



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:11 PM UTC

PDB ID : 7QH9 / pdb_00007qh9
Title : TarM(Se)_G117R-4RboP
Authors : Guo, Y.; Stehle, T.
Deposited on : 2021-12-10
Resolution : 2.69 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

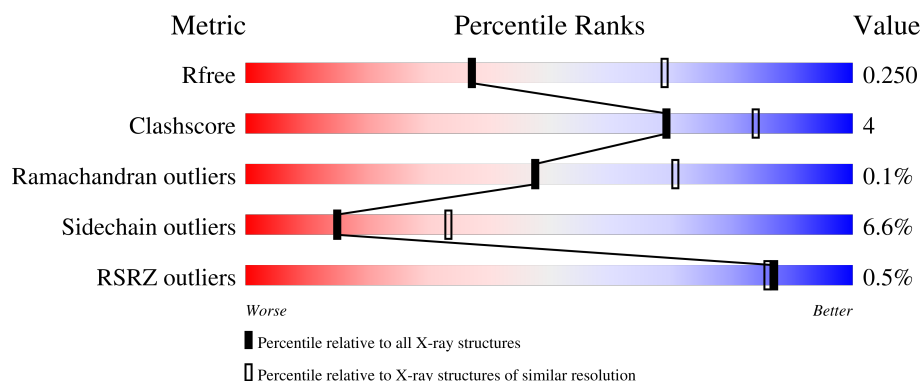
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	AAA	508	% 86% 11% .
1	BBB	508	86% 10% ..
1	CCC	508	% 87% 9% ..
1	DDD	508	% 87% 9% ..

2 Entry composition ⓘ

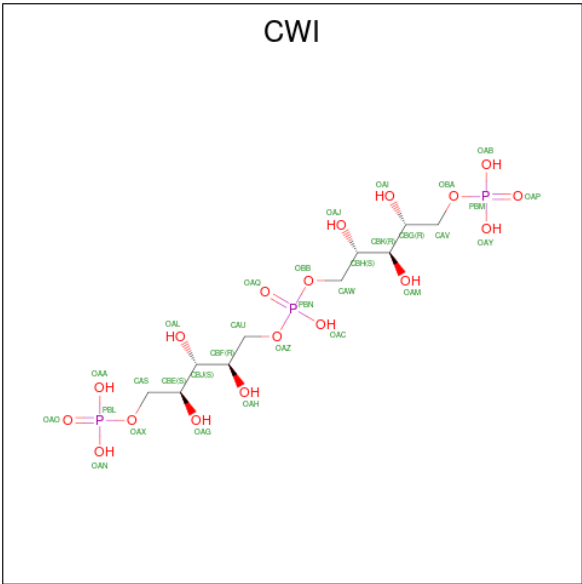
There are 5 unique types of molecules in this entry. The entry contains 14372 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TarM(Se)_G117R-4RboP.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	492	Total	C	N	O	S	0	0	0
			3518	2239	590	676	13			
1	BBB	492	Total	C	N	O	S	0	0	0
			3508	2220	588	684	16			
1	CCC	492	Total	C	N	O	S	0	0	0
			3503	2223	590	675	15			
1	DDD	491	Total	C	N	O	S	0	0	0
			3468	2204	582	669	13			

- Molecule 2 is [(2 {R},3 {S},4 {S})-2,3,4-tris(oxidanyl)-5-phosphonooxy-pentyl] [(2 {S},3 {R},4 {R})-2,3,4-tris(oxidanyl)-5-phosphonooxy-pentyl] hydrogen phosphate (CCD ID: CWI) (formula: C₁₀H₂₅O₁₈P₃) (labeled as "Ligand of Interest" by depositor).



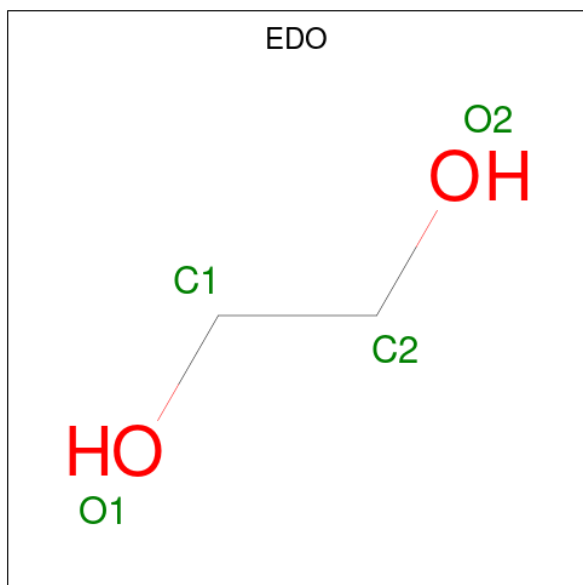
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	AAA	1	Total	C	O	P	0	0
			31	10	18	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	BBB	1	Total	C	O	P	0	0
			31	10	18	3		
2	CCC	1	Total	C	O	P	0	0
			31	10	18	3		
2	DDD	1	Total	C	O	P	0	0
			31	10	18	3		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	BBB	1	Total	C	O	0	0
			4	2	2		
3	DDD	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	CCC	2	Total	Cl	0	0
			2	2		
4	DDD	1	Total	Cl	0	0
			1	1		

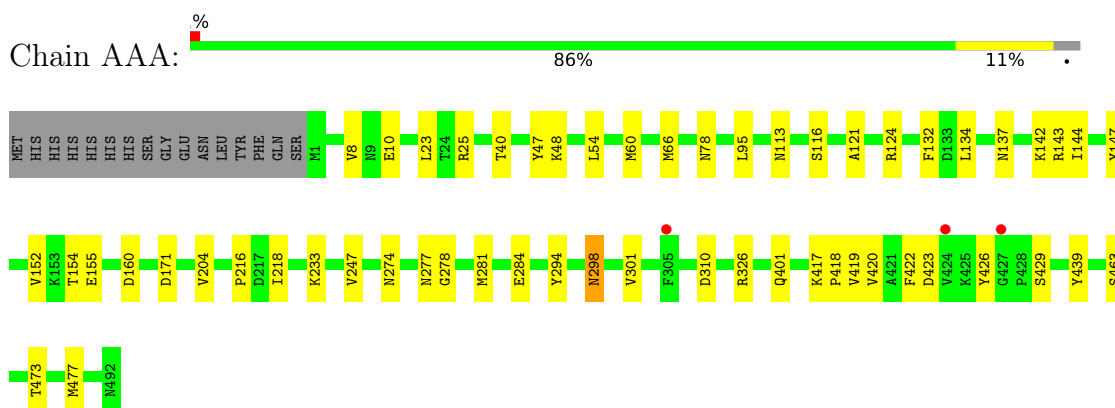
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	54	Total 54	O 54	0	0
5	BBB	71	Total 71	O 71	0	0
5	CCC	54	Total 54	O 54	0	0
5	DDD	61	Total 61	O 61	0	0

