



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 07:24 PM UTC

PDB ID : 6EY7 / pdb_00006ey7
Title : Human cytomegalovirus terminase nuclease domain, Mn soaked, inhibitor bound
Authors : Bongarzone, S.; Nadal, M.; Kaczmarska, Z.; Machon, C.; Alvarez, M.; Albericio, F.; Coll, M.
Deposited on : 2017-11-10
Resolution : 2.90 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

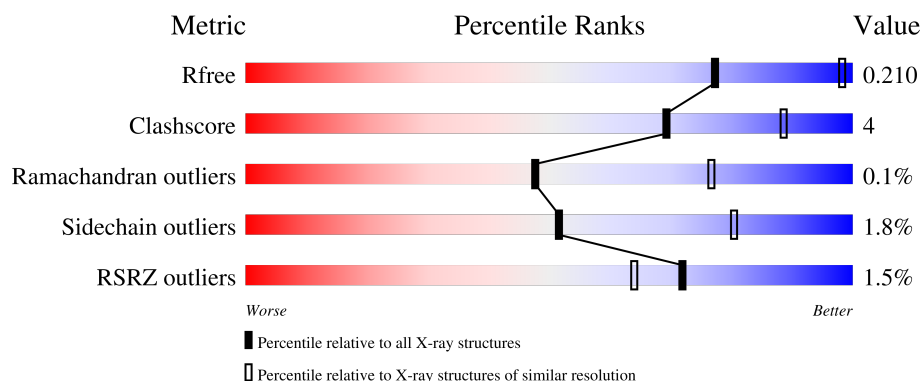
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	279	2% 71% 9% • 19%
1	B	279	% 70% 10% 19%
1	C	279	% 69% 10% • 21%
1	D	279	70% 7% 23%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6928 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 UL89 HCMV terminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	1	0	0
			1724	1110	294	314	6			
1	B	227	Total	C	N	O	S	1	1	0
			1775	1143	303	323	6			
1	C	221	Total	C	N	O	S	1	0	0
			1688	1086	281	315	6			
1	D	214	Total	C	N	O	S	0	0	0
			1633	1048	275	304	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	396	MET	-	initiating methionine	UNP P16732
A	397	GLY	-	expression tag	UNP P16732
A	398	HIS	-	expression tag	UNP P16732
A	399	HIS	-	expression tag	UNP P16732
A	400	HIS	VAL	conflict	UNP P16732
A	401	HIS	ARG	conflict	UNP P16732
A	402	HIS	LYS	conflict	UNP P16732
A	403	HIS	THR	conflict	UNP P16732
A	404	ASP	ALA	conflict	UNP P16732
A	405	TYR	ASN	conflict	UNP P16732
A	406	ASP	MET	conflict	UNP P16732
A	407	ILE	PHE	conflict	UNP P16732
A	408	PRO	MET	conflict	UNP P16732
A	409	THR	PRO	conflict	UNP P16732
A	410	THR	GLY	conflict	UNP P16732
A	411	GLU	ALA	conflict	UNP P16732
A	412	ASN	PHE	conflict	UNP P16732
A	413	LEU	MET	conflict	UNP P16732
A	414	TYR	ASP	conflict	UNP P16732
A	415	PHE	GLU	conflict	UNP P16732
A	416	GLN	ILE	conflict	UNP P16732

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Chain	Residue	Modelled	Actual	Comment	Reference
A	417	GLY	ILE	conflict	UNP P16732
B	396	MET	-	initiating methionine	UNP P16732
B	397	GLY	-	expression tag	UNP P16732
B	398	HIS	-	expression tag	UNP P16732
B	399	HIS	-	expression tag	UNP P16732
B	400	HIS	VAL	conflict	UNP P16732
B	401	HIS	ARG	conflict	UNP P16732
B	402	HIS	LYS	conflict	UNP P16732
B	403	HIS	THR	conflict	UNP P16732
B	404	ASP	ALA	conflict	UNP P16732
B	405	TYR	ASN	conflict	UNP P16732
B	406	ASP	MET	conflict	UNP P16732
B	407	ILE	PHE	conflict	UNP P16732
B	408	PRO	MET	conflict	UNP P16732
B	409	THR	PRO	conflict	UNP P16732
B	410	THR	GLY	conflict	UNP P16732
B	411	GLU	ALA	conflict	UNP P16732
B	412	ASN	PHE	conflict	UNP P16732
B	413	LEU	MET	conflict	UNP P16732
B	414	TYR	ASP	conflict	UNP P16732
B	415	PHE	GLU	conflict	UNP P16732
B	416	GLN	ILE	conflict	UNP P16732
B	417	GLY	ILE	conflict	UNP P16732
C	396	MET	-	initiating methionine	UNP P16732
C	397	GLY	-	expression tag	UNP P16732
C	398	HIS	-	expression tag	UNP P16732
C	399	HIS	-	expression tag	UNP P16732
C	400	HIS	VAL	conflict	UNP P16732
C	401	HIS	ARG	conflict	UNP P16732
C	402	HIS	LYS	conflict	UNP P16732
C	403	HIS	THR	conflict	UNP P16732
C	404	ASP	ALA	conflict	UNP P16732
C	405	TYR	ASN	conflict	UNP P16732
C	406	ASP	MET	conflict	UNP P16732
C	407	ILE	PHE	conflict	UNP P16732
C	408	PRO	MET	conflict	UNP P16732
C	409	THR	PRO	conflict	UNP P16732
C	410	THR	GLY	conflict	UNP P16732
C	411	GLU	ALA	conflict	UNP P16732
C	412	ASN	PHE	conflict	UNP P16732
C	413	LEU	MET	conflict	UNP P16732
C	414	TYR	ASP	conflict	UNP P16732

