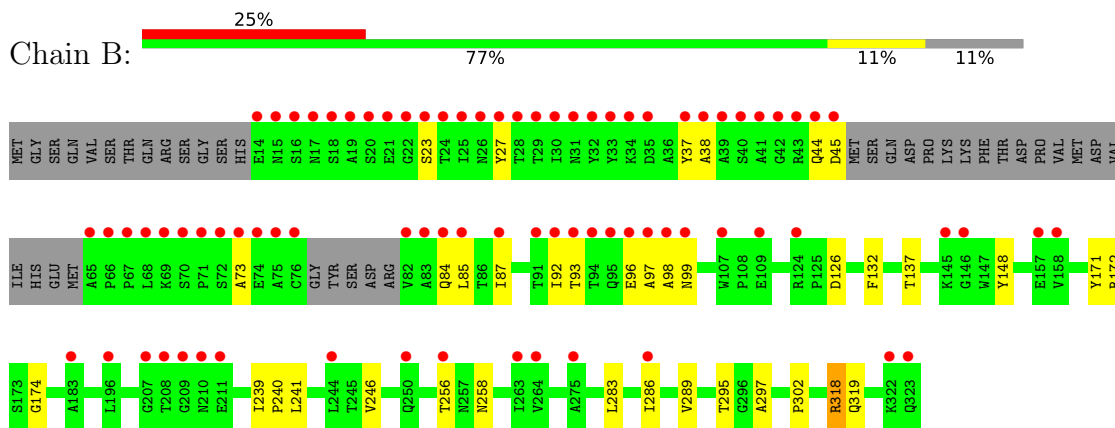
3 Residue-property plots [i](#)

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.

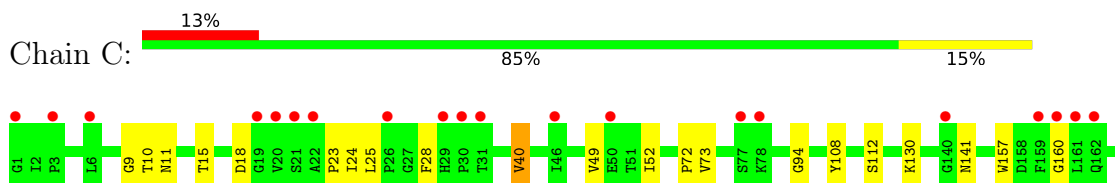
• Molecule 1: VP1

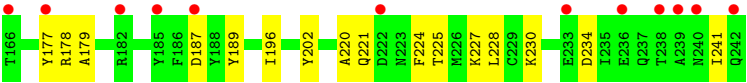


• Molecule 2: VP0



• Molecule 3: VP3





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 ₂ 3 2	Depositor
Cell constants a, b, c, α , β , γ	347.90Å 347.90Å 347.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.70 – 2.50 49.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.70-2.50) 100.0 (49.70-2.50)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.64 (at 2.51Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.164 , 0.172 0.160 , 0.159	Depositor DCC
R_{free} test set	12259 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.37	EDS
Total number of atoms	6642	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.17% 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: CL, STE, K