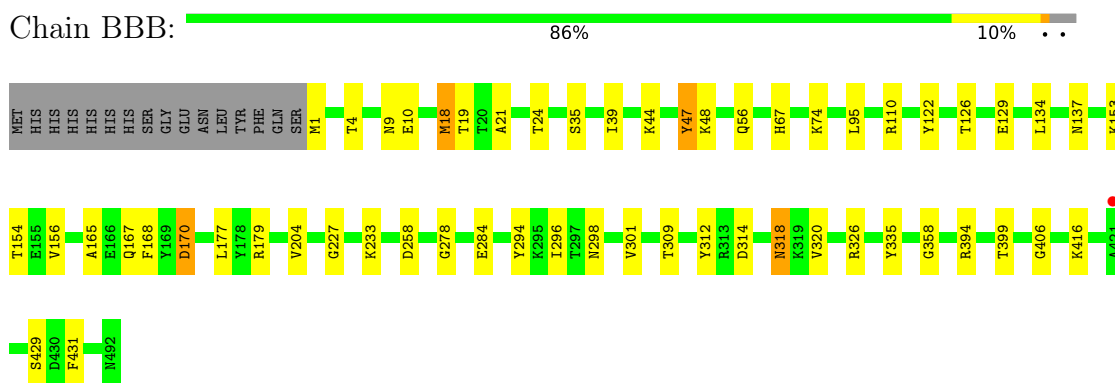
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

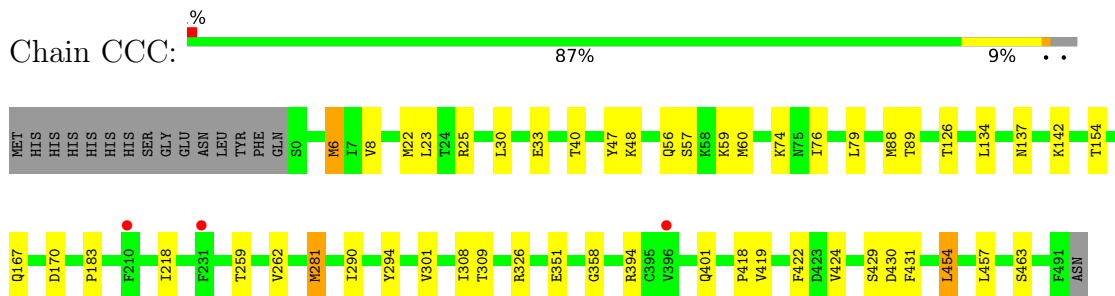
- Molecule 1: TarM(Se)_G117R-4RboP



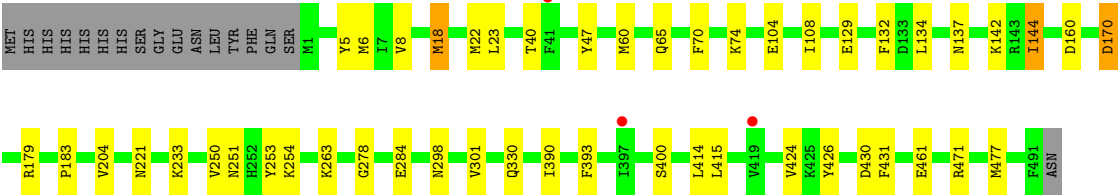
- Molecule 1: TarM(Se)_G117R-4RboP



- Molecule 1: TarM(Se)_G117R-4RboP



● Molecule 1: TarM(Se)_G117R-4RboP



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.87Å 70.57Å 137.38Å 89.97° 90.01° 90.02°	Depositor
Resolution (Å)	49.23 – 2.69 49.23 – 2.69	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.23-2.69) 95.1 (49.23-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.243 , 0.253 0.240 , 0.250	Depositor DCC
R_{free} test set	2924 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 151.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.449 for h,-k,-l 0.458 for -h,k,-l 0.457 for -h,-k,l	Xtriage
Reported twinning fraction	0.331 for H, K, L 0.198 for h,-k,-l 0.217 for -h,-k,l 0.254 for -H, K, -L	Depositor
Outliers	0 of 58472 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14372	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% 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: EDO, CL, CWI

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	AAA	1.04	0/3581	1.35	0/4876
1	BBB	1.06	0/3570	1.38	3/4862 (0.1%)
1	CCC	1.06	0/3564	1.35	2/4853 (0.0%)
1	DDD	1.06	0/3530	1.39	1/4805 (0.0%)
All	All	1.06	0/14245	1.37	6/19396 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	170	ASP	CA-CB-CG	5.28	117.88	112.60
1	BBB	358	GLY	CA-C-N	5.24	127.82	120.28
1	BBB	358	GLY	C-N-CA	5.24	127.82	120.28
1	CCC	358	GLY	CA-C-N	5.23	127.81	120.28
1	CCC	358	GLY	C-N-CA	5.23	127.81	120.28
1	DDD	170	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	3518	0	2839	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BBB	3508	0	2830	21	0
1	CCC	3503	0	2835	21	0
1	DDD	3468	0	2761	22	0
2	AAA	31	0	0	0	0
2	BBB	31	0	0	0	0
2	CCC	31	0	0	0	0
2	DDD	31	0	0	0	0
3	BBB	4	0	6	0	0
3	DDD	4	0	6	0	0
4	CCC	2	0	0	0	0
4	DDD	1	0	0	0	0
5	AAA	54	0	0	0	0
5	BBB	71	0	0	0	0
5	CCC	54	0	0	0	0
5	DDD	61	0	0	1	0
All	All	14372	0	11277	90	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 4.