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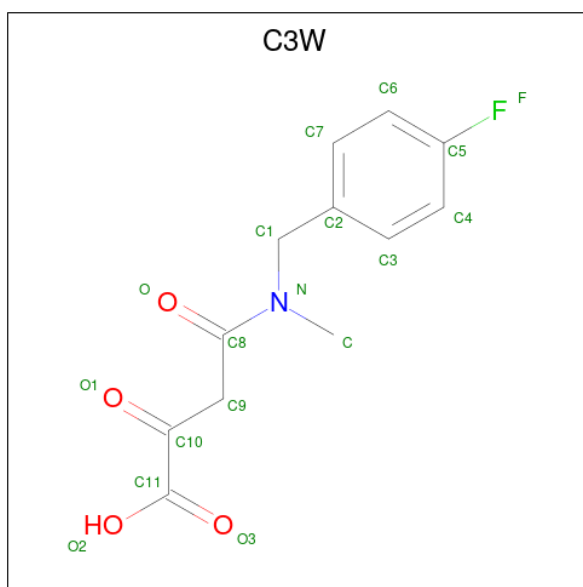
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Chain	Residue	Modelled	Actual	Comment	Reference
C	415	PHE	GLU	conflict	UNP P16732
C	416	GLN	ILE	conflict	UNP P16732
C	417	GLY	ILE	conflict	UNP P16732
D	396	MET	-	initiating methionine	UNP P16732
D	397	GLY	-	expression tag	UNP P16732
D	398	HIS	-	expression tag	UNP P16732
D	399	HIS	-	expression tag	UNP P16732
D	400	HIS	VAL	conflict	UNP P16732
D	401	HIS	ARG	conflict	UNP P16732
D	402	HIS	LYS	conflict	UNP P16732
D	403	HIS	THR	conflict	UNP P16732
D	404	ASP	ALA	conflict	UNP P16732
D	405	TYR	ASN	conflict	UNP P16732
D	406	ASP	MET	conflict	UNP P16732
D	407	ILE	PHE	conflict	UNP P16732
D	408	PRO	MET	conflict	UNP P16732
D	409	THR	PRO	conflict	UNP P16732
D	410	THR	GLY	conflict	UNP P16732
D	411	GLU	ALA	conflict	UNP P16732
D	412	ASN	PHE	conflict	UNP P16732
D	413	LEU	MET	conflict	UNP P16732
D	414	TYR	ASP	conflict	UNP P16732
D	415	PHE	GLU	conflict	UNP P16732
D	416	GLN	ILE	conflict	UNP P16732
D	417	GLY	ILE	conflict	UNP P16732

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Mn 3 3	0	0
2	B	2	Total Mn 2 2	0	0
2	C	3	Total Mn 3 3	0	0
2	D	2	Total Mn 2 2	0	0

- Molecule 3 is 4-[(4-fluorophenyl)methyl-methyl-amino]-2,4-bis(oxidanylidene)butanoic acid (CCD ID: C3W) (formula: C₁₂H₁₂FNO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 18	C 12	F 1	N 1	O 4	0	0
3	B	1	Total 18	C 12	F 1	N 1	O 4	0	0
3	C	1	Total 18	C 12	F 1	N 1	O 4	0	0
3	D	1	Total 18	C 12	F 1	N 1	O 4	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Cl	0	0
			1	1		

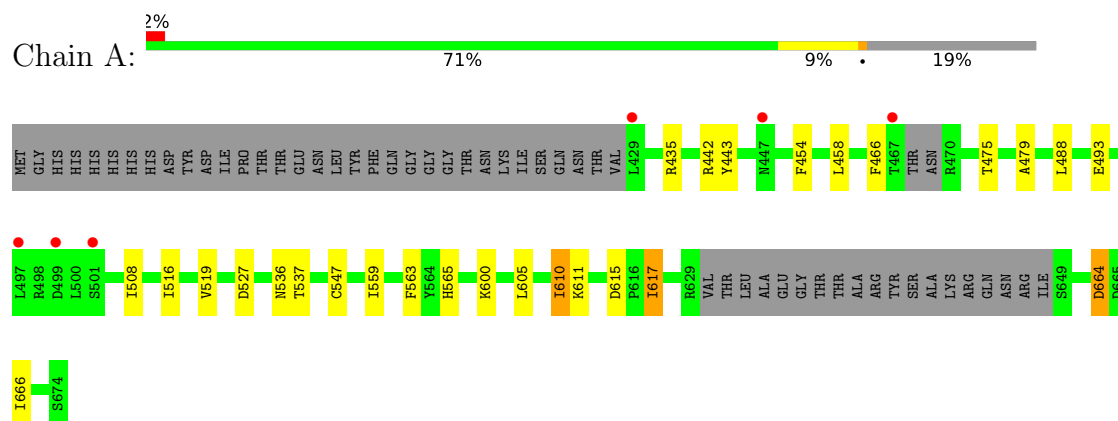
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	12	Total	O	0	0
			12	12		
5	C	3	Total	O	0	0
			3	3		
5	D	4	Total	O	0	0
			4	4		