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	0.59	1/2111 (0.0%)	1.04	15/2874 (0.5%)
2	B	0.54	0/2241	0.96	6/3073 (0.2%)
3	C	0.54	0/1929	1.04	10/2642 (0.4%)
All	All	0.56	1/6281 (0.0%)	1.01	31/8589 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	95	MET	SD-CE	6.41	1.95	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	179	ALA	N-CA-C	-9.60	98.14	110.53
1	A	213	GLU	N-CA-C	-9.06	98.32	110.55
1	A	60	ASP	N-CA-C	-7.62	102.91	111.14
2	B	240	PRO	N-CA-C	7.41	122.00	110.80
1	A	117	ALA	N-CA-C	7.04	119.55	111.11
1	A	197	PRO	N-CA-C	-6.81	105.35	113.86
2	B	126	ASP	N-CA-C	6.74	119.92	108.67
1	A	275	THR	N-CA-C	6.73	121.20	112.92
3	C	241	ILE	N-CA-C	-6.72	98.17	107.99
3	C	234	ASP	N-CA-C	6.72	120.45	112.93
2	B	289	VAL	N-CA-C	-6.63	100.51	107.60
1	A	237	THR	N-CA-C	-6.62	98.85	109.96
3	C	52	ILE	N-CA-C	6.60	117.55	109.30
1	A	132	ASP	N-CA-C	-6.52	100.81	110.46
2	B	174	GLY	N-CA-C	-6.31	104.11	112.81
1	A	125	LEU	N-CA-C	-6.13	105.06	112.54
1	A	195	MET	N-CA-C	6.08	121.44	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	160	GLY	N-CA-C	-6.05	105.17	112.49
3	C	202	TYR	N-CA-C	-5.87	100.27	109.25
1	A	258	VAL	N-CA-C	5.84	118.35	109.12
1	A	79	ALA	N-CA-C	-5.72	101.81	110.28
3	C	73	VAL	N-CA-C	-5.57	100.20	108.45
1	A	76	GLN	N-CA-C	5.52	117.30	111.28
2	B	297	ALA	N-CA-C	-5.39	103.28	110.55
3	C	9	GLY	N-CA-C	-5.38	107.60	114.37
1	A	113	LEU	N-CA-C	5.36	119.37	113.21
3	C	72	PRO	N-CA-C	5.27	120.48	111.68
1	A	201	TYR	N-CA-C	-5.26	102.70	110.48
2	B	98	ALA	N-CA-C	-5.25	106.71	113.02
1	A	247	ILE	N-CA-C	5.03	115.16	108.11
3	C	15	THR	N-CA-C	5.00	117.46	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2055	0	2002	31	0
2	B	2182	0	2102	25	0
3	C	1876	0	1838	22	0
4	A	20	0	35	4	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	1	0	0	0	0
7	A	155	0	0	0	0
7	B	187	0	0	2	2
7	C	164	0	0	4	1
All	All	6642	0	5977	66	2

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 5.