All (90) 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:AAA:294:TYR:CZ	1:AAA:294:TYR:CD1	2.50	0.94
1:DDD:65:GLN:OE1	5:DDD:601:HOH:O	2.12	0.67
1:DDD:431:PHE:HA	1:DDD:477:MET:HE1	1.77	0.65
1:BBB:278:GLY:HA2	1:BBB:298:ASN:HB2	1.77	0.64
1:CCC:154:THR:OG1	1:CCC:167:GLN:HB2	2.03	0.59
1:AAA:147:TYR:HB3	1:AAA:152:VAL:HG11	1.84	0.58
1:AAA:278:GLY:HA2	1:AAA:298:ASN:HB3	1.85	0.58
1:AAA:54:LEU:HB3	1:AAA:60:MET:HB2	1.89	0.55
1:AAA:78:ASN:HD21	1:AAA:171:ASP:HB2	1.74	0.53
1:DDD:23:LEU:HD22	1:DDD:60:MET:HG3	1.92	0.52
1:DDD:5:TYR:HE2	1:DDD:221:ASN:HD22	1.56	0.51
1:AAA:204:VAL:HA	1:AAA:233:LYS:HG2	1.91	0.51
1:CCC:394:ARG:HG2	1:CCC:457:LEU:HD23	1.93	0.50
1:CCC:401:GLN:O	1:CCC:424:VAL:CG1	2.59	0.50
1:CCC:401:GLN:C	1:CCC:424:VAL:HG11	2.36	0.50
1:AAA:420:VAL:HG22	1:AAA:439:TYR:HB2	1.92	0.50
1:AAA:473:THR:HG22	1:AAA:477:MET:HE2	1.91	0.50
1:BBB:39:ILE:HG12	1:BBB:67:HIS:HB2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:126:THR:OG1	1:BBB:129:GLU:HB3	2.12	0.50
1:CCC:401:GLN:O	1:CCC:424:VAL:HG11	2.12	0.50
1:BBB:406:GLY:HA3	1:BBB:431:PHE:HZ	1.76	0.50
1:DDD:6:MET:HB3	1:DDD:22:MET:HE3	1.93	0.50
1:BBB:95:LEU:CD2	1:BBB:134:LEU:HD22	2.41	0.50
1:CCC:57:SER:C	1:CCC:59:LYS:H	2.19	0.50
1:CCC:74:LYS:HG3	1:CCC:170:ASP:HA	1.93	0.49
1:DDD:132:PHE:HB2	1:DDD:144:ILE:HB	1.93	0.49
1:AAA:121:ALA:HB2	1:AAA:134:LEU:HD23	1.95	0.49
1:BBB:156:VAL:HB	1:BBB:165:ALA:HB3	1.95	0.48
1:BBB:204:VAL:HA	1:BBB:233:LYS:HG2	1.95	0.48
1:BBB:4:THR:HB	1:BBB:35:SER:O	2.14	0.48
1:DDD:251:ASN:HD21	1:DDD:253:TYR:HD2	1.62	0.48
1:DDD:6:MET:HB3	1:DDD:22:MET:CE	2.44	0.48
1:AAA:284:GLU:HG2	1:AAA:301:VAL:HG11	1.95	0.48
1:BBB:284:GLU:HA	1:BBB:301:VAL:HG21	1.94	0.48
1:DDD:400:SER:O	1:DDD:424:VAL:HG11	2.14	0.47
1:CCC:23:LEU:HD22	1:CCC:60:MET:HG3	1.97	0.47
1:CCC:418:PRO:HG3	1:CCC:463:SER:HB2	1.96	0.47
1:BBB:44:LYS:HB2	1:BBB:47:TYR:CD2	2.50	0.47
1:CCC:134:LEU:HD12	1:CCC:142:LYS:HB3	1.95	0.47
1:AAA:417:LYS:HD3	1:AAA:417:LYS:HA	1.56	0.47
1:CCC:422:PHE:HB3	1:CCC:424:VAL:HG23	1.97	0.47
1:BBB:154:THR:OG1	1:BBB:167:GLN:HB2	2.16	0.46
1:DDD:278:GLY:HA2	1:DDD:298:ASN:HB2	1.96	0.46
1:CCC:281:MET:O	1:CCC:301:VAL:HA	2.15	0.46
1:BBB:18:MET:HE1	1:BBB:227:GLY:HA2	1.98	0.46
1:BBB:168:PHE:HB2	1:BBB:177:LEU:HB3	1.98	0.46
1:BBB:318:ASN:O	1:BBB:394:ARG:HB2	2.16	0.46
1:CCC:8:VAL:O	1:CCC:40:THR:HA	2.15	0.45
1:AAA:113:ASN:HB3	1:AAA:116:SER:HB2	1.98	0.45
1:DDD:204:VAL:HA	1:DDD:233:LYS:HG2	1.98	0.45
1:AAA:144:ILE:HA	1:AAA:154:THR:HG22	1.99	0.45
1:BBB:312:TYR:O	1:BBB:416:LYS:CE	2.65	0.45
1:DDD:18:MET:HE3	1:DDD:18:MET:HB2	1.75	0.45
1:AAA:23:LEU:HD22	1:AAA:60:MET:HG3	1.99	0.44
1:AAA:298:ASN:HD22	1:AAA:298:ASN:HA	1.64	0.44
1:DDD:284:GLU:HA	1:DDD:301:VAL:HG21	1.99	0.44
1:DDD:8:VAL:O	1:DDD:40:THR:HA	2.18	0.44
1:CCC:290:ILE:O	1:CCC:294:TYR:HB2	2.18	0.43
1:BBB:21:ALA:HA	1:BBB:24:THR:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:154:THR:HG1	1:CCC:167:GLN:HB2	1.82	0.43
1:AAA:418:PRO:HG3	1:AAA:463:SER:HB2	2.00	0.43
1:CCC:6:MET:HB3	1:CCC:22:MET:CE	2.48	0.43
1:CCC:308:ILE:O	1:CCC:309:THR:HG23	2.18	0.43
1:DDD:70:PHE:O	1:DDD:74:LYS:HB2	2.18	0.43
1:DDD:390:ILE:HG21	1:DDD:415:LEU:HD12	2.01	0.43
1:AAA:66:MET:HE2	1:AAA:66:MET:HB3	1.79	0.43
1:AAA:132:PHE:O	1:AAA:143:ARG:HA	2.18	0.42
1:DDD:134:LEU:HD12	1:DDD:142:LYS:HB3	2.01	0.42
1:AAA:216:PRO:O	1:AAA:218:ILE:HG22	2.19	0.42
1:AAA:134:LEU:HD12	1:AAA:142:LYS:HB3	2.02	0.42
1:AAA:8:VAL:O	1:AAA:40:THR:HA	2.20	0.42
1:BBB:95:LEU:HD23	1:BBB:134:LEU:HD22	2.00	0.42
1:AAA:419:VAL:HG23	1:AAA:419:VAL:O	2.19	0.42
1:BBB:9:ASN:HB3	1:BBB:10:GLU:OE1	2.19	0.42
1:CCC:419:VAL:O	1:CCC:419:VAL:HG23	2.20	0.42
1:DDD:74:LYS:HG3	1:DDD:170:ASP:HA	2.01	0.41
1:AAA:78:ASN:ND2	1:AAA:171:ASP:HB2	2.36	0.41
1:DDD:390:ILE:HA	1:DDD:393:PHE:CD2	2.55	0.41
1:AAA:143:ARG:HB3	1:AAA:155:GLU:HB2	2.03	0.41
1:DDD:414:LEU:HA	1:DDD:471:ARG:HA	2.02	0.41
1:CCC:57:SER:C	1:CCC:59:LYS:N	2.76	0.41
1:CCC:76:ILE:HA	1:CCC:79:LEU:HD12	2.03	0.41
1:CCC:454:LEU:HD12	1:CCC:454:LEU:HA	1.83	0.41
1:DDD:254:LYS:HA	1:DDD:263:LYS:HG2	2.03	0.41
1:BBB:335:TYR:HB2	1:BBB:399:THR:HB	2.03	0.41
1:BBB:74:LYS:HG3	1:BBB:170:ASP:HA	2.04	0.40
1:BBB:314:ASP:OD1	1:BBB:416:LYS:CE	2.69	0.40
1:AAA:95:LEU:HD23	1:AAA:134:LEU:HD22	2.03	0.40
1:AAA:121:ALA:CB	1:AAA:134:LEU:HD23	2.51	0.40
1:DDD:104:GLU:HB2	1:DDD:108:ILE:HG23	2.03	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	AAA	490/508 (96%)	457 (93%)	33 (7%)	0	100	100
1	BBB	490/508 (96%)	442 (90%)	48 (10%)	0	100	100
1	CCC	490/508 (96%)	449 (92%)	40 (8%)	1 (0%)	43	65
1	DDD	489/508 (96%)	446 (91%)	42 (9%)	1 (0%)	43	65
All	All	1959/2032 (96%)	1794 (92%)	163 (8%)	2 (0%)	48	71

