



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 AM UTC

PDB ID : 7C18 / pdb_00007c18
Title : Crystal structure of FumaraseC from Mannheimia succiniciproducens in complex with Fumarate
Authors : Kim, B.; Lee, S.H.; Kim, K.-J.
Deposited on : 2020-05-02
Resolution : 2.12 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

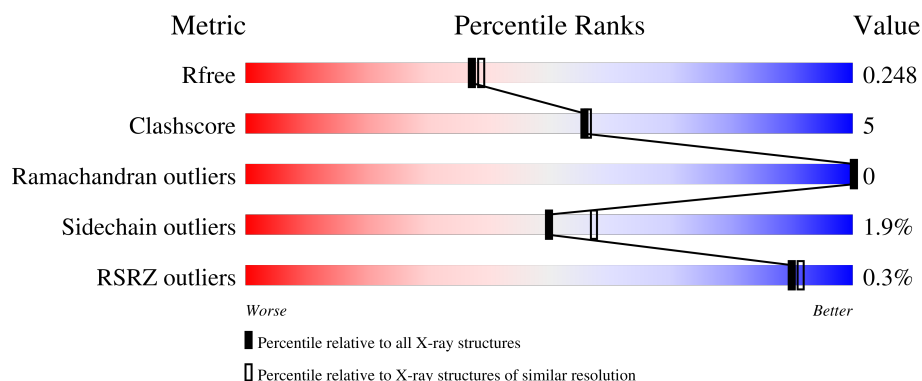
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	467	 85% 13% .
1	B	467	 87% 11% ..
1	C	467	 84% 14% ..
1	D	467	 83% 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
2	FUM	C	502	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14312 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.

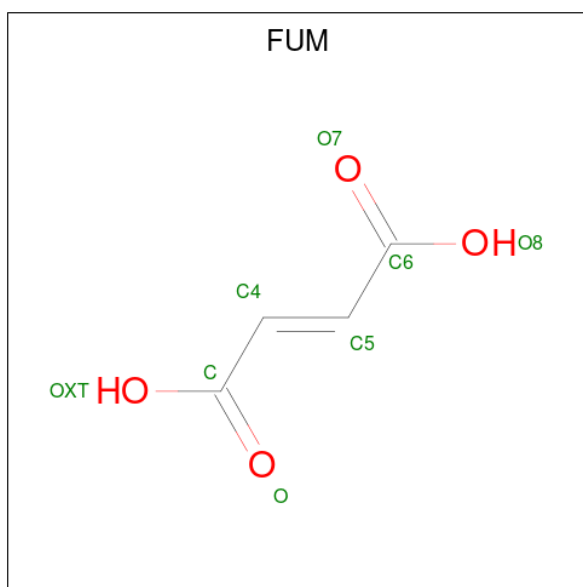
- Molecule 1 is a protein called Fumarate hydratase class II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3500	2212	604	667	17			
1	B	464	Total	C	N	O	S	0	0	0
			3507	2216	605	669	17			
1	C	461	Total	C	N	O	S	0	0	0
			3490	2206	602	665	17			
1	D	460	Total	C	N	O	S	0	0	0
			3481	2200	601	663	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q65UJ3
A	0	ALA	-	expression tag	UNP Q65UJ3
A	319	CYS	SER	engineered mutation	UNP Q65UJ3
B	-1	GLY	-	expression tag	UNP Q65UJ3
B	0	ALA	-	expression tag	UNP Q65UJ3
B	319	CYS	SER	engineered mutation	UNP Q65UJ3
C	-1	GLY	-	expression tag	UNP Q65UJ3
C	0	ALA	-	expression tag	UNP Q65UJ3
C	319	CYS	SER	engineered mutation	UNP Q65UJ3
D	-1	GLY	-	expression tag	UNP Q65UJ3
D	0	ALA	-	expression tag	UNP Q65UJ3
D	319	CYS	SER	engineered mutation	UNP Q65UJ3

- Molecule 2 is FUMARIC ACID (CCD ID: FUM) (formula: C₄H₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	4	4		
2	A	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		
2	C	1	Total	C	O	0	0
			8	4	4		

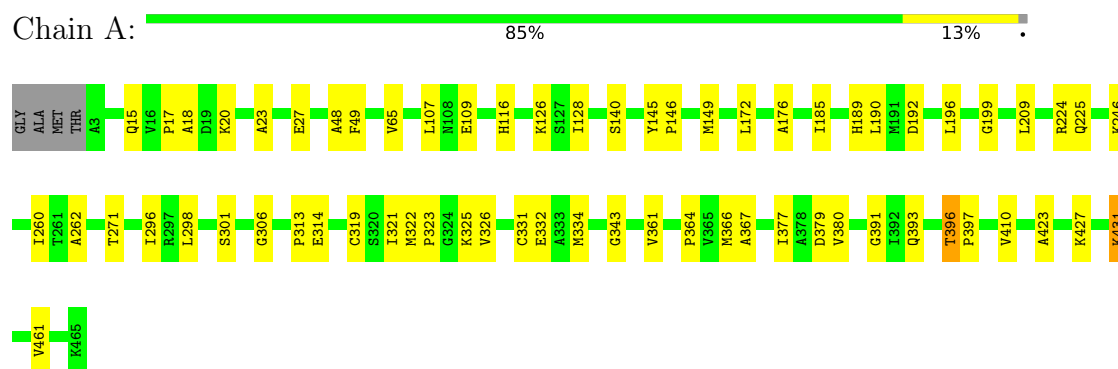
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	77	Total	O	0	0
			77	77		
3	B	84	Total	O	0	0
			84	84		
3	C	66	Total	O	0	0
			66	66		
3	D	75	Total	O	0	0
			75	75		

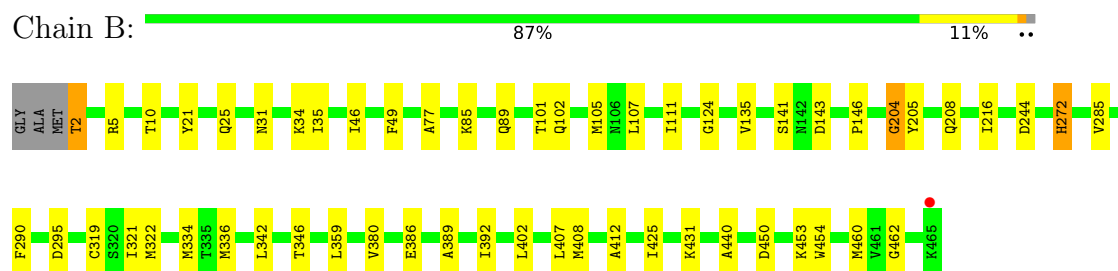
3 Residue-property plots [i](#)

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.