All (66) 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:59:SER:HB2	3:C:221:GLN:HE22	1.35	0.92
1:A:59:SER:HB2	3:C:221:GLN:NE2	1.90	0.85
2:B:44:GLN:O	2:B:45:ASP:HB2	1.74	0.84
1:A:113:LEU:O	1:A:114:MET:HE2	1.81	0.81
2:B:295:THR:CB	7:B:501:HOH:O	2.26	0.74
2:B:96:GLU:HB2	2:B:99:ASN:ND2	2.03	0.73
2:B:84:GLN:HG2	2:B:93:THR:HG22	1.73	0.69
2:B:85:LEU:HD22	2:B:92:ILE:HD11	1.76	0.68
1:A:254:ARG:NH2	3:C:18:ASP:OD1	2.34	0.61
2:B:258:ASN:HB3	7:B:661:HOH:O	2.04	0.58
1:A:111:ILE:HD12	1:A:231:GLY:C	2.30	0.57
3:C:178:ARG:HD2	3:C:189:TYR:O	2.05	0.56
2:B:27:TYR:HE1	2:B:44:GLN:HG2	1.70	0.56
1:A:192:VAL:HG11	4:A:301:STE:H92	1.88	0.56
1:A:228:ASN:HB3	4:A:301:STE:H21	1.88	0.55
2:B:27:TYR:CE1	2:B:44:GLN:HG2	2.43	0.54
2:B:85:LEU:HD12	2:B:85:LEU:N	2.23	0.53
3:C:141:ASN:HB3	7:C:431:HOH:O	2.10	0.52
1:A:113:LEU:N	1:A:113:LEU:HD23	2.24	0.52
1:A:151:LEU:HD21	1:A:247:ILE:HD13	1.92	0.51
1:A:167:ASP:OD1	1:A:240:THR:HG22	2.11	0.51
3:C:112:SER:O	3:C:224:PHE:HA	2.11	0.50
3:C:24:ILE:HG13	3:C:25:LEU:HG	1.94	0.50
1:A:229:MET:C	1:A:230:MET:HE2	2.36	0.50
1:A:230:MET:HE2	1:A:230:MET:HA	1.94	0.49
1:A:192:VAL:CG1	1:A:195:MET:HE2	2.44	0.48
1:A:263:PRO:HG3	3:C:40:VAL:HG11	1.96	0.48
2:B:96:GLU:CB	2:B:99:ASN:ND2	2.76	0.48
2:B:73:ALA:HB3	2:B:97:ALA:O	2.15	0.47
1:A:230:MET:HG3	4:A:301:STE:H81	1.96	0.47
1:A:229:MET:O	1:A:230:MET:HE2	2.16	0.46
1:A:288:SER:HB2	3:C:94:GLY:O	2.17	0.45
1:A:203:TRP:HZ3	4:A:301:STE:H32	1.82	0.45
2:B:241:LEU:HD13	2:B:286:ILE:HD12	1.97	0.45
2:B:171:TYR:CG	2:B:172:ARG:N	2.83	0.45
1:A:26:LEU:HB3	1:A:27:PRO:HD2	1.99	0.45
1:A:29:ALA:HB2	3:C:225:THR:HG23	1.99	0.45
1:A:95:MET:HG2	1:A:107:VAL:HG23	1.99	0.44
1:A:24:GLN:HG3	7:C:385:HOH:O	2.15	0.44
3:C:227:LYS:HG2	3:C:228:LEU:N	2.31	0.44
2:B:137:THR:CG2	2:B:302:PRO:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:TYR:O	1:A:223:GLY:HA2	2.17	0.43
1:A:193:PRO:HB3	2:B:37:TYR:CD2	2.54	0.43
1:A:137:PHE:HB3	1:A:249:LEU:HD11	2.01	0.43
3:C:10:THR:O	3:C:11:ASN:HB2	2.18	0.42
3:C:178:ARG:NH2	7:C:304:HOH:O	2.51	0.42
1:A:61:LYS:HB3	1:A:66:THR:OG1	2.19	0.42
2:B:23:SER:HB2	7:C:411:HOH:O	2.19	0.42
1:A:113:LEU:C	1:A:114:MET:HE2	2.43	0.42
2:B:84:GLN:HE21	2:B:93:THR:HG22	1.84	0.42
3:C:130:LYS:HA	3:C:157:TRP:O	2.19	0.42
3:C:178:ARG:CD	3:C:189:TYR:O	2.67	0.42
1:A:265:PRO:HB2	2:B:239:ILE:HB	2.00	0.42
2:B:171:TYR:CD1	2:B:172:ARG:N	2.88	0.41
1:A:73:HIS:HB3	3:C:177:TYR:OH	2.20	0.41
1:A:232:THR:HG22	1:A:233:PHE:N	2.36	0.41
2:B:318:ARG:HB2	2:B:319:GLN:H	1.75	0.41
1:A:254:ARG:NH2	3:C:18:ASP:HA	2.35	0.41
2:B:96:GLU:HG2	2:B:99:ASN:ND2	2.36	0.41
3:C:220:ALA:HB1	3:C:224:PHE:CG	2.55	0.41
3:C:108:TYR:O	3:C:230:LYS:HE3	2.21	0.41
2:B:38:ALA:HB2	3:C:23:PRO:HB3	2.02	0.40
2:B:148:TYR:HA	2:B:283:LEU:O	2.21	0.40
3:C:28:PHE:CD1	3:C:28:PHE:C	2.98	0.40
2:B:246:VAL:HA	3:C:49:VAL:HG11	2.03	0.40
2:B:87:ILE:HG22	2:B:132:PHE:CE2	2.57	0.40

All (2) 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)
7:B:639:HOH:O	7:C:404:HOH:O[9_555]	0.47	1.73
7:B:501:HOH:O	7:B:501:HOH:O[19_555]	1.76	0.44

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	253/297 (85%)	240 (95%)	13 (5%)	0	100	100
2	B	280/323 (87%)	268 (96%)	12 (4%)	0	100	100
3	C	240/242 (99%)	233 (97%)	7 (3%)	0	100	100
All	All	773/862 (90%)	741 (96%)	32 (4%)	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	228/257 (89%)	226 (99%)	2 (1%)	70	87
2	B	237/271 (88%)	235 (99%)	2 (1%)	73	88
3	C	204/204 (100%)	201 (98%)	3 (2%)	57	80
All	All	669/732 (91%)	662 (99%)	7 (1%)	68	86

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	235	ILE
2	B	256	THR
2	B	318	ARG
3	C	40	VAL
3	C	187	ASP
3	C	196	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN