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	183	PRO
1	CCC	183	PRO

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	AAA	269/471 (57%)	250 (93%)	19 (7%)	13	30
1	BBB	272/471 (58%)	253 (93%)	19 (7%)	14	31
1	CCC	268/471 (57%)	247 (92%)	21 (8%)	11	26
1	DDD	260/471 (55%)	248 (95%)	12 (5%)	24	48
All	All	1069/1884 (57%)	998 (93%)	71 (7%)	15	33

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	10	GLU
1	AAA	25	ARG
1	AAA	47	TYR
1	AAA	48	LYS
1	AAA	124	ARG
1	AAA	137	ASN

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Mol	Chain	Res	Type
1	AAA	160	ASP
1	AAA	247	VAL
1	AAA	274	ASN
1	AAA	277	ASN
1	AAA	281	MET
1	AAA	298	ASN
1	AAA	310	ASP
1	AAA	326	ARG
1	AAA	401	GLN
1	AAA	422	PHE
1	AAA	423	ASP
1	AAA	426	TYR
1	AAA	429	SER
1	BBB	1	MET
1	BBB	18	MET
1	BBB	19	THR
1	BBB	47	TYR
1	BBB	48	LYS
1	BBB	56	GLN
1	BBB	110	ARG
1	BBB	122	TYR
1	BBB	137	ASN
1	BBB	153	LYS
1	BBB	179	ARG
1	BBB	258	ASP
1	BBB	294	TYR
1	BBB	296	ILE
1	BBB	309	THR
1	BBB	318	ASN
1	BBB	320	VAL
1	BBB	326	ARG
1	BBB	429	SER
1	CCC	6	MET
1	CCC	25	ARG
1	CCC	30	LEU
1	CCC	33	GLU
1	CCC	47	TYR
1	CCC	48	LYS
1	CCC	56	GLN
1	CCC	88	MET
1	CCC	89	THR
1	CCC	126	THR

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Mol	Chain	Res	Type
1	CCC	137	ASN
1	CCC	218	ILE
1	CCC	259	THR
1	CCC	262	VAL
1	CCC	281	MET
1	CCC	326	ARG
1	CCC	351	GLU
1	CCC	429	SER
1	CCC	430	ASP
1	CCC	431	PHE
1	CCC	454	LEU
1	DDD	18	MET
1	DDD	47	TYR
1	DDD	129	GLU
1	DDD	137	ASN
1	DDD	144	ILE
1	DDD	160	ASP
1	DDD	179	ARG
1	DDD	250	VAL
1	DDD	330	GLN
1	DDD	426	TYR
1	DDD	430	ASP
1	DDD	461	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	EDO	DDD	502	-	3,3,3	0.28	0	2,2,2	0.20	0
2	CWI	CCC	501	-	30,30,30	1.57	5 (16%)	41,44,44	1.03	3 (7%)
3	EDO	BBB	501	-	3,3,3	0.24	0	2,2,2	0.17	0
2	CWI	BBB	502	-	30,30,30	1.65	7 (23%)	41,44,44	1.06	2 (4%)
2	CWI	AAA	501	-	30,30,30	1.59	6 (20%)	41,44,44	1.02	3 (7%)
2	CWI	DDD	501	-	30,30,30	1.80	8 (26%)	41,44,44	1.02	3 (7%)

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
3	EDO	DDD	502	-	-	1/1/1/1	-
2	CWI	CCC	501	-	-	28/40/40/40	-
3	EDO	BBB	501	-	-	1/1/1/1	-
2	CWI	BBB	502	-	-	16/40/40/40	-
2	CWI	AAA	501	-	-	22/40/40/40	-
2	CWI	DDD	501	-	-	18/40/40/40	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	DDD	501	CWI	PBM-OAP	3.91	1.62	1.50
2	DDD	501	CWI	PBN-OAQ	3.87	1.64	1.50
2	BBB	502	CWI	PBL-OAO	3.79	1.62	1.50
2	CCC	501	CWI	PBM-OAP	3.75	1.62	1.50
2	BBB	502	CWI	PBM-OAP	3.73	1.62	1.50
2	CCC	501	CWI	PBL-OAO	3.68	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	CWI	PBL-OAO	3.65	1.61	1.50
2	AAA	501	CWI	PBM-OAP	3.64	1.61	1.50
2	DDD	501	CWI	PBL-OAO	3.51	1.61	1.50
2	BBB	502	CWI	PBN-OAQ	3.34	1.62	1.50
2	CCC	501	CWI	PBN-OAQ	3.07	1.61	1.50
2	AAA	501	CWI	PBN-OAQ	2.70	1.60	1.50
2	DDD	501	CWI	CBG-CBK	2.59	1.58	1.53
2	DDD	501	CWI	CAV-CBG	2.22	1.54	1.51
2	BBB	502	CWI	PBL-OAN	2.19	1.62	1.54
2	BBB	502	CWI	CAS-CBE	2.18	1.54	1.51
2	AAA	501	CWI	CBG-CBK	2.17	1.57	1.53
2	DDD	501	CWI	CAW-CBH	2.16	1.54	1.51
2	DDD	501	CWI	PBL-OAN	2.14	1.62	1.54
2	AAA	501	CWI	PBL-OAN	2.13	1.62	1.54
2	CCC	501	CWI	CAS-CBE	2.12	1.54	1.51
2	DDD	501	CWI	CAS-CBE	2.10	1.54	1.51
2	CCC	501	CWI	PBL-OAN	2.08	1.62	1.54
2	BBB	502	CWI	CBE-CBJ	2.02	1.57	1.53
2	AAA	501	CWI	CBH-CBK	2.01	1.56	1.53
2	BBB	502	CWI	CBG-CBK	2.01	1.56	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	DDD	501	CWI	CAV-CBG-CBK	2.86	117.62	112.22
2	DDD	501	CWI	OAA-PBL-OAX	2.61	113.48	106.67
2	BBB	502	CWI	CAU-CBF-CBJ	-2.47	107.55	112.22
2	CCC	501	CWI	CAU-CBF-CBJ	-2.38	107.72	112.22
2	AAA	501	CWI	CAV-CBG-CBK	2.36	116.67	112.22
2	CCC	501	CWI	CBG-CBK-CBH	-2.34	109.68	113.57
2	DDD	501	CWI	CAU-CBF-CBJ	-2.31	107.86	112.22
2	AAA	501	CWI	OAA-PBL-OAX	2.16	112.30	106.67
2	BBB	502	CWI	OAI-CBG-CAV	-2.07	105.42	109.99
2	CCC	501	CWI	OAA-PBL-OAX	2.03	111.96	106.67
2	AAA	501	CWI	OAB-PBM-OBA	2.01	111.90	106.67