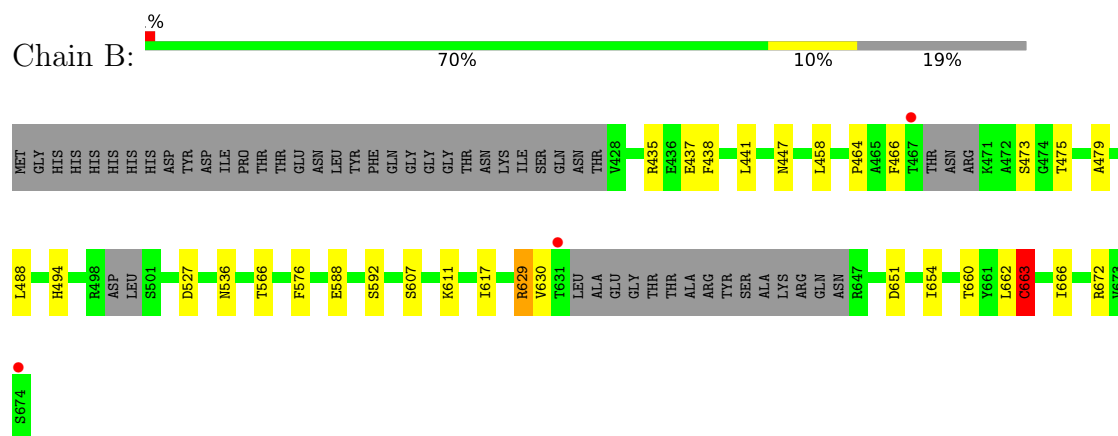
3 Residue-property plots [i](#)

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.

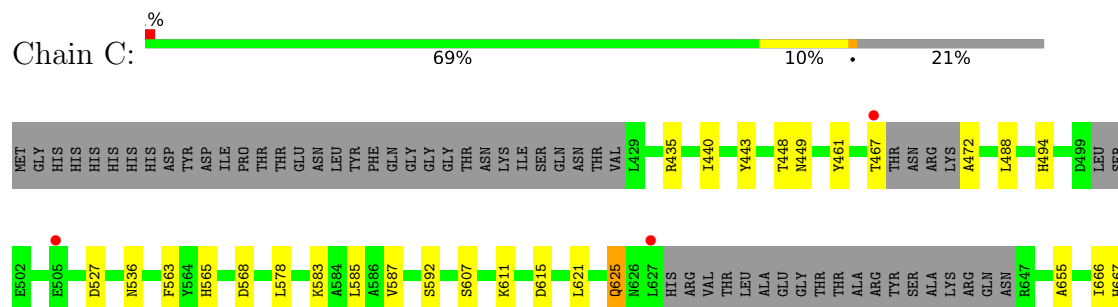
• Molecule 1: UL89 HCMV terminase



• Molecule 1: UL89 HCMV terminase

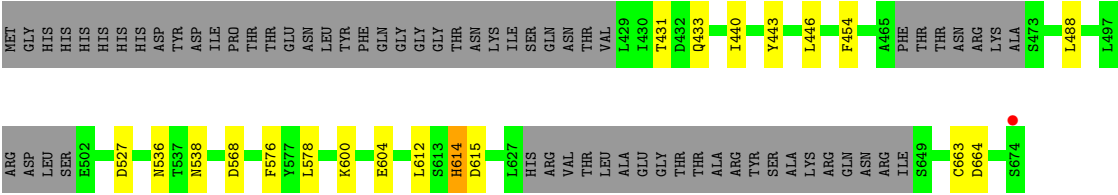


• Molecule 1: UL89 HCMV terminase





- Molecule 1: UL89 HCMV terminase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.65Å 87.65Å 186.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.90 29.87 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.87-2.90) 98.7 (29.87-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.90Å)	Xtriage
Refinement program	BUSTER 2.10.3, REFMAC	Depositor
R, R_{free}	0.175 , 0.198 0.191 , 0.210	Depositor DCC
R_{free} test set	1503 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	84.9	Xtriage
Anisotropy	0.257	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6928	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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: C3W, CL, MN