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Mol	Chain	Res	Type
1	A	102	ASN
1	A	202	GLN
2	B	84	GLN
2	B	99	ASN
2	B	164	ASN
2	B	210	ASN
2	B	280	ASN
2	B	294	ASN
3	C	56	ASN
3	C	221	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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	STE	A	301	-	19,19,19	0.41	0	19,19,19	0.90	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	STE	A	301	-	-	9/17/17/17	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

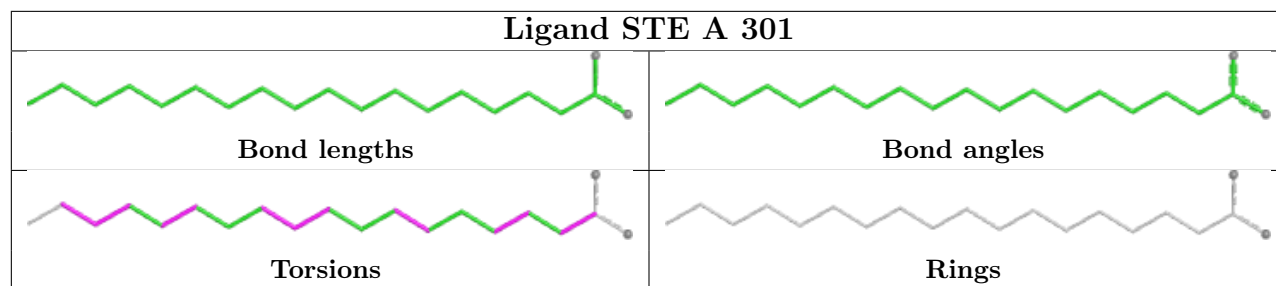
Mol	Chain	Res	Type	Atoms
4	A	301	STE	C2-C3-C4-C5
4	A	301	STE	C11-C10-C9-C8
4	A	301	STE	C14-C15-C16-C17
4	A	301	STE	C9-C10-C11-C12
4	A	301	STE	C5-C6-C7-C8
4	A	301	STE	C12-C13-C14-C15
4	A	301	STE	C15-C16-C17-C18
4	A	301	STE	O2-C1-C2-C3
4	A	301	STE	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	STE	4	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

6.1 Protein, DNA and RNA chains

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	259/297 (87%)	2.16	74 (28%)  	9, 18, 77, 125	0
2	B	286/323 (88%)	2.15	80 (27%)  	9, 15, 87, 121	0
3	C	242/242 (100%)	1.17	32 (13%)  	9, 15, 35, 55	0
All	All	787/862 (91%)	1.86	186 (23%)  	9, 16, 75, 125	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLY	17.5
2	B	45	ASP	14.7
2	B	74	GLU	13.4
1	A	23	LEU	13.2
1	A	2	ASP	12.5
1	A	61	LYS	11.8
2	B	65	ALA	11.8
2	B	98	ALA	11.3
2	B	82	VAL	11.0
1	A	59	SER	11.0
1	A	35	SER	10.7
2	B	75	ALA	10.5
1	A	3	PRO	10.5
2	B	76	CYS	10.4
1	A	33	GLU	10.2
2	B	26	ASN	10.2
2	B	95	GLN	10.0
2	B	44	GLN	10.0
2	B	14	GLU	9.9
2	B	69	LYS	9.8
1	A	72	HIS	9.5
1	A	62	ASN	9.4
1	A	5	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
2	B	83	ALA	9.3
2	B	96	GLU	9.1
2	B	27	TYR	9.1
1	A	101	GLN	8.8
1	A	27	PRO	8.8
2	B	25	ILE	8.4
2	B	24	THR	8.4
2	B	43	ARG	8.3
1	A	24	GLN	8.2
2	B	73	ALA	8.2
1	A	100	THR	8.1
2	B	84	GLN	8.1
2	B	67	PRO	8.0
1	A	60	ASP	7.9
2	B	99	ASN	7.7
2	B	72	SER	7.7
3	C	238	THR	7.6
2	B	71	PRO	7.4
1	A	6	ASP	7.4
1	A	26	LEU	7.4
2	B	94	THR	7.3
2	B	34	LYS	7.3
1	A	31	ASN	7.1
2	B	16	SER	7.1
1	A	34	ALA	7.0
1	A	29	ALA	6.8
2	B	23	SER	6.5
2	B	70	SER	6.5
2	B	68	LEU	6.5
1	A	4	ILE	6.4
2	B	66	PRO	6.4
1	A	32	THR	6.3
1	A	99	GLY	6.3
2	B	28	THR	6.3
2	B	22	GLY	6.2
1	A	7	MET	6.2
2	B	30	ILE	6.1
2	B	97	ALA	5.9
2	B	21	GLU	5.8
2	B	93	THR	5.7
2	B	33	TYR	5.5
1	A	28	THR	5.4