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	501	CWI	CAS-OAX-PBL-OAN
2	AAA	501	CWI	CAS-OAX-PBL-OAA

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Mol	Chain	Res	Type	Atoms
2	AAA	501	CWI	OAX-CAS-CBE-CBJ
2	AAA	501	CWI	OAH-CBF-CBJ-CBE
2	AAA	501	CWI	CAU-CBF-CBJ-CBE
2	AAA	501	CWI	OAH-CBF-CBJ-OAL
2	AAA	501	CWI	CAU-CBF-CBJ-OAL
2	AAA	501	CWI	OAZ-CAU-CBF-CBJ
2	AAA	501	CWI	OAZ-CAU-CBF-OAH
2	AAA	501	CWI	CAU-OAZ-PBN-OAC
2	AAA	501	CWI	CAU-OAZ-PBN-OB
2	AAA	501	CWI	CAW-OB-PBN-OAQ
2	AAA	501	CWI	OBA-CAV-CBG-CBK
2	BBB	502	CWI	CAS-OAX-PBL-OAO
2	BBB	502	CWI	CAS-CBE-CBJ-OAL
2	BBB	502	CWI	CAS-CBE-CBJ-CBF
2	BBB	502	CWI	OAG-CBE-CBJ-OAL
2	BBB	502	CWI	OAG-CBE-CBJ-CBF
2	BBB	502	CWI	OAZ-CAU-CBF-CBJ
2	BBB	502	CWI	CAW-OB-PBN-OAQ
2	CCC	501	CWI	CAS-OAX-PBL-OAN
2	CCC	501	CWI	CAS-OAX-PBL-OAA
2	CCC	501	CWI	OAG-CBE-CBJ-OAL
2	CCC	501	CWI	OAG-CBE-CBJ-CBF
2	CCC	501	CWI	CAU-OAZ-PBN-OAC
2	CCC	501	CWI	CAW-CBH-CBK-OAM
2	CCC	501	CWI	CAV-OBA-PBM-OAB
2	DDD	501	CWI	CAS-OAX-PBL-OAN
2	DDD	501	CWI	CAS-OAX-PBL-OAO
2	DDD	501	CWI	CAS-OAX-PBL-OAA
2	DDD	501	CWI	CAS-CBE-CBJ-OAL
2	DDD	501	CWI	CAS-CBE-CBJ-CBF
2	DDD	501	CWI	OAG-CBE-CBJ-OAL
2	DDD	501	CWI	OAG-CBE-CBJ-CBF
2	DDD	501	CWI	OAZ-CAU-CBF-CBJ
2	DDD	501	CWI	OAZ-CAU-CBF-OAH
2	DDD	501	CWI	CAW-OB-PBN-OAZ
2	DDD	501	CWI	CAW-OB-PBN-OAQ
2	DDD	501	CWI	OAI-CBG-CBK-CBH
2	DDD	501	CWI	OAI-CBG-CBK-OAM
2	DDD	501	CWI	CAV-CBG-CBK-OAM
2	CCC	501	CWI	CAS-CBE-CBJ-OAL
2	CCC	501	CWI	CAS-CBE-CBJ-CBF
2	CCC	501	CWI	CAV-CBG-CBK-CBH