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	0.89	0/1760	1.35	10/2394 (0.4%)
1	B	0.91	1/1814 (0.1%)	1.32	13/2463 (0.5%)
1	C	0.88	0/1721	1.35	13/2341 (0.6%)
1	D	0.88	0/1664	1.34	13/2262 (0.6%)
All	All	0.89	1/6959 (0.0%)	1.34	49/9460 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	630	VAL	CA-C	5.19	1.58	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	ASP	CA-CB-CG	7.35	119.95	112.60
1	B	663	CYS	CA-C-N	7.25	131.47	120.82
1	B	663	CYS	C-N-CA	7.25	131.47	120.82
1	C	527	ASP	CA-CB-CG	7.16	119.75	112.60
1	D	527	ASP	CA-CB-CG	7.02	119.62	112.60
1	B	662	LEU	CA-C-N	6.95	129.90	120.38
1	B	662	LEU	C-N-CA	6.95	129.90	120.38
1	C	449	ASN	N-CA-C	-6.79	105.55	114.31
1	A	527	ASP	CA-CB-CG	6.56	119.16	112.60
1	B	527	ASP	CA-CB-CG	6.46	119.06	112.60
1	B	494	HIS	CA-C-N	6.46	131.01	122.30
1	B	494	HIS	C-N-CA	6.46	131.01	122.30
1	D	538	ASN	CA-CB-CG	6.37	118.97	112.60
1	D	568	ASP	CA-CB-CG	6.26	118.86	112.60
1	C	568	ASP	CA-CB-CG	6.20	118.80	112.60
1	A	536	ASN	CA-C-N	6.00	128.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ASN	C-N-CA	6.00	128.24	120.44
1	C	435	ARG	CA-C-N	5.91	128.13	120.44
1	C	435	ARG	C-N-CA	5.91	128.13	120.44
1	A	615	ASP	N-CA-C	-5.91	100.42	109.64
1	D	615	ASP	CA-CB-CG	5.85	118.45	112.60
1	D	536	ASN	CA-C-N	5.82	128.08	120.28
1	D	536	ASN	C-N-CA	5.82	128.08	120.28
1	C	615	ASP	N-CA-C	-5.78	100.86	109.42
1	D	664	ASP	CA-CB-CG	5.76	118.36	112.60
1	D	614	HIS	CA-C-N	5.65	129.10	121.20
1	D	614	HIS	C-N-CA	5.65	129.10	121.20
1	A	454	PHE	CA-C-N	5.36	125.19	120.10
1	A	454	PHE	C-N-CA	5.36	125.19	120.10
1	C	667	HIS	CA-C-N	5.36	127.73	120.38
1	C	667	HIS	C-N-CA	5.36	127.73	120.38
1	C	536	ASN	CA-C-N	5.34	127.44	120.28
1	C	536	ASN	C-N-CA	5.34	127.44	120.28
1	D	454	PHE	CA-C-N	5.31	125.14	120.10
1	D	454	PHE	C-N-CA	5.31	125.14	120.10
1	B	435	ARG	CA-C-N	5.30	127.33	120.44
1	B	435	ARG	C-N-CA	5.30	127.33	120.44
1	A	435	ARG	CA-C-N	5.26	127.28	120.44
1	A	435	ARG	C-N-CA	5.26	127.28	120.44
1	C	625	GLN	CB-CG-CD	5.25	121.53	112.60
1	B	536	ASN	CA-C-N	5.23	127.29	120.28
1	B	536	ASN	C-N-CA	5.23	127.29	120.28
1	B	629	ARG	CA-C-N	5.21	127.59	120.77
1	B	629	ARG	C-N-CA	5.21	127.59	120.77
1	A	493	GLU	CB-CG-CD	5.09	121.25	112.60
1	D	663	CYS	CA-C-N	5.08	128.28	120.82
1	D	663	CYS	C-N-CA	5.08	128.28	120.82
1	C	494	HIS	CA-C-N	5.01	129.64	122.72
1	C	494	HIS	C-N-CA	5.01	129.64	122.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1724	0	1630	13	0
1	B	1775	0	1717	12	0
1	C	1688	0	1594	17	0
1	D	1633	0	1548	13	0
2	A	3	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
3	A	18	0	0	0	0
3	B	18	0	0	0	0
3	C	18	0	0	0	0