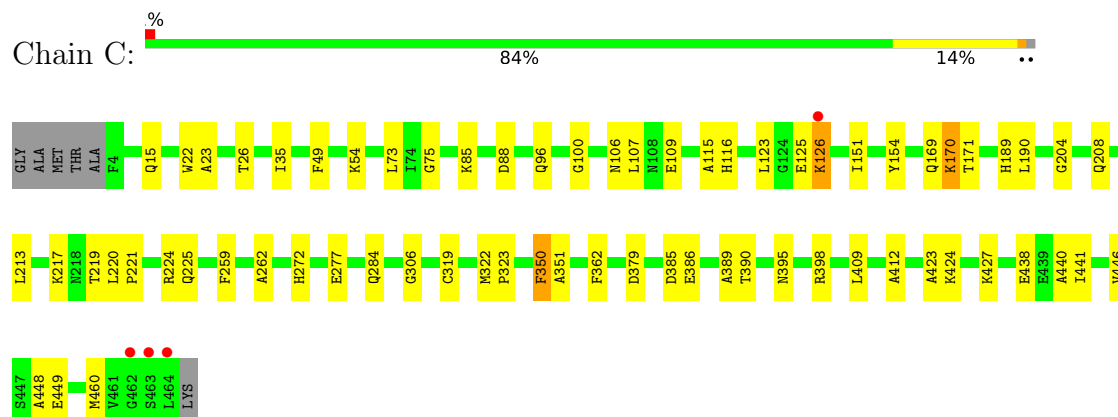
- Molecule 1: Fumarate hydratase class II



- Molecule 1: Fumarate hydratase class II



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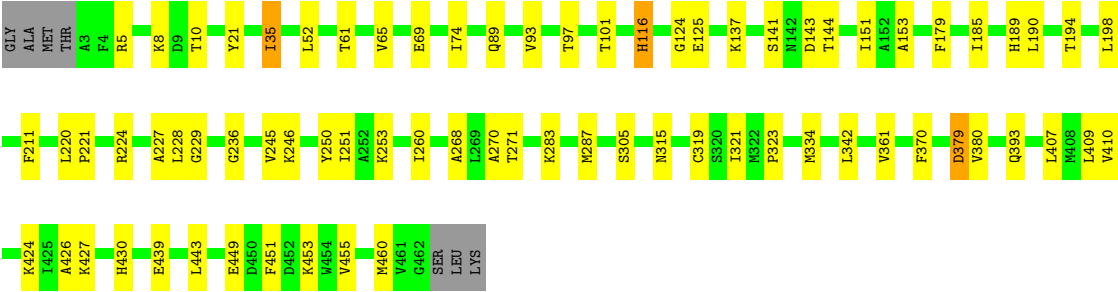
- Molecule 1: Fumarate hydratase class II

Chain D:

83%

15%

..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.09Å 104.28Å 125.33Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	32.57 – 2.12 32.57 – 2.12	Depositor EDS
% Data completeness (in resolution range)	96.9 (32.57-2.12) 97.4 (32.57-2.12)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.95 (at 2.12Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.185 , 0.241 0.194 , 0.248	Depositor DCC
R_{free} test set	4190 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 29.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14312	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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: FUM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.17	2/3565 (0.1%)	1.52	12/4837 (0.2%)
1	B	1.16	2/3572 (0.1%)	1.56	10/4847 (0.2%)
1	C	1.18	1/3555 (0.0%)	1.56	7/4823 (0.1%)
1	D	1.18	5/3546 (0.1%)	1.56	14/4811 (0.3%)
All	All	1.17	10/14238 (0.1%)	1.55	43/19318 (0.2%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	323	PRO	C-O	-7.32	1.16	1.23
1	B	359	LEU	C-O	6.58	1.31	1.23
1	A	301	SER	C-O	6.38	1.31	1.23
1	D	260	ILE	C-O	5.79	1.29	1.23
1	D	379	ASP	C-O	5.72	1.30	1.24
1	D	270	ALA	C-O	5.46	1.31	1.24
1	D	35	ILE	C-O	5.36	1.30	1.24
1	D	361	VAL	C-O	5.26	1.30	1.24
1	A	260	ILE	C-O	5.05	1.29	1.23
1	B	462	GLY	C-O	5.03	1.29	1.23

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2	THR	CB-CA-C	7.53	125.67	109.10
1	D	211	PHE	CA-C-N	7.15	128.07	119.99
1	D	211	PHE	C-N-CA	7.15	128.07	119.99
1	D	143	ASP	CA-CB-CG	6.06	118.66	112.60
1	C	395	ASN	CA-C-N	5.91	128.19	120.26
1	C	395	ASN	C-N-CA	5.91	128.19	120.26
1	D	61	THR	CA-C-O	-5.87	114.65	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	ILE	N-CA-C	-5.87	104.79	110.72
1	C	440	ALA	CA-C-N	5.72	127.88	120.56
1	C	440	ALA	C-N-CA	5.72	127.88	120.56
1	C	350	PHE	CA-CB-CG	5.60	119.40	113.80
1	A	396	THR	CA-CB-OG1	-5.53	101.31	109.60
1	C	272	HIS	CA-CB-CG	-5.50	108.30	113.80
1	D	93	VAL	CA-C-N	5.46	127.65	120.60
1	D	93	VAL	C-N-CA	5.46	127.65	120.60
1	A	192	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	135	VAL	O-C-N	5.41	127.41	121.83
1	C	284	GLN	N-CA-C	-5.40	105.39	111.28
1	B	204	GLY	CA-C-N	5.35	127.39	120.44
1	B	204	GLY	C-N-CA	5.35	127.39	120.44
1	A	48	ALA	CA-C-N	5.34	127.44	120.28
1	A	48	ALA	C-N-CA	5.34	127.44	120.28
1	D	116	HIS	CA-C-N	5.33	127.99	120.42
1	D	116	HIS	C-N-CA	5.33	127.99	120.42
1	B	244	ASP	CA-CB-CG	5.32	117.92	112.60
1	A	366	MET	CA-C-N	5.29	128.14	120.79
1	A	366	MET	C-N-CA	5.29	128.14	120.79
1	B	342	LEU	CA-C-O	-5.29	115.26	120.70
1	B	143	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	393	GLN	CB-CA-C	5.27	117.04	108.87
1	A	18	ALA	CA-C-N	5.26	128.31	120.31
1	A	18	ALA	C-N-CA	5.26	128.31	120.31
1	A	149	MET	CA-C-O	-5.22	115.34	120.82
1	D	74	ILE	CA-C-N	5.20	125.85	120.03
1	D	74	ILE	C-N-CA	5.20	125.85	120.03
1	A	306	GLY	CA-C-O	-5.20	117.05	121.78
1	A	377	ILE	N-CA-C	-5.17	105.46	110.42
1	D	250	TYR	CA-C-O	-5.15	115.41	120.82
1	D	393	GLN	CB-CA-C	5.14	116.83	108.87
1	D	427	LYS	CA-C-N	5.12	127.10	120.44
1	D	427	LYS	C-N-CA	5.12	127.10	120.44
1	B	272	HIS	CA-CB-CG	-5.07	108.73	113.80
1	B	102	GLN	CB-CA-C	5.06	119.45	110.85

