



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:13 AM UTC

PDB ID : 9EMK / pdb_00009emk
Title : DupA from legionella covalently bound to ubiquitin-based probe
Authors : Kim, R.Q.; Kloet, M.S.; van der Heden van Noort, G.
Deposited on : 2024-03-08
Resolution : 2.17 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

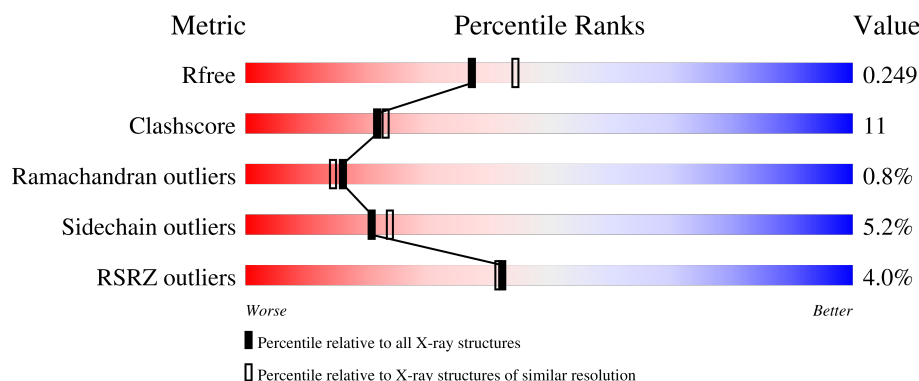
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	347	<div> <div>16%</div> <div>70%</div> <div>16%</div> <div>10%</div> </div>
1	C	347	<div> <div>73%</div> <div>14%</div> <div>10%</div> </div>
1	E	347	<div> <div>2%</div> <div>68%</div> <div>18%</div> <div>11%</div> </div>
2	B	76	<div> <div>16%</div> <div>63%</div> <div>29%</div> <div>7%</div> </div>
2	D	76	<div> <div>25%</div> <div>51%</div> <div>37%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	76	

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	ABA	D	42	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18701 atoms, of which 9174 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 Septation initiation protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	312	Total	C	H	N	O	S	89	0	0
			4944	1584	2446	441	463	10			
1	C	312	Total	C	H	N	O	S	89	0	0
			4957	1588	2454	442	463	10			
1	E	308	Total	C	H	N	O	S	89	0	0
			4901	1572	2424	437	459	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A0A3A6VVK6
A	0	ALA	-	expression tag	UNP A0A3A6VVK6
A	1	MET	-	expression tag	UNP A0A3A6VVK6
A	2	GLY	-	expression tag	UNP A0A3A6VVK6
A	3	SER	-	expression tag	UNP A0A3A6VVK6
A	228	ASP	ALA	conflict	UNP A0A3A6VVK6
C	-1	GLY	-	expression tag	UNP A0A3A6VVK6
C	0	ALA	-	expression tag	UNP A0A3A6VVK6
C	1	MET	-	expression tag	UNP A0A3A6VVK6
C	2	GLY	-	expression tag	UNP A0A3A6VVK6
C	3	SER	-	expression tag	UNP A0A3A6VVK6
C	228	ASP	ALA	conflict	UNP A0A3A6VVK6
E	-1	GLY	-	expression tag	UNP A0A3A6VVK6
E	0	ALA	-	expression tag	UNP A0A3A6VVK6
E	1	MET	-	expression tag	UNP A0A3A6VVK6
E	2	GLY	-	expression tag	UNP A0A3A6VVK6
E	3	SER	-	expression tag	UNP A0A3A6VVK6
E	228	ASP	ALA	conflict	UNP A0A3A6VVK6

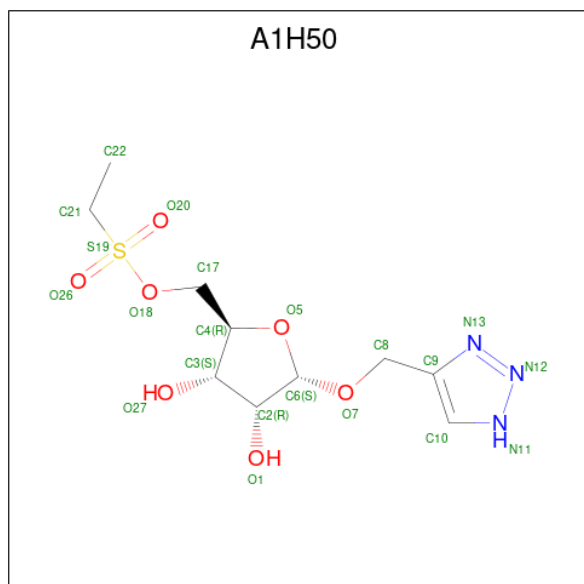
- Molecule 2 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	76	Total	C	H	N	O	S	13	0	0
			1217	376	620	102	118	1			
2	D	73	Total	C	H	N	O		13	0	0
			1162	360	590	98	114				
2	F	73	Total	C	H	N	O	S	13	0	0
			1178	366	601	96	114	1			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	ABA	ARG	engineered mutation	UNP P0CG47
D	42	ABA	ARG	engineered mutation	UNP P0CG47
F	42	ABA	ARG	engineered mutation	UNP P0CG47