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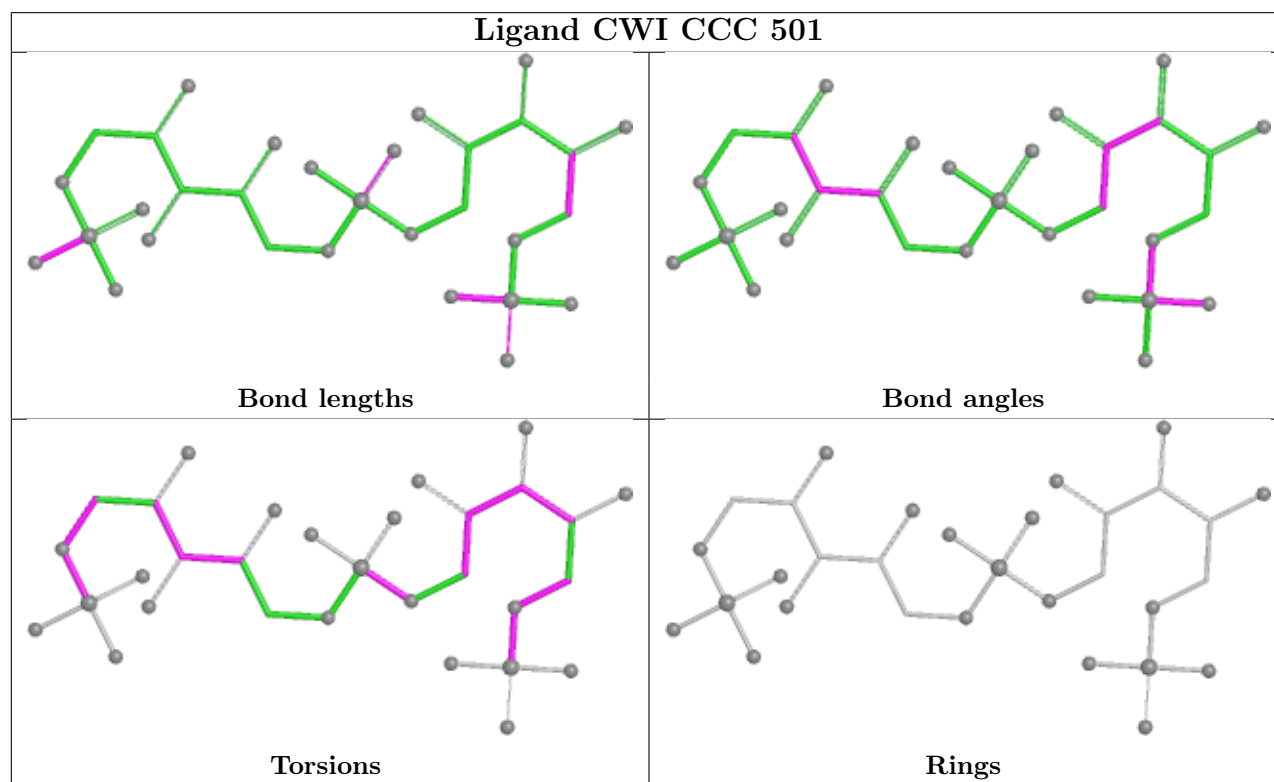
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Mol	Chain	Res	Type	Atoms
2	DDD	501	CWI	CAV-CBG-CBK-CBH
2	BBB	502	CWI	OAI-CBG-CBK-OAM
2	CCC	501	CWI	OAH-CBF-CBJ-OAL
2	CCC	501	CWI	OAJ-CBH-CBK-OAM
2	BBB	502	CWI	OAI-CBG-CBK-CBH
2	CCC	501	CWI	OAH-CBF-CBJ-CBE
2	CCC	501	CWI	OAJ-CBH-CBK-CBG
2	CCC	501	CWI	OAI-CBG-CBK-CBH
2	AAA	501	CWI	CAV-CBG-CBK-OAM
2	BBB	502	CWI	CAV-CBG-CBK-OAM
2	AAA	501	CWI	CAV-CBG-CBK-CBH
2	BBB	502	CWI	CAV-CBG-CBK-CBH
2	CCC	501	CWI	CAU-CBF-CBJ-CBE
2	CCC	501	CWI	CAW-CBH-CBK-CBG
2	AAA	501	CWI	OAI-CBG-CBK-OAM
2	CCC	501	CWI	CAU-CBF-CBJ-OAL
2	CCC	501	CWI	OAI-CBG-CBK-OAM
2	AAA	501	CWI	OBA-CAV-CBG-OAI
2	CCC	501	CWI	CAV-CBG-CBK-OAM
2	AAA	501	CWI	OAI-CBG-CBK-CBH
3	BBB	501	EDO	O1-C1-C2-O2
2	AAA	501	CWI	CAS-OAX-PBL-OAO
2	CCC	501	CWI	CAS-OAX-PBL-OAO
2	CCC	501	CWI	CAV-OBA-PBM-OAP
2	AAA	501	CWI	OAX-CAS-CBE-OAG
2	BBB	502	CWI	OAZ-CAU-CBF-OAH
2	BBB	502	CWI	CAS-OAX-PBL-OAA
3	DDD	502	EDO	O1-C1-C2-O2
2	CCC	501	CWI	OAZ-CAU-CBF-CBJ
2	DDD	501	CWI	CAU-CBF-CBJ-OAL
2	BBB	502	CWI	CAW-OBB-PBN-OAZ
2	CCC	501	CWI	CAU-OAZ-PBN-OAQ
2	CCC	501	CWI	CAU-OAZ-PBN-OB
2	DDD	501	CWI	OAH-CBF-CBJ-OAL
2	CCC	501	CWI	CBG-CAV-OBA-PBM
2	AAA	501	CWI	CBE-CAS-OAX-PBL
2	CCC	501	CWI	CBE-CAS-OAX-PBL
2	BBB	502	CWI	CAS-OAX-PBL-OAN
2	CCC	501	CWI	CAV-OBA-PBM-OAY
2	DDD	501	CWI	CAW-CBH-CBK-CBG
2	AAA	501	CWI	CBH-CAW-OBB-PBN
2	BBB	502	CWI	CBH-CAW-OBB-PBN

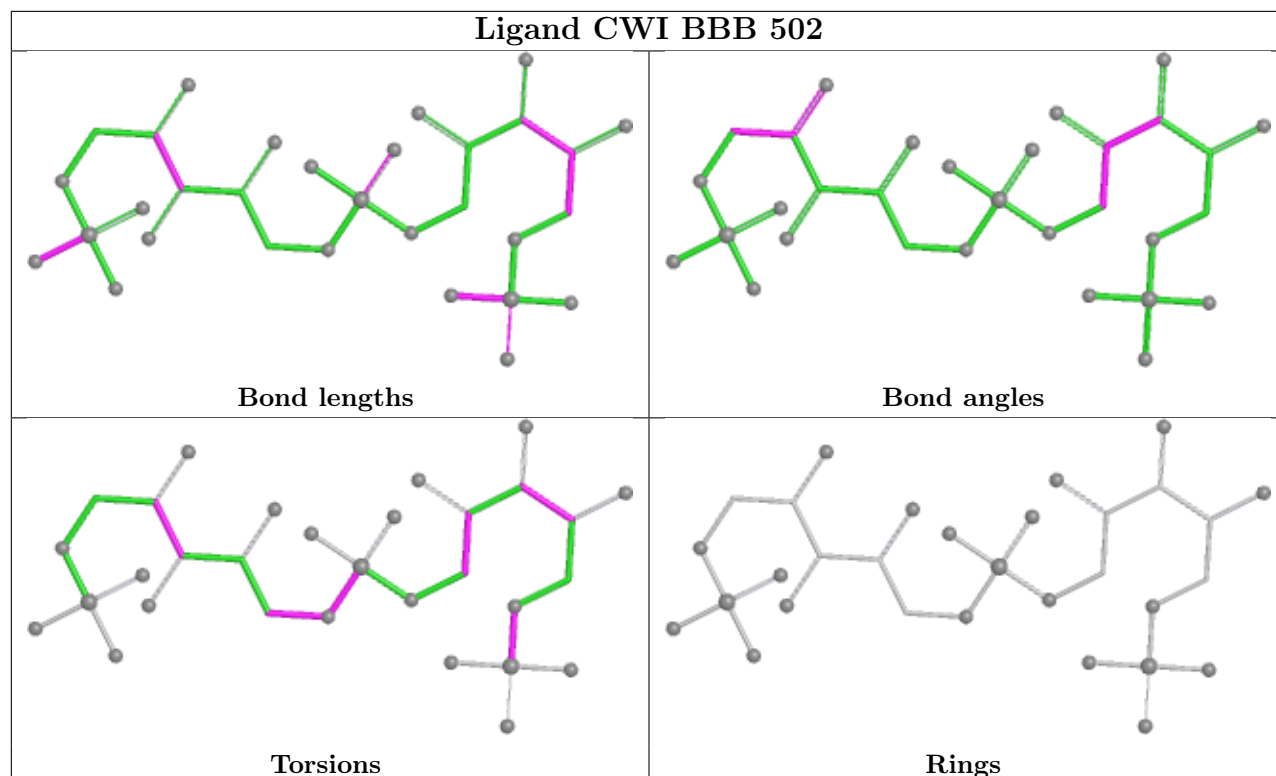
There are no ring outliers.