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	3500	0	3515	36	0
1	B	3507	0	3522	30	0
1	C	3490	0	3508	41	0
1	D	3481	0	3497	40	0
2	A	16	0	2	6	0
2	C	16	0	2	7	0
3	A	77	0	0	1	0
3	B	84	0	0	0	0
3	C	66	0	0	0	0
3	D	75	0	0	2	0
All	All	14312	0	14046	133	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 5.

All (133) 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:319:CYS:SG	2:C:501:FUM:C5	2.45	1.05
2:A:502:FUM:C5	1:B:319:CYS:SG	2.51	0.98
1:A:319:CYS:SG	2:A:501:FUM:C5	2.57	0.93
2:C:502:FUM:C4	1:D:319:CYS:SG	2.59	0.90
1:D:21:TYR:H	1:D:89:GLN:HE22	1.30	0.79
1:D:21:TYR:H	1:D:89:GLN:NE2	1.83	0.76
1:C:319:CYS:SG	2:C:501:FUM:C4	2.74	0.75
2:C:502:FUM:C5	1:D:319:CYS:SG	2.79	0.71
2:A:502:FUM:C4	1:B:319:CYS:SG	2.80	0.70
1:A:319:CYS:SG	2:A:501:FUM:C4	2.82	0.68
1:C:379:ASP:HB3	1:D:35:ILE:HA	1.80	0.64
1:A:49:PHE:HB3	1:A:107:LEU:HG	1.79	0.63
1:B:21:TYR:H	1:B:89:GLN:NE2	1.97	0.62
1:D:116:HIS:HE1	1:D:125:GLU:HB2	1.65	0.61
2:A:502:FUM:C6	1:B:319:CYS:SG	2.88	0.61
1:D:65:VAL:O	1:D:137:LYS:HE3	1.99	0.61
1:D:315:ASN:ND2	3:D:501:HOH:O	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:THR:HG21	1:D:101:THR:HB	1.85	0.59
1:D:271:THR:HA	3:D:524:HOH:O	2.05	0.57
1:C:23:ALA:HB3	1:C:109:GLU:CD	2.30	0.56
1:D:151:ILE:HD11	1:D:251:ILE:HG21	1.86	0.56
1:A:361:VAL:HG22	3:A:668:HOH:O	2.04	0.56
1:A:313:PRO:HG3	1:A:391:GLY:HA3	1.89	0.55
1:C:319:CYS:SG	1:C:322:MET:HB2	2.48	0.54
1:D:451:PHE:CE1	1:D:455:VAL:HG21	2.43	0.54
1:D:410:VAL:HG11	1:D:426:ALA:HB2	1.90	0.53
1:C:151:ILE:HA	1:C:259:PHE:CZ	2.43	0.53
1:D:21:TYR:HB2	1:D:89:GLN:NE2	2.23	0.53
1:B:334:MET:HA	1:B:380:VAL:HG21	1.89	0.53
1:C:319:CYS:SG	2:C:501:FUM:C6	2.97	0.52
1:B:205:TYR:OH	1:B:295:ASP:OD2	2.19	0.52
1:B:10:THR:O	1:C:427:LYS:HE2	2.09	0.52
1:A:334:MET:HA	1:A:380:VAL:HG21	1.92	0.52
1:B:407:LEU:C	1:B:408:MET:HE2	2.35	0.52
1:D:220:LEU:N	1:D:221:PRO:CD	2.72	0.52
1:C:126:LYS:HD2	1:C:126:LYS:C	2.35	0.51
1:A:319:CYS:SG	2:A:501:FUM:C6	2.99	0.51
1:C:220:LEU:N	1:C:221:PRO:CD	2.73	0.51
1:B:49:PHE:HB3	1:B:107:LEU:HG	1.93	0.51
1:A:140:SER:HB2	1:B:321:ILE:HG21	1.92	0.51
1:D:334:MET:HA	1:D:380:VAL:HG21	1.93	0.50
1:D:5:ARG:HD2	1:D:124:GLY:HA2	1.94	0.50
1:C:441:ILE:HD11	1:C:448:ALA:HA	1.94	0.50
1:D:101:THR:HA	1:D:141:SER:OG	2.12	0.50
1:C:412:ALA:HB2	1:C:460:MET:HE3	1.94	0.50
1:A:176:ALA:HA	1:A:199:GLY:HA2	1.94	0.50
1:C:219:THR:HB	1:C:277:GLU:HG2	1.92	0.49
1:C:350:PHE:CD2	1:D:342:LEU:HD23	2.47	0.49
1:A:322:MET:HE3	1:A:325:LYS:HD3	1.92	0.49
1:D:221:PRO:HA	1:D:224:ARG:HD3	1.94	0.49
1:C:73:LEU:HD22	1:C:115:ALA:O	2.12	0.49
1:A:116:HIS:HD2	1:A:128:ILE:HG22	1.77	0.49
1:A:321:ILE:O	1:A:323:PRO:HD3	2.12	0.49
1:A:396:THR:N	1:A:397:PRO:HD2	2.28	0.49
1:A:323:PRO:HB3	1:C:423:ALA:HB2	1.95	0.49
1:C:96:GLN:OE1	1:C:100:GLY:HA2	2.13	0.48
1:D:283:LYS:O	1:D:287:MET:HG2	2.13	0.48
1:B:425:ILE:HD13	1:B:440:ALA:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:HA	1:B:141:SER:OG	2.13	0.48
1:C:170:LYS:HD2	1:C:171:THR:N	2.29	0.48
1:C:409:LEU:HA	1:C:460:MET:HE1	1.96	0.48
1:A:423:ALA:O	1:A:427:LYS:HG3	2.13	0.48
1:A:332:GLU:OE2	1:C:189:HIS:HD2	1.97	0.47
1:C:116:HIS:HE2	1:C:125:GLU:HB2	1.79	0.47
1:D:153:ALA:HB1	1:D:370:PHE:CE1	2.50	0.47
1:A:23:ALA:HB3	1:A:109:GLU:CD	2.39	0.47
1:D:407:LEU:CD1	1:D:430:HIS:HB2	2.45	0.47
1:B:146:PRO:HB3	1:B:272:HIS:HE1	1.79	0.47