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Mol	Chain	Res	Type	RSRZ
2	B	35	ASP	5.4
3	C	240	ASN	5.3
2	B	32	TYR	5.3
1	A	231	GLY	5.2
1	A	25	VAL	5.2
1	A	70	LEU	5.0
3	C	161	LEU	5.0
3	C	239	ALA	4.9
2	B	20	SER	4.8
1	A	167	ASP	4.8
1	A	103	THR	4.8
2	B	15	ASN	4.8
1	A	102	ASN	4.8
2	B	31	ASN	4.7
1	A	233	PHE	4.7
3	C	233	GLU	4.6
1	A	98	THR	4.4
1	A	71	ASN	4.4
1	A	76	GLN	4.3
1	A	213	GLU	4.2
1	A	97	THR	4.1
1	A	63	LEU	4.0
2	B	17	ASN	3.9
2	B	157	GLU	3.9
3	C	19	GLY	3.7
3	C	160	GLY	3.7
1	A	288	SER	3.7
2	B	42	GLY	3.6
2	B	18	SER	3.6
2	B	29	THR	3.5
1	A	30	ALA	3.4
3	C	162	GLN	3.4
2	B	85	LEU	3.4
1	A	133	ALA	3.4
1	A	220	LEU	3.3
1	A	65	GLU	3.3
2	B	40	SER	3.3
3	C	29	HIS	3.2
1	A	293	LYS	3.2
1	A	104	ASP	3.2
1	A	297	LEU	3.2
3	C	177	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
3	C	20	VAL	3.2
2	B	39	ALA	3.1
1	A	139	VAL	3.1
2	B	19	ALA	3.1
3	C	222	ASP	3.1
2	B	146	GLY	3.1
3	C	78	LYS	3.1
1	A	95	MET	3.1
2	B	211	GLU	3.1
1	A	112	ASP	3.1
2	B	37	TYR	3.0
1	A	242	LYS	3.0
2	B	208	THR	3.0
3	C	77	SER	3.0
1	A	258	VAL	3.0
2	B	91	THR	3.0
3	C	30	PRO	3.0
3	C	21	SER	3.0
1	A	155	TYR	2.9
3	C	242	GLN	2.9
1	A	282	ASN	2.8
3	C	3	PRO	2.8
2	B	41	ALA	2.8
3	C	236	GLU	2.8
3	C	187	ASP	2.8
1	A	162	LYS	2.7
2	B	87	ILE	2.7
1	A	109	TRP	2.7
2	B	38	ALA	2.7
3	C	31	THR	2.7
3	C	182	ARG	2.7
2	B	264	VAL	2.6
1	A	226	PRO	2.6
1	A	191	SER	2.6
1	A	74	SER	2.5
3	C	22	ALA	2.5
2	B	323	GLN	2.5
1	A	73	HIS	2.5
2	B	124	ARG	2.5
1	A	164	THR	2.5
3	C	185	TYR	2.4
1	A	118	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	322	LYS	2.4
1	A	111	ILE	2.4
2	B	92	ILE	2.4
1	A	113	LEU	2.4
2	B	158	VAL	2.4
3	C	1	GLY	2.4
3	C	140	GLY	2.4
2	B	145	LYS	2.3
2	B	183	ALA	2.3
2	B	275	ALA	2.3
3	C	50	GLU	2.3
1	A	239	GLY	2.3
2	B	107	TRP	2.3
2	B	210	ASN	2.2
1	A	240	THR	2.2
2	B	207	GLY	2.2
1	A	69	VAL	2.2
2	B	250	GLN	2.2
2	B	209	GLY	2.2
2	B	256	THR	2.2
2	B	286	ILE	2.2
2	B	109	GLU	2.2
3	C	159	PHE	2.2
1	A	200	ALA	2.1
2	B	244	LEU	2.1
3	C	166	THR	2.1
3	C	6	LEU	2.1
1	A	78	THR	2.1
1	A	175	THR	2.1
2	B	263	ILE	2.1
1	A	91	SER	2.1
2	B	196	LEU	2.0
1	A	145	GLU	2.0
3	C	46	ILE	2.0
1	A	110	ASP	2.0
1	A	247	ILE	2.0
3	C	26	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