3	D	18	0	0	0	0
4	D	1	0	0	0	0
5	A	6	0	0	0	0
5	B	12	0	0	1	0
5	C	3	0	0	0	0
5	D	4	0	0	0	0
All	All	6928	0	6489	47	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 (47) 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:B:566:THR:HG22	1:B:576:PHE:O	1.78	0.82
1:C:440:ILE:CG2	1:D:443:TYR:HD1	1.97	0.78
1:A:664:ASP:HB3	1:A:666:ILE:HD12	1.67	0.76
1:C:440:ILE:HG22	1:D:443:TYR:HD1	1.51	0.75
1:C:669:ILE:H	1:C:669:ILE:HD12	1.61	0.66
1:D:612:LEU:C	1:D:614:HIS:H	2.05	0.64
1:A:610:ILE:HG22	1:A:611:LYS:H	1.63	0.64
1:D:576:PHE:HE1	1:D:578:LEU:HG	1.67	0.59
1:B:607:SER:O	1:B:611:LYS:HB2	2.04	0.58
1:D:443:TYR:CE2	1:D:600:LYS:HB2	2.39	0.57
1:C:607:SER:O	1:C:611:LYS:HB2	2.04	0.57
1:D:446:LEU:HD22	1:D:604:GLU:HG2	1.88	0.56
1:C:440:ILE:CG2	1:D:443:TYR:CD1	2.86	0.54
1:C:467:THR:HG22	1:C:472:ALA:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LYS:O	1:C:587:VAL:HG23	2.09	0.52
1:C:448:THR:HB	1:D:440:ILE:HG21	1.92	0.52
1:A:443:TYR:CE2	1:A:600:LYS:HB2	2.45	0.51
1:A:443:TYR:HE2	1:A:600:LYS:HB2	1.75	0.51
1:B:464:PRO:HA	1:B:475:THR:HG23	1.92	0.51
1:D:443:TYR:HE2	1:D:600:LYS:HB2	1.75	0.51
1:C:440:ILE:HG22	1:D:443:TYR:CD1	2.39	0.50
1:C:563:PHE:O	1:C:565:HIS:HD2	1.95	0.49
1:D:431:THR:HG22	1:D:433:GLN:H	1.76	0.49
1:C:448:THR:HB	1:D:440:ILE:CG2	2.42	0.49
1:B:588:GLU:HG2	1:C:592:SER:HA	1.94	0.49
1:A:563:PHE:O	1:A:565:HIS:HD2	1.94	0.49
1:C:461:TYR:HD2	1:C:655:ALA:HA	1.78	0.48
1:B:458:LEU:HD11	1:B:479:ALA:HB1	1.95	0.47
1:A:458:LEU:HD11	1:A:479:ALA:HB1	1.96	0.46
1:A:466:PHE:HD1	1:A:537:THR:HG23	1.80	0.46
1:A:488:LEU:HA	1:A:600:LYS:O	2.16	0.46
1:C:621:LEU:O	1:C:625:GLN:HG2	2.16	0.46
1:B:660:THR:O	1:B:663:CYS:HB2	2.17	0.45
1:A:664:ASP:HB3	1:A:666:ILE:CD1	2.44	0.45
1:D:488:LEU:HA	1:D:600:LYS:O	2.17	0.45
1:A:516:ILE:O	1:A:519:VAL:HG22	2.17	0.44
1:B:466:PHE:O	1:B:473:SER:HB3	2.17	0.44
1:C:443:TYR:HB2	1:C:488:LEU:HD21	1.98	0.44
1:B:437:GLU:HG2	1:B:441:LEU:HD12	1.99	0.44
1:B:438:PHE:CE2	1:B:617:ILE:HG23	2.52	0.43
1:A:605:LEU:HD13	1:A:617:ILE:HD11	2.00	0.42
1:B:588:GLU:OE2	1:B:629:ARG:HD3	2.19	0.42
1:B:666:ILE:HA	1:C:666:ILE:HD11	2.02	0.42
1:A:442:ARG:NH1	1:A:617:ILE:HD13	2.35	0.42
1:C:461:TYR:CD2	1:C:655:ALA:HA	2.55	0.41
1:B:654:ILE:HD12	5:B:805:HOH:O	2.19	0.41
1:A:475:THR:HG21	1:A:508: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	A	219/279 (78%)	211 (96%)	7 (3%)	1 (0%)	24	54
1	B	220/279 (79%)	213 (97%)	7 (3%)	0	100	100
1	C	213/279 (76%)	208 (98%)	5 (2%)	0	100	100
1	D	206/279 (74%)	196 (95%)	10 (5%)	0	100	100
All	All	858/1116 (77%)	828 (96%)	29 (3%)	1 (0%)	48	77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	610	ILE