- Molecule 3 is [(2 {R},3 {S},4 {R},5 {S})-5-[(1-ethyl-1,2,3-triazol-4-yl)methoxy]-3,4-bis(oxidanyl)oxolan-2-yl]methyl ethanesulfonate (CCD ID: A1H50) (formula: C₁₀H₁₇N₃O₇S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S	2	0
			34	10	13	3	7	1		
3	C	1	Total	C	H	N	O	S	2	0
			34	10	13	3	7	1		
3	E	1	Total	C	H	N	O	S	2	0
			34	10	13	3	7	1		

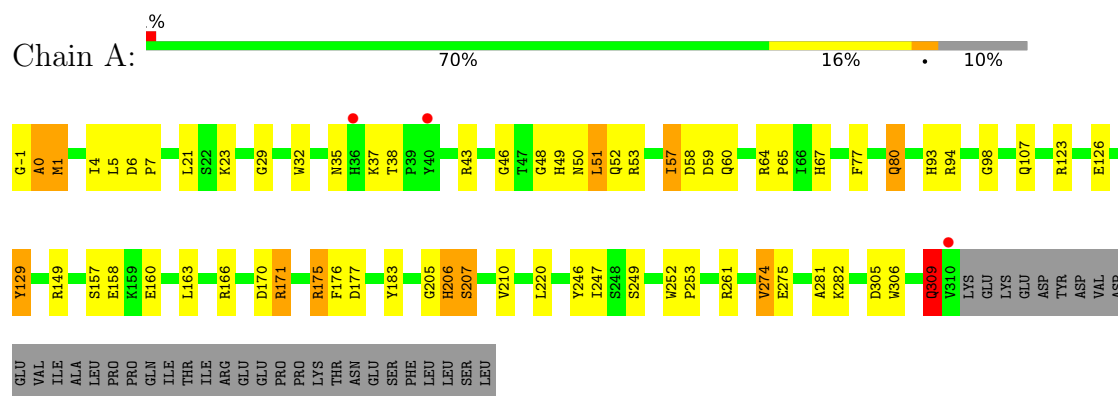
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	3	Total 3	O 3	0	0
4	C	54	Total 54	O 54	0	0
4	D	1	Total 1	O 1	0	0
4	E	59	Total 59	O 59	0	0
4	F	2	Total 2	O 2	0	0

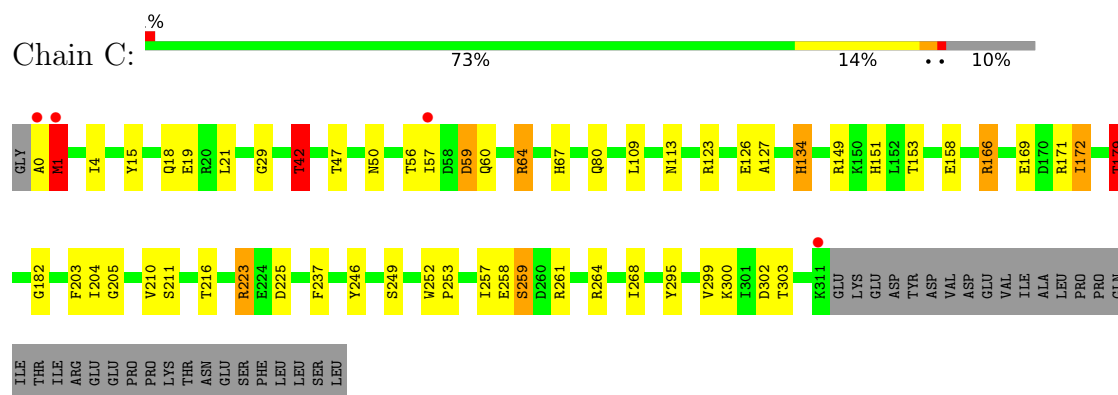
3 Residue-property plots

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.