No monomer is involved in short contacts.

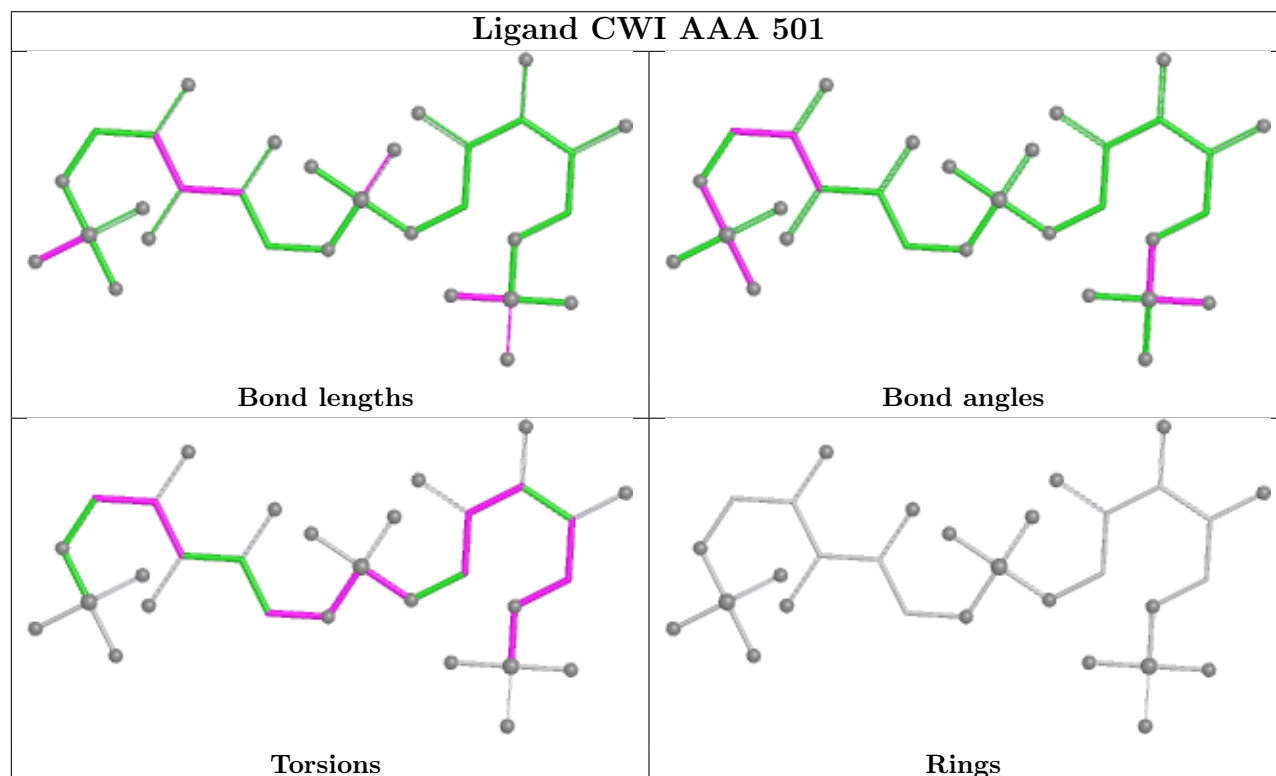
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

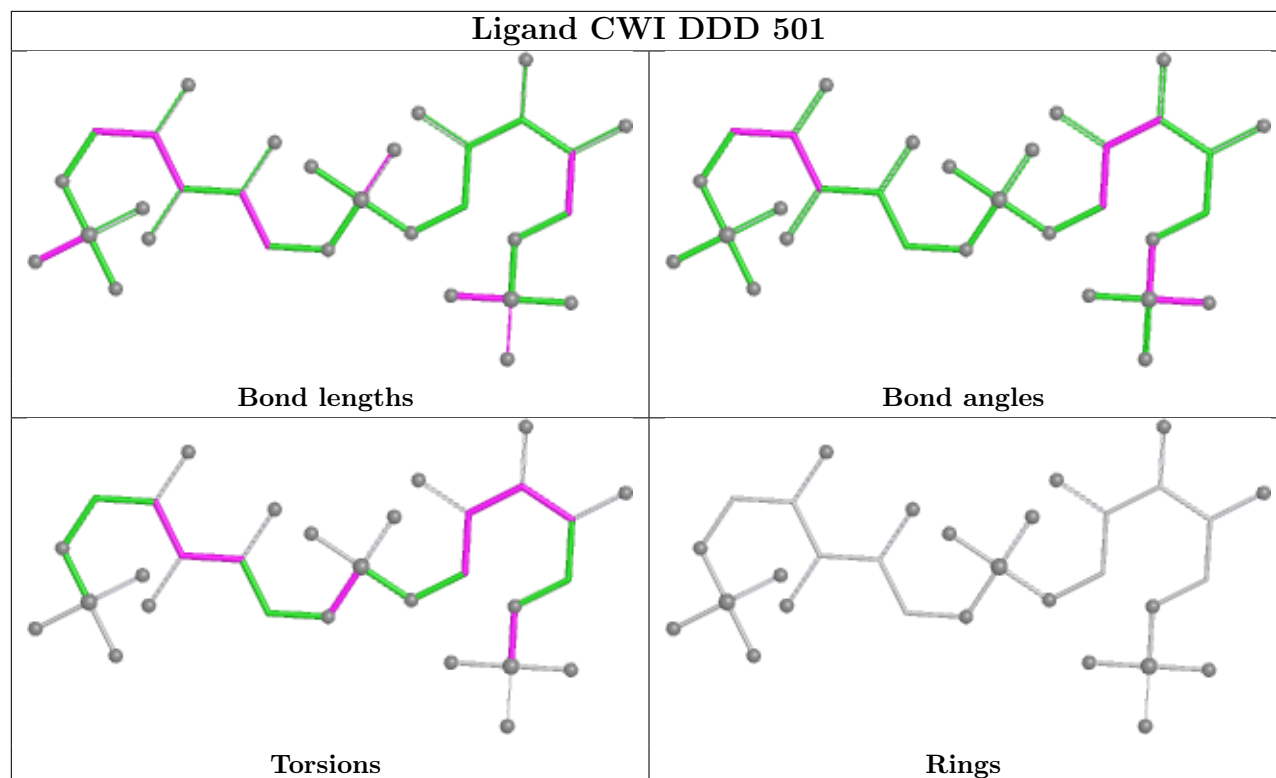


Ligand CWI BBB 502



Ligand CWI AAA 501





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	AAA	492/508 (96%)	-0.71	3 (0%) 85 84	54, 98, 142, 167	0
1	BBB	492/508 (96%)	-0.80	1 (0%) 91 90	54, 99, 132, 161	0
1	CCC	492/508 (96%)	-0.79	3 (0%) 85 84	60, 99, 137, 182	0
1	DDD	491/508 (96%)	-0.80	3 (0%) 85 84	43, 98, 130, 172	0
All	All	1967/2032 (96%)	-0.77	10 (0%) 87 86	43, 99, 135, 182	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	424	VAL	3.4
1	DDD	397	ILE	3.0
1	CCC	396	VAL	2.7
1	DDD	41	PHE	2.7
1	AAA	305	PHE	2.6
1	AAA	427	GLY	2.4
1	BBB	421	ALA	2.4
1	CCC	210	PHE	2.4
1	CCC	231	PHE	2.3
1	DDD	419	VAL	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 ⓘ