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	170/242 (70%)	167 (98%)	3 (2%)	51	80
1	B	183/242 (76%)	177 (97%)	6 (3%)	33	67
1	C	169/242 (70%)	166 (98%)	3 (2%)	51	80
1	D	164/242 (68%)	164 (100%)	0	100	100
All	All	686/968 (71%)	674 (98%)	12 (2%)	51	82

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	547	CYS
1	A	559	ILE
1	A	617	ILE
1	B	447	ASN
1	B	488	LEU
1	B	592	SER
1	B	651	ASP
1	B	663	CYS
1	B	672	ARG
1	C	578	LEU
1	C	585	LEU
1	C	669	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	538	ASN
1	A	539	GLN
1	A	554	GLN
1	A	565	HIS
1	A	628	HIS
1	B	447	ASN
1	B	538	ASN
1	B	614	HIS
1	B	625	GLN
1	C	514	HIS
1	C	538	ASN
1	C	554	GLN
1	C	565	HIS
1	C	574	GLN
1	C	614	HIS
1	D	589	GLN
1	D	603	GLN
1	D	623	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 11 are monoatomic - leaving 4 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	C3W	C	704	2	18,18,18	1.09	2 (11%)	22,24,24	1.49	2 (9%)
3	C3W	A	704	2	18,18,18	1.09	2 (11%)	22,24,24	1.40	2 (9%)
3	C3W	B	703	2	18,18,18	0.43	0	22,24,24	0.51	0
3	C3W	D	703	2	18,18,18	1.24	2 (11%)	22,24,24	1.11	2 (9%)