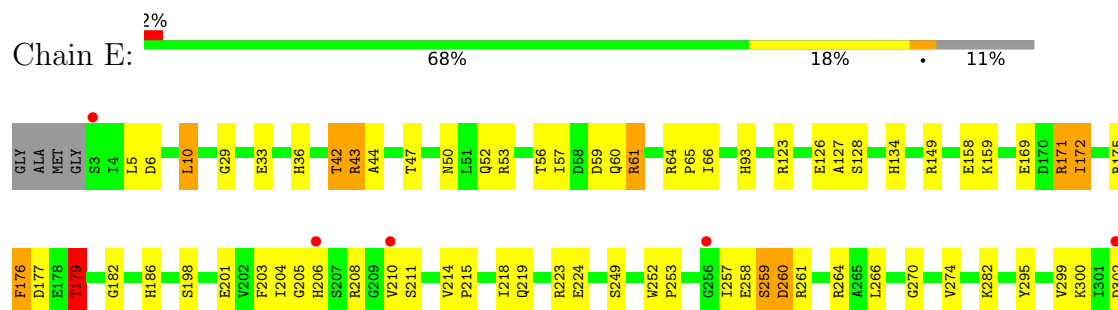
• Molecule 1: Septation initiation protein

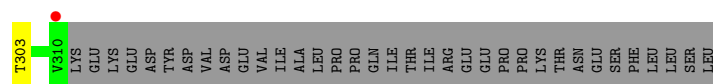


• Molecule 1: Septation initiation protein

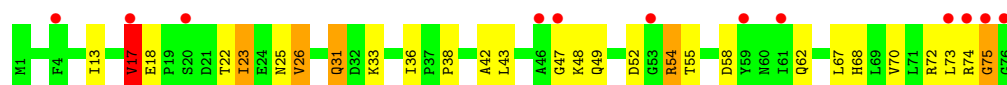


• Molecule 1: Septation initiation protein

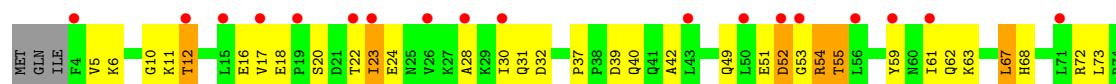




• Molecule 2: Polyubiquitin-B



• Molecule 2: Polyubiquitin-B



• Molecule 2: Polyubiquitin-B



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	86.81Å 86.81Å 146.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	75.29 – 2.17 75.18 – 2.17	Depositor EDS
% Data completeness (in resolution range)	100.0 (75.29-2.17) 99.9 (75.18-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.185 , 0.239 0.190 , 0.249	Depositor DCC
R_{free} test set	3239 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for -h,-k,l 0.093 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18701	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: A1H50, ABA

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	0.76	0/2561	1.27	14/3465 (0.4%)
1	C	0.69	0/2566	1.22	13/3471 (0.4%)
1	E	0.67	0/2540	1.22	11/3438 (0.3%)
2	B	0.57	0/596	1.29	1/799 (0.1%)
2	D	0.54	0/571	1.23	1/766 (0.1%)
2	F	0.58	0/576	1.22	4/775 (0.5%)
All	All	0.68	0/9410	1.24	44/12714 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	4
1	C	0	3
1	E	0	4
2	B	1	1
2	D	2	0
All	All	4	12