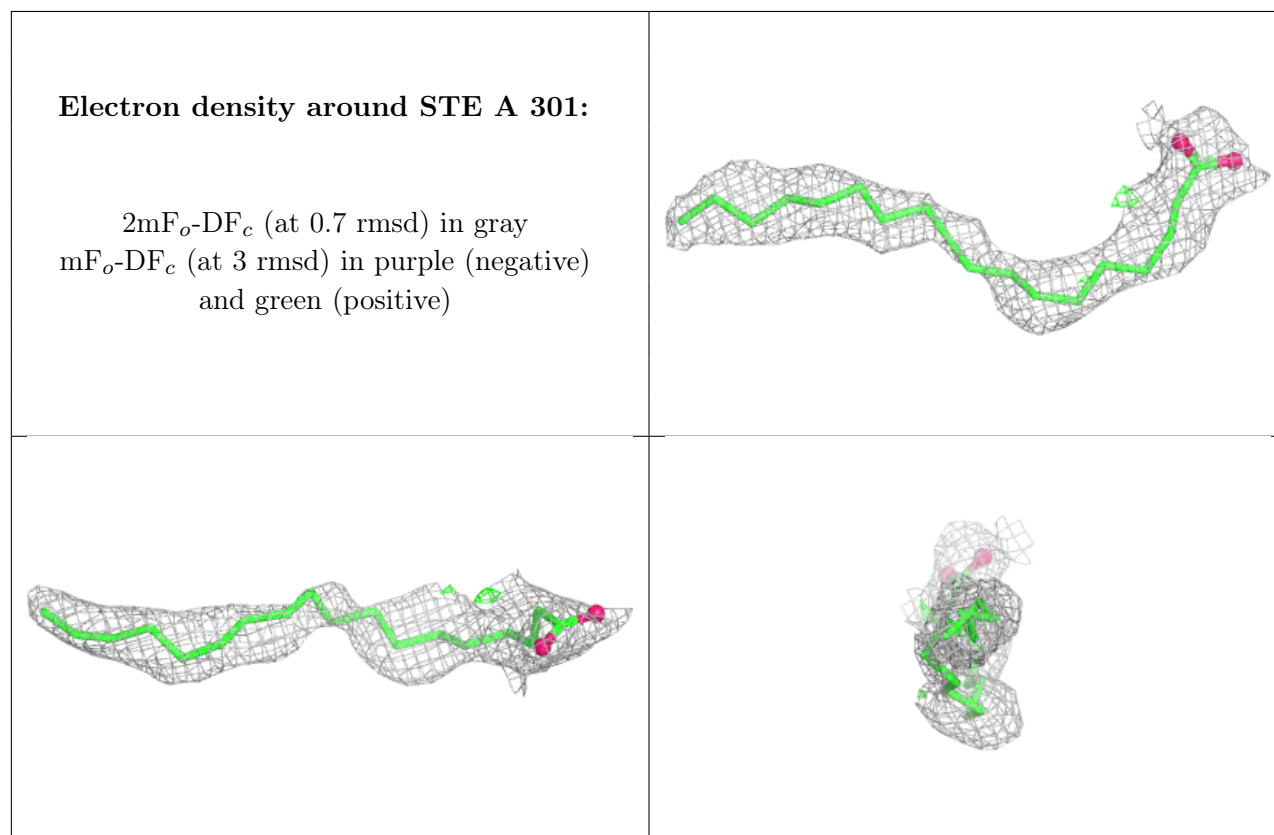
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
6	K	A	303	1/1	0.42	0.55	101,101,101,101	0
4	STE	A	301	20/20	0.80	0.30	22,38,72,85	0
5	CL	A	302	1/1	0.94	0.14	26,26,26,26	0
5	CL	B	401	1/1	0.98	0.06	33,33,33,33	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.