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	C3W	C	704	2	-	0/16/16/16	0/1/1/1
3	C3W	A	704	2	-	0/16/16/16	0/1/1/1
3	C3W	B	703	2	-	0/16/16/16	0/1/1/1
3	C3W	D	703	2	-	0/16/16/16	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	703	C3W	O3-C11	3.51	1.31	1.22
3	A	704	C3W	O3-C11	3.40	1.31	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	704	C3W	O3-C11	3.36	1.30	1.22
3	D	703	C3W	O2-C11	-3.04	1.22	1.30
3	A	704	C3W	O2-C11	-2.75	1.23	1.30
3	C	704	C3W	O2-C11	-2.60	1.23	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	704	C3W	O3-C11-C10	-5.73	114.69	121.81
3	A	704	C3W	O3-C11-C10	-5.41	115.08	121.81
3	D	703	C3W	O3-C11-C10	-4.18	116.61	121.81
3	C	704	C3W	O2-C11-C10	3.26	122.64	113.59
3	A	704	C3W	O2-C11-C10	3.21	122.49	113.59
3	D	703	C3W	O2-C11-C10	2.50	120.53	113.59

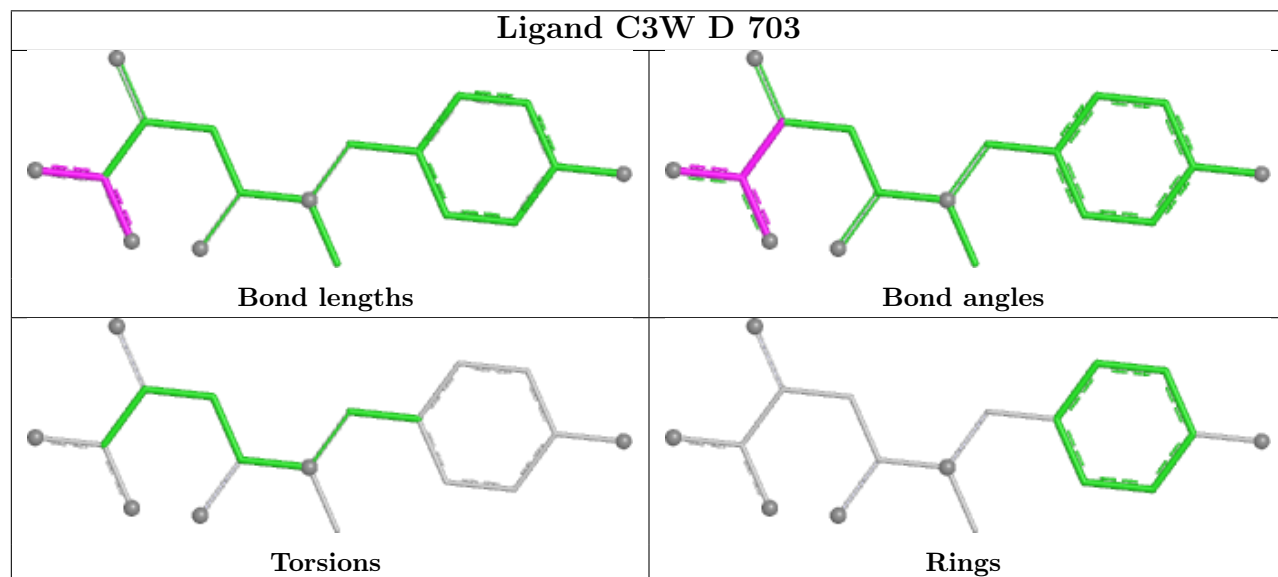
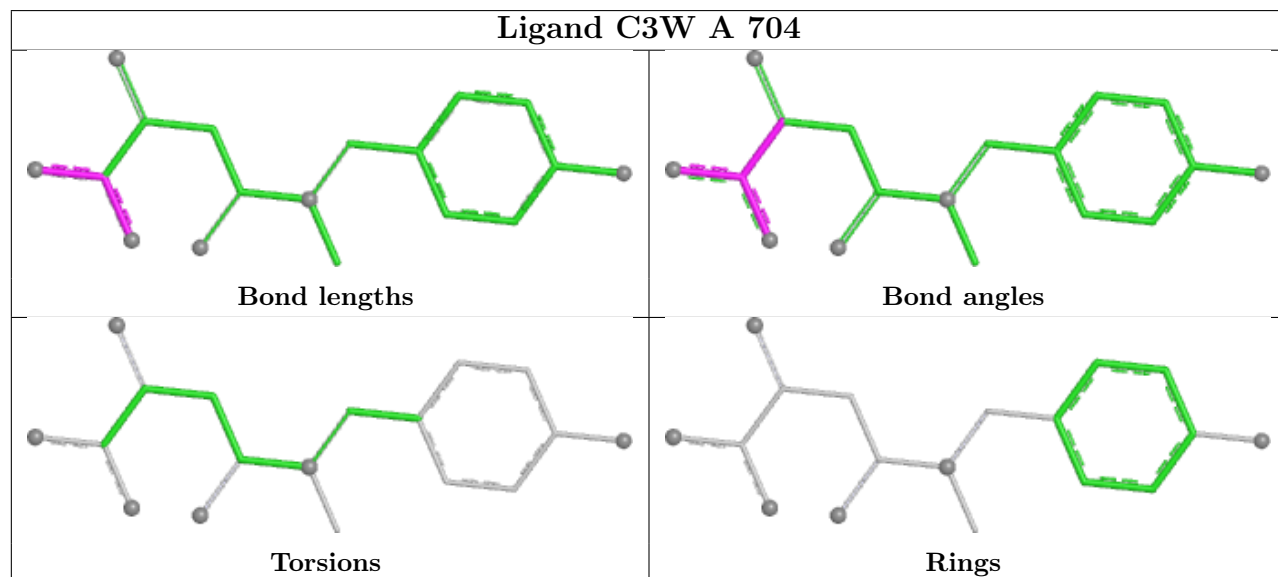
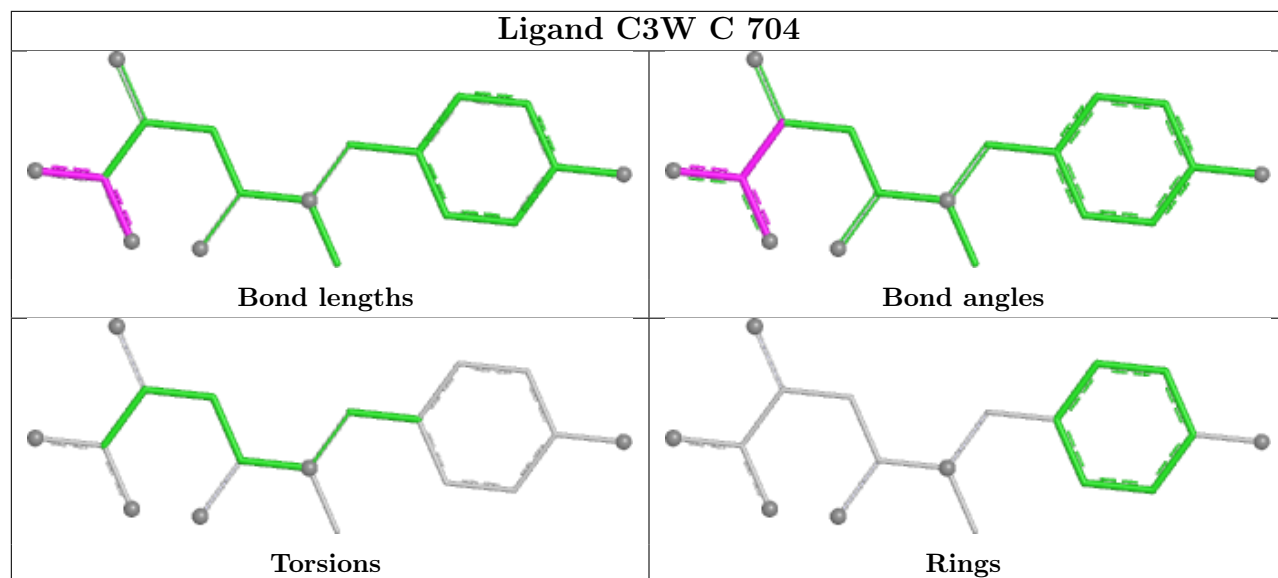
There are no chirality outliers.