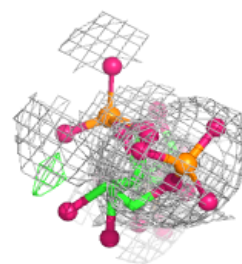
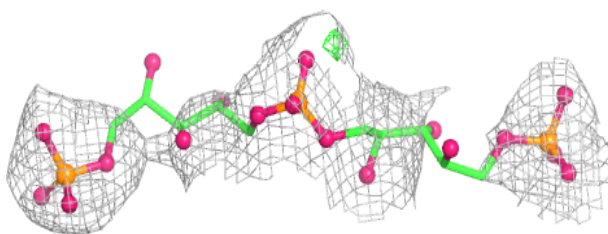
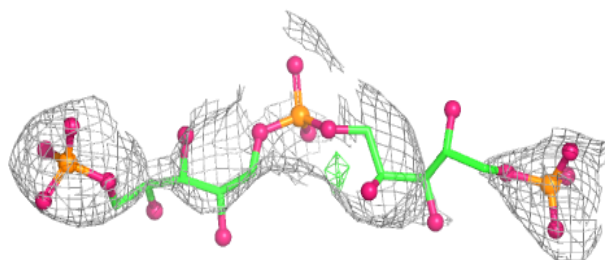
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CWI	BBB	502	31/31	0.97	0.06	69,96,118,127	0
2	CWI	CCC	501	31/31	0.97	0.06	70,84,142,144	0
2	CWI	DDD	501	31/31	0.97	0.06	70,87,113,120	0
3	EDO	BBB	501	4/4	0.97	0.06	24,25,27,31	0
3	EDO	DDD	502	4/4	0.97	0.08	24,29,31,32	0
2	CWI	AAA	501	31/31	0.98	0.07	82,113,135,147	0
4	CL	CCC	502	1/1	0.99	0.06	37,37,37,37	0
4	CL	CCC	503	1/1	0.99	0.12	40,40,40,40	0
4	CL	DDD	503	1/1	0.99	0.05	37,37,37,37	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.

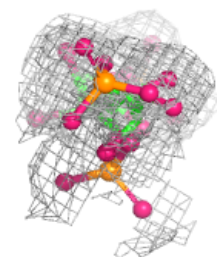
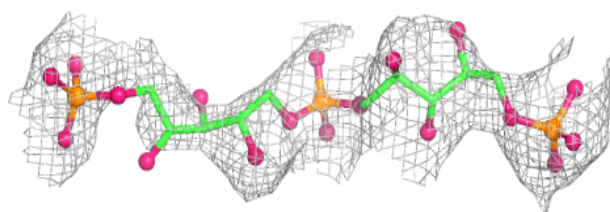
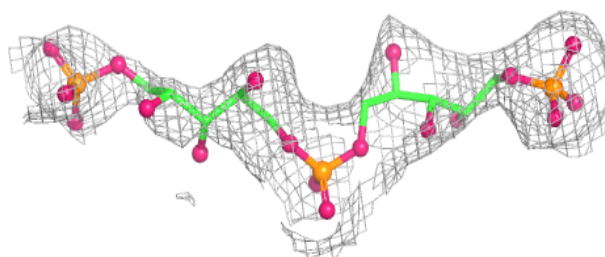
Electron density around CWI BBB 502:

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

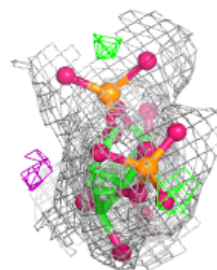
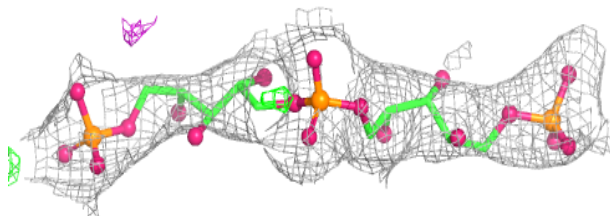
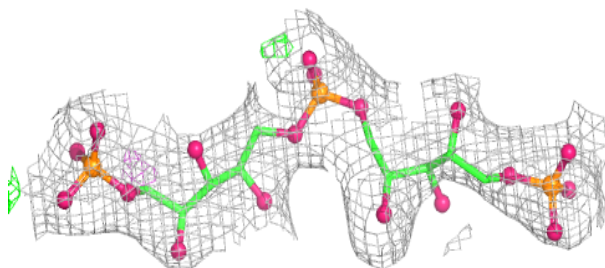


Electron density around CWI CCC 501:

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

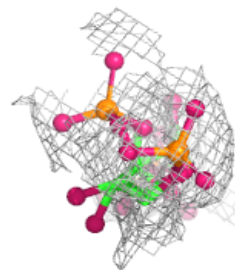
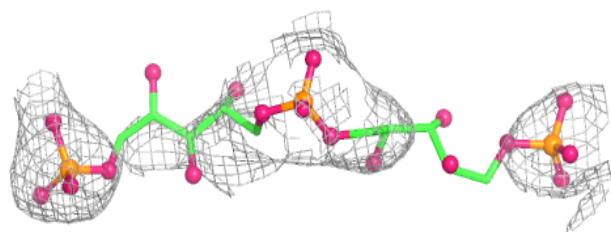
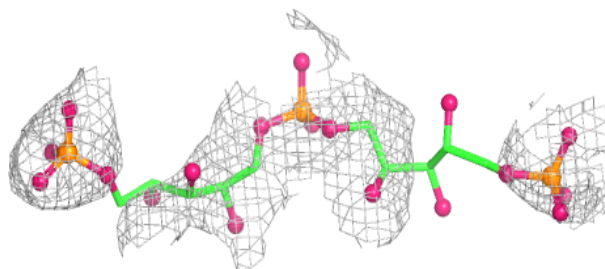
**Electron density around CWI DDD 501:**

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



Electron density around CWI AAA 501:

$2mF_o - DF_c$ (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.