1:C:126:LYS:CE	1:C:126:LYS:O	2.63	0.47
1:B:389:ALA:HA	1:B:392:ILE:HD12	1.97	0.47
1:B:402:LEU:HD22	1:D:305:SER:HA	1.97	0.47
1:D:229:GLY:O	1:D:236:GLY:HA2	2.15	0.47
1:A:189:HIS:O	1:A:190:LEU:HB2	2.16	0.46
1:B:290:PHE:CD1	1:B:290:PHE:C	2.94	0.46
1:C:154:TYR:CE2	1:C:224:ARG:HB3	2.50	0.46
1:C:225:GLN:HB3	1:C:262:ALA:HA	1.98	0.45
1:A:364:PRO:O	1:A:367:ALA:HB3	2.15	0.45
1:A:17:PRO:HB2	1:A:20:LYS:HG2	1.98	0.45
1:C:126:LYS:C	1:C:126:LYS:CD	2.90	0.45
1:D:52:LEU:HD12	1:D:52:LEU:C	2.42	0.45
1:D:409:LEU:HA	1:D:460:MET:HE1	1.98	0.45
1:A:296:ILE:HG22	1:A:331:CYS:SG	2.57	0.45
2:C:502:FUM:C	1:D:319:CYS:SG	3.05	0.45
1:A:379:ASP:HB3	1:B:35:ILE:HA	1.98	0.45
1:B:386:GLU:HA	1:B:386:GLU:OE1	2.17	0.45
1:C:170:LYS:HD2	1:C:170:LYS:C	2.42	0.45
1:C:54:LYS:HG3	1:C:75:GLY:HA2	1.99	0.44
1:A:185:ILE:HA	1:A:185:ILE:HD12	1.76	0.44
1:B:21:TYR:H	1:B:89:GLN:HE22	1.64	0.44
1:B:25:GLN:NE2	1:B:105:MET:HG3	2.32	0.44
1:B:450:ASP:HB3	1:B:454:TRP:CZ3	2.52	0.44
1:C:385:ASP:HA	1:C:389:ALA:HB3	1.99	0.44
1:A:185:ILE:O	1:A:185:ILE:HG23	2.18	0.44
1:A:225:GLN:HB3	1:A:262:ALA:HA	1.98	0.44
1:C:26:THR:OG1	1:C:106:ASN:HA	2.17	0.44
1:B:5:ARG:HD2	1:B:124:GLY:HA2	2.00	0.44
1:B:204:GLY:O	1:B:208:GLN:HG3	2.18	0.44
2:C:502:FUM:C	1:D:319:CYS:HG	2.31	0.44
1:A:196:LEU:HA	1:A:461:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:LYS:HG2	1:D:443:LEU:HD13	2.00	0.43
1:C:351:ALA:HB1	1:C:362:PHE:HB3	1.99	0.43
1:A:343:GLY:HA2	1:B:346:THR:HB	2.01	0.43
1:B:412:ALA:HB2	1:B:460:MET:HE3	2.01	0.43
1:C:22:TRP:HB2	1:C:26:THR:HG21	2.00	0.43
1:C:35:ILE:HA	1:D:379:ASP:HB3	2.01	0.43
1:D:439:GLU:HA	1:D:439:GLU:OE1	2.19	0.43
1:D:189:HIS:O	1:D:190:LEU:HB2	2.19	0.43
1:A:314:GLU:HG2	1:A:326:VAL:HG11	2.01	0.43
1:A:427:LYS:O	1:A:431:LYS:HB2	2.19	0.42
1:A:364:PRO:HD2	1:B:336:MET:SD	2.60	0.42
1:D:321:ILE:O	1:D:323:PRO:HD3	2.19	0.42
1:B:216:ILE:HD11	1:B:285:VAL:HG21	2.02	0.42
1:C:49:PHE:CG	1:C:107:LEU:HG	2.54	0.42
1:A:322:MET:HE3	1:A:325:LYS:CD	2.49	0.42
1:C:213:LEU:O	1:C:217:LYS:HG3	2.19	0.42
1:A:172:LEU:HD12	1:A:209:LEU:HD12	2.02	0.42
1:C:49:PHE:HB3	1:C:107:LEU:CD1	2.50	0.41
1:C:169:GLN:NE2	1:C:169:GLN:C	2.77	0.41
1:A:298:LEU:HD23	1:C:190:LEU:HD13	2.02	0.41
1:B:77:ALA:HB3	1:B:111:ILE:HG23	2.00	0.41
1:C:88:ASP:OD1	1:C:88:ASP:N	2.51	0.41
1:A:15:GLN:O	1:A:27:GLU:HG2	2.20	0.41
1:C:204:GLY:O	1:C:208:GLN:HG3	2.21	0.41
1:D:179:PHE:CD2	1:D:198:LEU:HD23	2.56	0.41
1:D:227:ALA:HB2	1:D:268:ALA:HB1	2.02	0.41
1:A:145:TYR:HB3	1:A:146:PRO:HD3	2.03	0.41
1:C:306:GLY:O	1:C:398:ARG:NH2	2.54	0.41
1:D:185:ILE:HD12	1:D:185:ILE:HA	1.91	0.41
1:C:15:GLN:HE21	1:C:15:GLN:HB3	1.54	0.40
1:A:427:LYS:HE2	1:D:10:THR:O	2.20	0.40
1:B:322:MET:SD	1:D:194:THR:HG23	2.61	0.40
1:B:31:ASN:O	1:B:34:LYS:HE2	2.21	0.40
1:D:144:THR:HG22	1:D:228:LEU:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	461/467 (99%)	443 (96%)	18 (4%)	0	100	100
1	B	462/467 (99%)	448 (97%)	14 (3%)	0	100	100
1	C	459/467 (98%)	440 (96%)	19 (4%)	0	100	100
1	D	458/467 (98%)	440 (96%)	18 (4%)	0	100	100
All	All	1840/1868 (98%)	1771 (96%)	69 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	370/373 (99%)	363 (98%)	7 (2%)	50	57
1	B	371/373 (100%)	367 (99%)	4 (1%)	65	74
1	C	370/373 (99%)	360 (97%)	10 (3%)	39	44
1	D	368/373 (99%)	361 (98%)	7 (2%)	50	57
All	All	1479/1492 (99%)	1451 (98%)	28 (2%)	50	57