There are no torsion outliers.

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.



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	225/279 (80%)	-0.02	6 (2%) 56 47	58, 87, 138, 168	1 (0%)
1	B	227/279 (81%)	-0.19	3 (1%) 75 67	51, 80, 123, 154	2 (0%)
1	C	221/279 (79%)	-0.03	3 (1%) 73 65	61, 88, 128, 166	1 (0%)
1	D	214/279 (76%)	-0.12	1 (0%) 87 83	60, 85, 126, 153	1 (0%)
All	All	887/1116 (79%)	-0.09	13 (1%) 72 64	51, 85, 134, 168	5 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	627	LEU	3.0
1	B	467	THR	2.7
1	B	631	THR	2.7
1	A	429	LEU	2.6
1	D	674	SER	2.5
1	A	501	SER	2.4
1	B	674	SER	2.4
1	A	467	THR	2.4
1	A	499	ASP	2.3
1	A	447	ASN	2.2
1	C	467	THR	2.2
1	A	497	LEU	2.1
1	C	505	GLU	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](#)

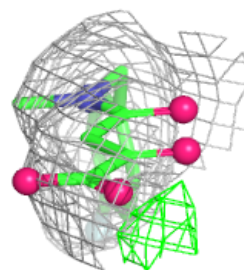
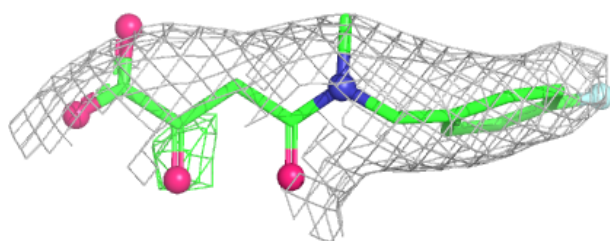
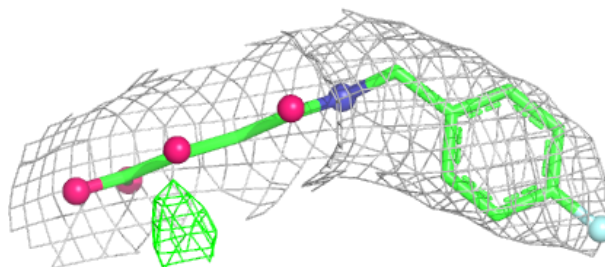
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	D	704	1/1	0.85	0.23	131,131,131,131	0
3	C3W	D	703	18/18	0.86	0.13	119,122,132,132	0
3	C3W	C	704	18/18	0.89	0.10	114,119,127,127	0
3	C3W	B	703	18/18	0.91	0.11	121,127,133,133	0
2	MN	C	703	1/1	0.91	0.06	133,133,133,133	0
3	C3W	A	704	18/18	0.94	0.11	128,132,138,138	0
2	MN	A	703	1/1	0.95	0.07	140,140,140,140	0
2	MN	D	702	1/1	0.98	0.06	91,91,91,91	0
2	MN	A	701	1/1	0.98	0.08	96,96,96,96	0
2	MN	B	701	1/1	0.99	0.05	80,80,80,80	0
2	MN	B	702	1/1	0.99	0.02	81,81,81,81	0
2	MN	C	701	1/1	0.99	0.06	87,87,87,87	0
2	MN	C	702	1/1	0.99	0.03	94,94,94,94	0
2	MN	A	702	1/1	0.99	0.05	93,93,93,93	0
2	MN	D	701	1/1	0.99	0.06	101,101,101,101	0

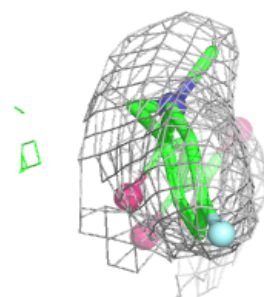
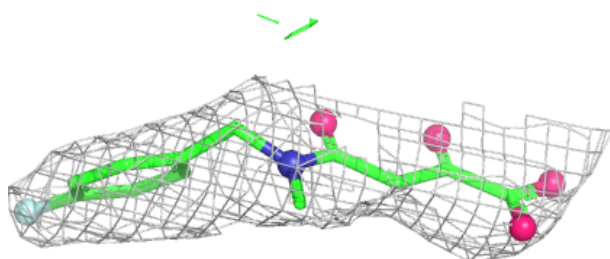
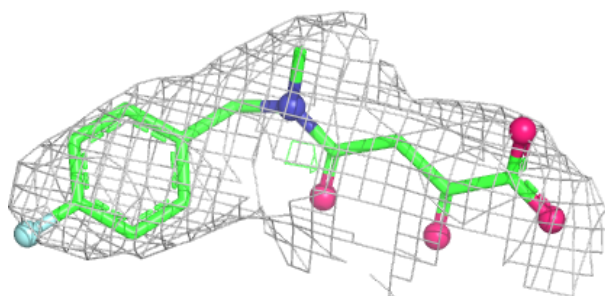
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around C3W D 703:

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

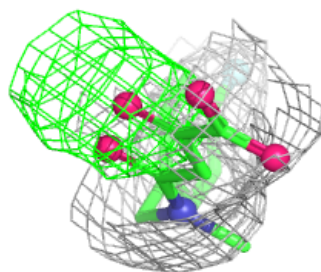
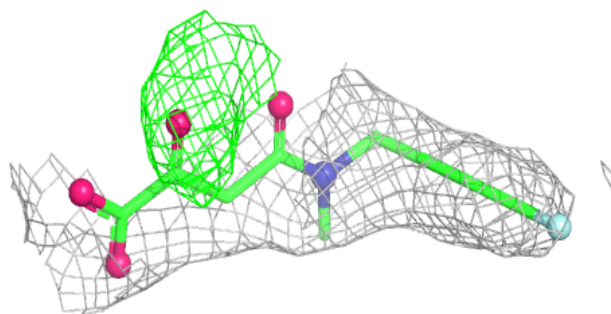
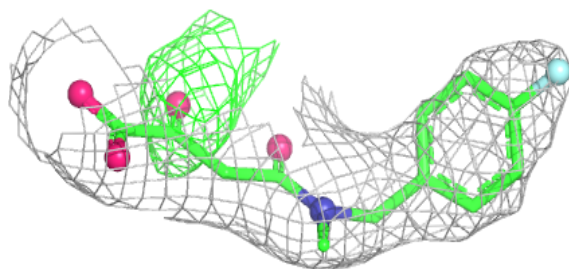
**Electron density around C3W C 704:**

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



Electron density around C3W A 704:

$2mF_o-DF_c$ (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.