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	VAL
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	224	ARG
1	A	246	LYS
1	A	271	THR
1	A	410	VAL
1	A	431	LYS
1	B	2	THR
1	B	85	LYS
1	B	431	LYS
1	B	453	LYS
1	C	85	LYS
1	C	123	LEU
1	C	126	LYS
1	C	170	LYS
1	C	386	GLU
1	C	390	THR
1	C	424	LYS
1	C	438	GLU
1	C	446	VAL
1	C	449	GLU
1	D	8	LYS
1	D	69	GLU
1	D	245	VAL
1	D	246	LYS
1	D	253	LYS
1	D	449	GLU
1	D	453	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	102	GLN
1	A	116	HIS
1	A	315	ASN
1	B	25	GLN
1	B	31	ASN
1	B	76	GLN
1	B	89	GLN
1	B	102	GLN
1	B	150	HIS
1	B	169	GLN
1	B	284	GLN

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Mol	Chain	Res	Type
1	B	315	ASN
1	B	330	GLN
1	B	375	GLN
1	B	416	HIS
1	C	15	GLN
1	C	76	GLN
1	C	102	GLN
1	C	119	ASN
1	C	169	GLN
1	C	315	ASN
1	C	369	ASN
1	C	430	HIS
1	D	31	ASN
1	D	89	GLN
1	D	102	GLN
1	D	116	HIS
1	D	119	ASN
1	D	132	ASN
1	D	169	GLN
1	D	315	ASN
1	D	340	GLN
1	D	400	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](#)

4 ligands are modelled in this entry.

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	FUM	C	502	-	7,7,7	1.38	0	8,8,8	0.81	0
2	FUM	A	502	-	7,7,7	1.21	1 (14%)	8,8,8	1.44	1 (12%)
2	FUM	A	501	-	7,7,7	1.47	1 (14%)	8,8,8	1.58	1 (12%)
2	FUM	C	501	-	7,7,7	1.52	1 (14%)	8,8,8	1.32	1 (12%)

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	FUM	C	502	-	-	0/5/5/5	-
2	FUM	A	502	-	-	0/5/5/5	-
2	FUM	A	501	-	-	2/5/5/5	-
2	FUM	C	501	-	-	2/5/5/5	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	FUM	OXT-C	-2.17	1.24	1.30
2	A	502	FUM	O7-C6	2.09	1.28	1.23
2	C	501	FUM	OXT-C	-2.05	1.25	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	FUM	OXT-C-O	-3.45	115.67	122.70
2	A	502	FUM	O-C-C4	-2.71	112.76	121.06
2	C	501	FUM	OXT-C-O	-2.50	117.60	122.70

There are no chirality outliers.

All (4) torsion outliers are listed below:

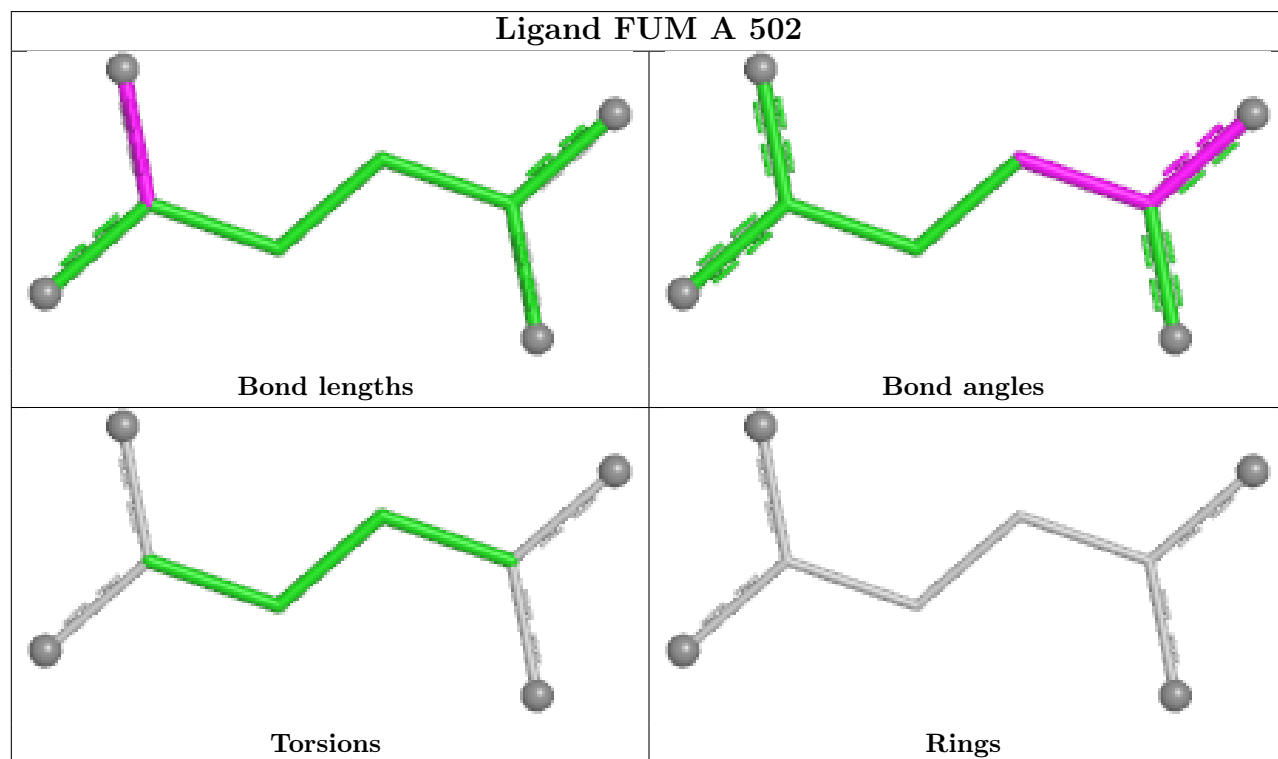
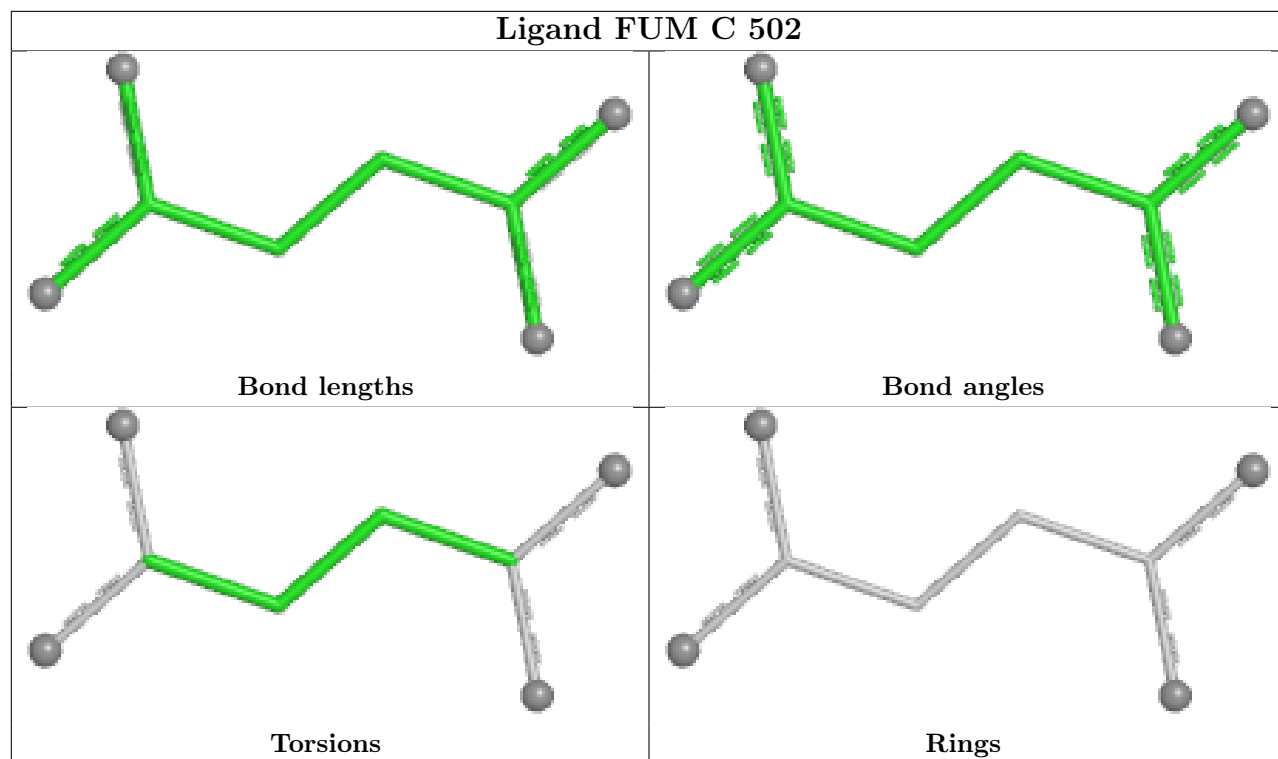
Mol	Chain	Res	Type	Atoms
2	C	501	FUM	OXT-C-C4-C5
2	A	501	FUM	OXT-C-C4-C5
2	C	501	FUM	O-C-C4-C5
2	A	501	FUM	O-C-C4-C5

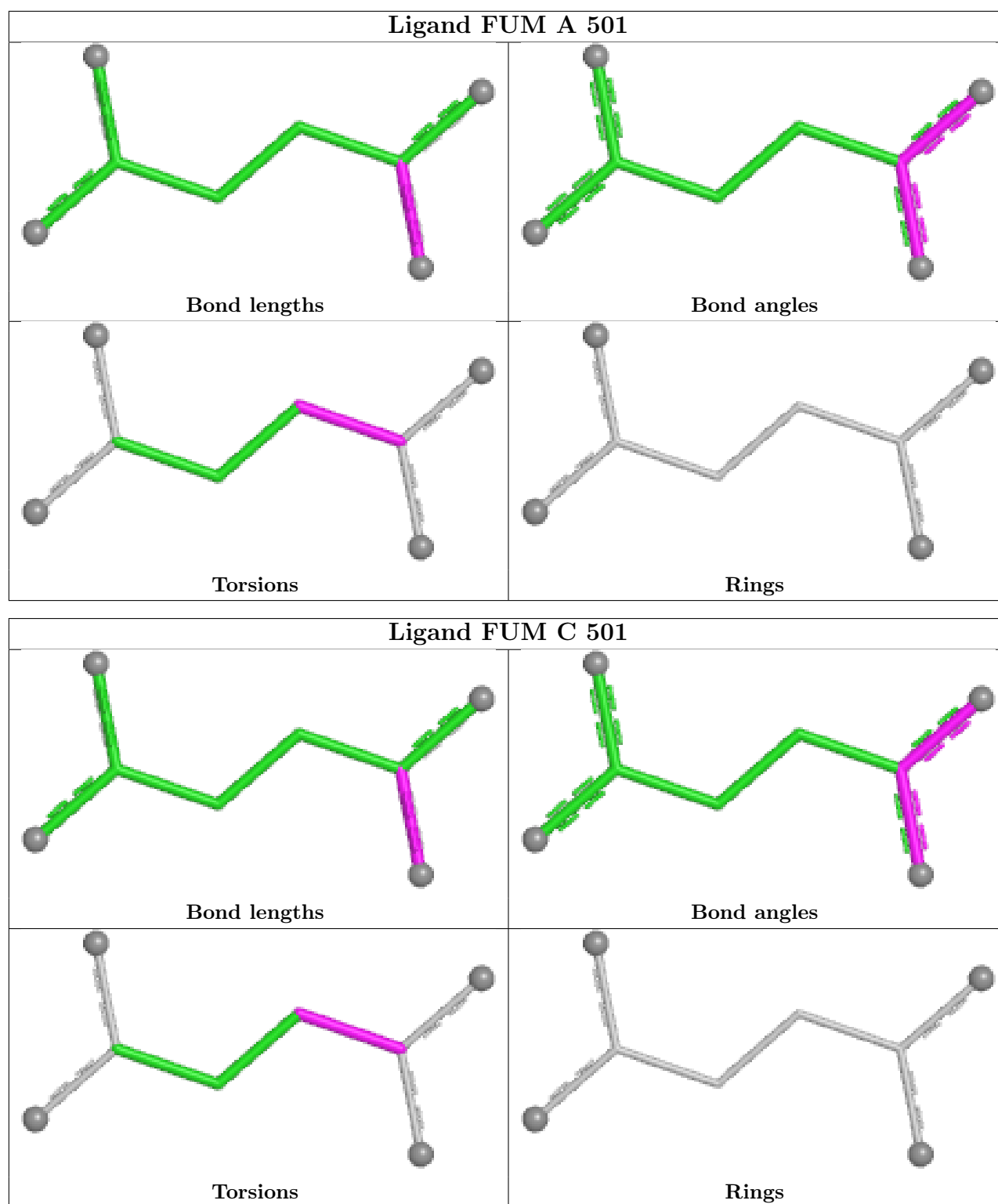
There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	FUM	4	0
2	A	502	FUM	3	0
2	A	501	FUM	3	0
2	C	501	FUM	3	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	463/467 (99%)	-0.12	0 100 100	13, 20, 30, 49	0
1	B	464/467 (99%)	-0.13	1 (0%) 91 92	13, 20, 30, 47	0
1	C	461/467 (98%)	-0.01	4 (0%) 81 83	12, 21, 36, 58	0
1	D	460/467 (98%)	-0.08	0 100 100	13, 21, 32, 50	0
All	All	1848/1868 (98%)	-0.08	5 (0%) 90 91	12, 20, 32, 58	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	464	LEU	3.9
1	C	463	SER	3.2
1	C	126	LYS	3.0
1	C	462	GLY	2.3
1	B	465	LYS	2.1

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.

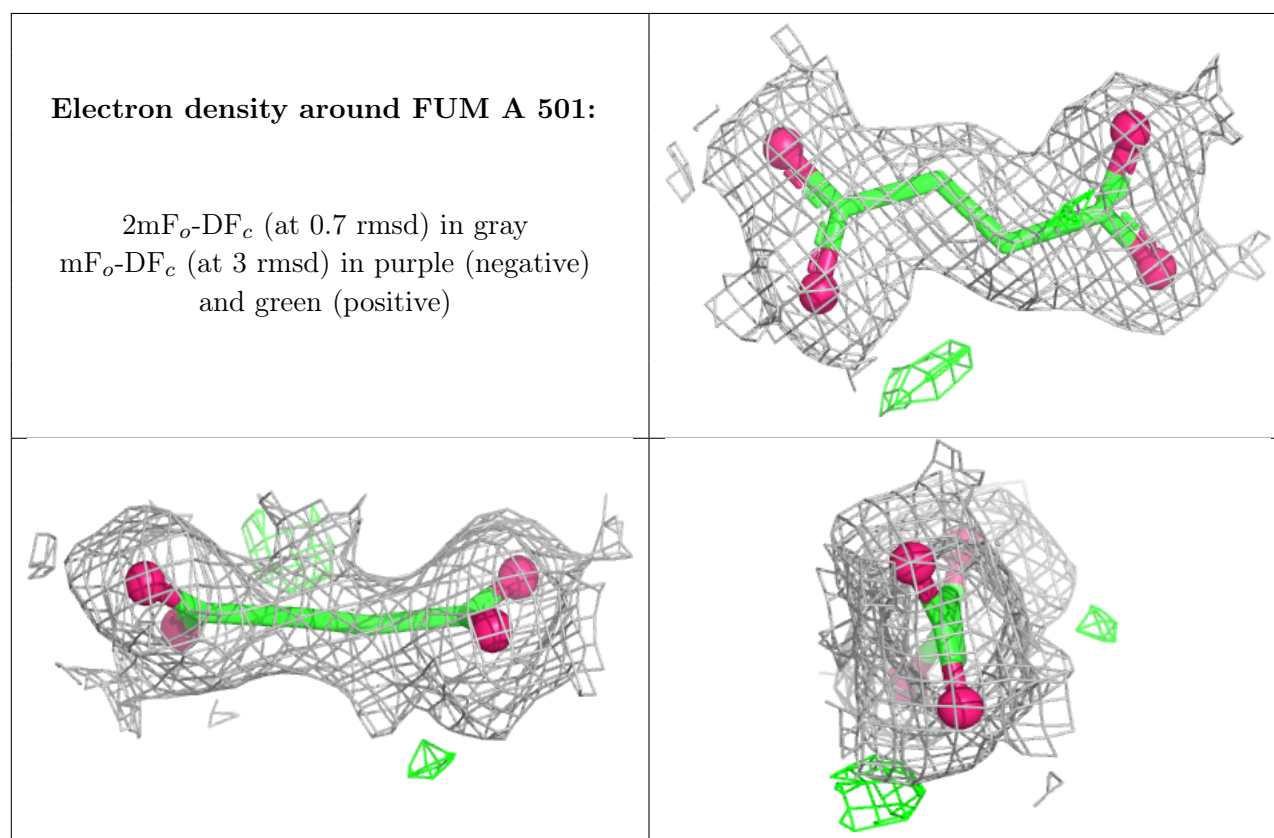
6.4 Ligands [i](#)

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.

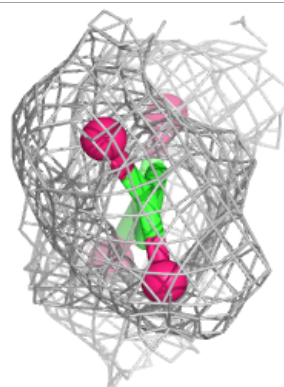
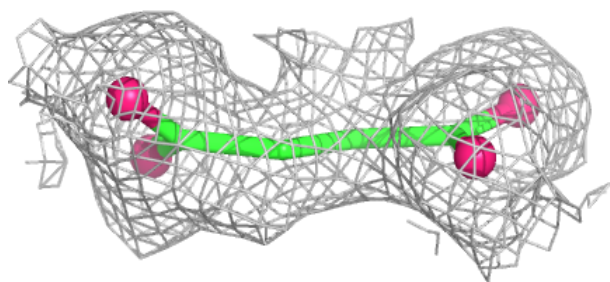
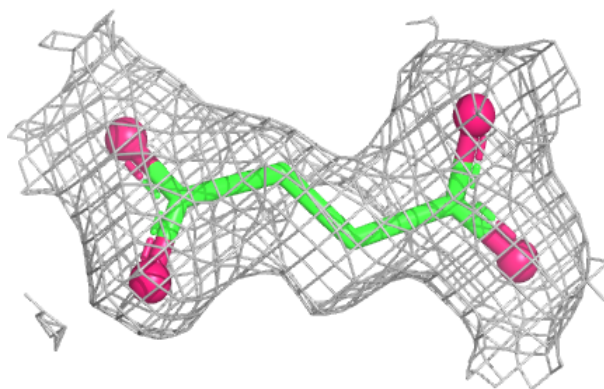
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	FUM	A	501	8/8	0.94	0.07	23,27,28,30	0
2	FUM	C	501	8/8	0.94	0.07	17,22,27,27	0
2	FUM	A	502	8/8	0.95	0.07	21,23,26,28	0
2	FUM	C	502	8/8	0.95	0.07	21,23,25,25	0

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.

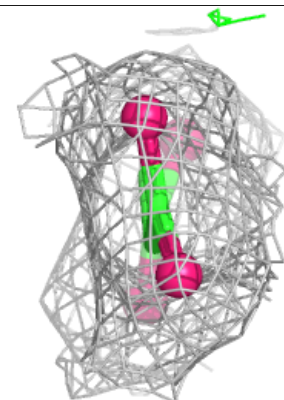
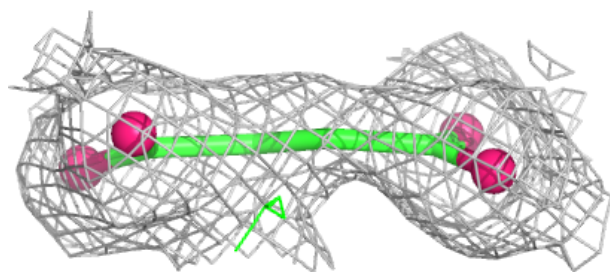
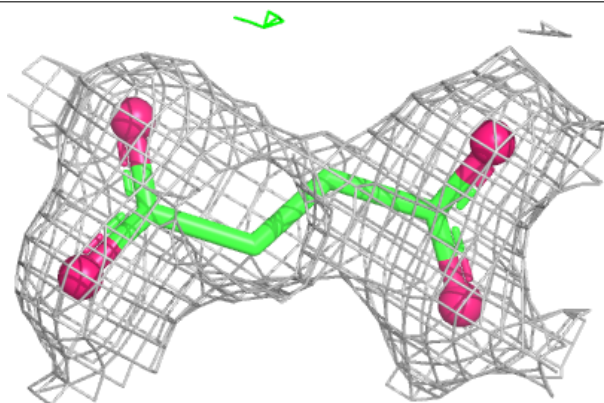


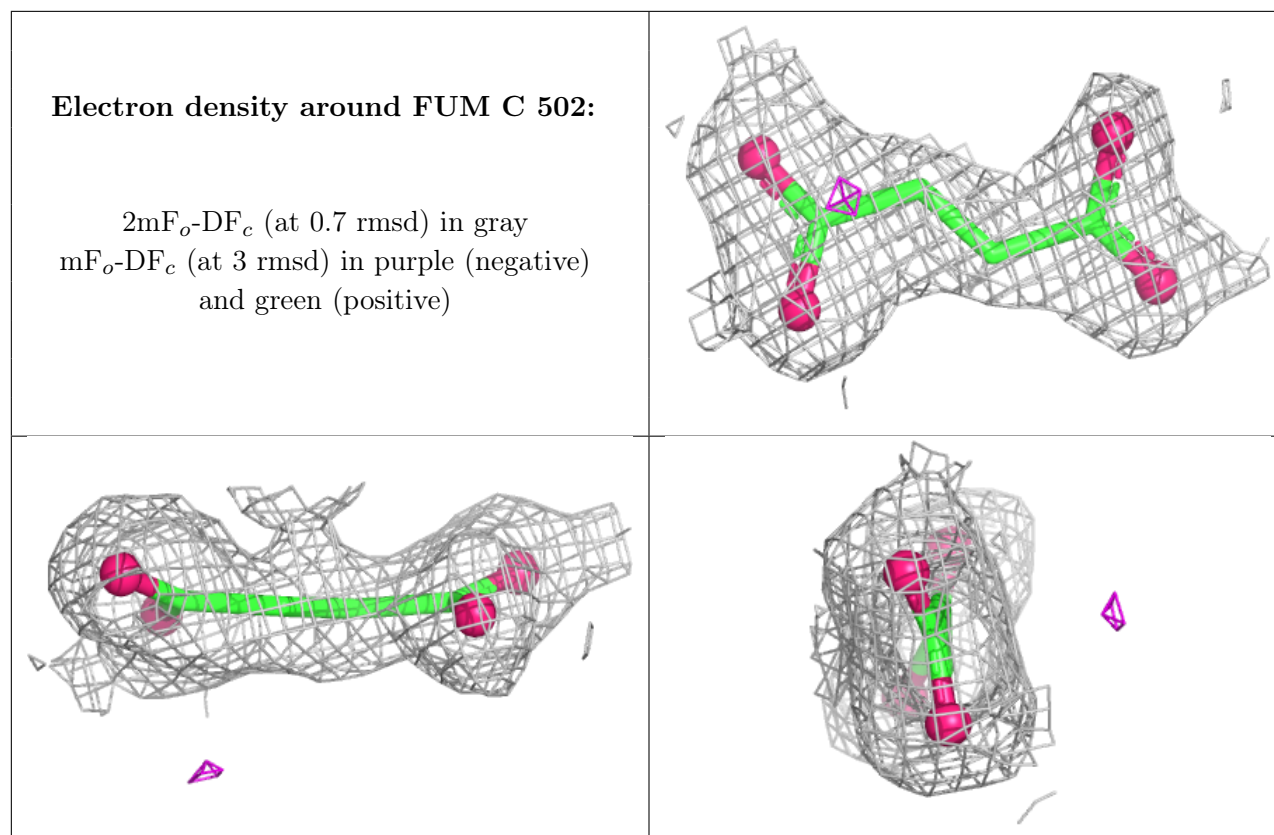
Electron density around FUM C 501:

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

**Electron density around FUM A 502:**

$2mF_o-DF_c$ (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.