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	302	ASP	CB-CA-C	10.93	128.00	109.53
2	B	17	VAL	N-CA-CB	10.91	129.24	111.23
1	C	1	MET	CG-SD-CE	7.68	117.79	100.90
1	A	175	ARG	N-CA-CB	-7.53	99.00	110.45
1	E	176	PHE	CB-CA-C	6.98	122.38	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	309	GLN	N-CA-CB	6.66	120.57	110.45
1	C	42	THR	OG1-CB-CG2	-6.58	96.13	109.30
1	E	179	THR	N-CA-CB	-6.55	99.34	111.53
1	E	47	THR	CA-CB-OG1	-6.37	100.04	109.60
1	A	58	ASP	CA-CB-CG	6.27	118.87	112.60
1	C	56	THR	CA-CB-OG1	-6.26	100.22	109.60
2	F	52	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	1	MET	CB-CA-C	6.21	123.77	111.22
1	A	60	GLN	CB-CA-C	6.12	120.31	109.72
1	E	56	THR	CA-CB-OG1	-6.03	100.56	109.60
1	E	59	ASP	CA-CB-CG	6.01	118.61	112.60
1	A	206	HIS	CA-CB-CG	6.00	119.80	113.80
1	E	158	GLU	CB-CG-CD	5.94	122.70	112.60
1	E	61	ARG	CB-CA-C	-5.86	100.69	110.29
1	A	305	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	207	SER	CB-CA-C	5.84	120.24	110.43
1	C	59	ASP	CA-CB-CG	5.83	118.44	112.60
1	E	171	ARG	N-CA-CB	-5.79	101.09	109.83
1	A	129	TYR	CA-C-N	5.71	126.28	119.94
1	A	129	TYR	C-N-CA	5.71	126.28	119.94
1	C	134	HIS	CA-CB-CG	-5.68	108.12	113.80
1	A	23	LYS	N-CA-CB	5.68	117.71	110.04
2	F	69	LEU	CA-C-N	-5.67	117.35	123.08
2	F	69	LEU	C-N-CA	-5.67	117.35	123.08
1	A	59	ASP	CB-CA-C	-5.61	100.45	111.06
1	C	153	THR	CA-CB-OG1	-5.56	101.25	109.60
2	F	32	ASP	CA-CB-CG	5.55	118.15	112.60
1	C	64	ARG	CD-NE-CZ	5.55	132.16	124.40
1	A	1	MET	CG-SD-CE	-5.40	89.02	100.90
1	C	179	THR	N-CA-CB	-5.35	101.58	111.53
1	E	224	GLU	N-CA-CB	5.30	117.67	109.98
1	E	176	PHE	N-CA-CB	-5.25	102.40	110.12
1	A	275	GLU	CB-CG-CD	5.24	121.51	112.60
2	D	12	THR	CA-CB-OG1	-5.24	101.74	109.60
1	C	18	GLN	CB-CA-C	-5.21	102.14	110.79
1	C	203	PHE	CA-CB-CG	-5.15	108.65	113.80
1	A	176	PHE	CA-CB-CG	5.10	118.90	113.80
1	C	225	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	237	PHE	N-CA-CB	5.03	117.30	110.01

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	207	SER	CA
2	B	17	VAL	CA
2	D	17	VAL	CA
2	D	42	ABA	CA

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	123	ARG	Sidechain
1	A	171	ARG	Sidechain
1	A	175	ARG	Sidechain
1	A	43	ARG	Sidechain
2	B	54	ARG	Sidechain
1	C	123	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	223	ARG	Sidechain
1	E	123	ARG	Sidechain
1	E	149	ARG	Sidechain
1	E	175	ARG	Sidechain
1	E	43	ARG	Sidechain

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	2498	2446	2429	51	0
1	C	2503	2454	2439	42	0
1	E	2477	2424	2406	41	0
2	B	597	620	621	31	0
2	D	572	590	588	32	0
2	F	577	601	602	11	0
3	A	21	13	0	0	0
3	C	21	13	0	1	0
3	E	21	13	0	0	0
4	A	121	0	0	4	0
4	B	3	0	0	0	0
4	C	54	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	59	0	0	0	0
4	F	2	0	0	0	0
All	All	9527	9174	9085	199	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 11.

All (199) 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:179:THR:HG22	1:C:182:GLY:H	1.30	0.95
1:E:33:GLU:O	1:E:42:THR:HG21	1.66	0.95
1:E:179:THR:HG22	1:E:182:GLY:H	1.32	0.95
2:D:23:ILE:HD11	2:D:52:ASP:HA	1.49	0.94
1:A:29:GLY:H	1:A:50:ASN:HD21	0.99	0.93
1:C:29:GLY:H	1:C:50:ASN:HD21	1.07	0.93
2:F:70:VAL:O	2:F:71:LEU:HB2	1.65	0.93
1:A:1:MET:CE	1:A:4:ILE:HD13	2.00	0.91
2:D:23:ILE:CD1	2:D:52:ASP:HA	2.01	0.90
1:E:29:GLY:H	1:E:50:ASN:HD21	1.21	0.89
1:A:4:ILE:HG13	1:A:5:LEU:HD13	1.58	0.84
1:C:205:GLY:O	1:C:261:ARG:NH2	2.09	0.83
1:E:42:THR:HG23	1:E:44:ALA:H	1.44	0.83
1:C:1:MET:CE	1:C:302:ASP:OD1	2.28	0.81
1:A:1:MET:HE1	1:A:4:ILE:HD13	1.61	0.79
1:C:1:MET:HE3	1:C:302:ASP:OD1	1.83	0.79
1:A:52:GLN:OE1	2:B:73:LEU:HB3	1.84	0.78
1:C:1:MET:HE2	1:C:300:LYS:O	1.85	0.77
1:A:306:TRP:HA	1:A:309:GLN:HG2	1.68	0.76
2:D:23:ILE:HD11	2:D:52:ASP:CA	2.15	0.76
1:E:205:GLY:O	1:E:261:ARG:NH2	2.19	0.75
1:A:1:MET:HE3	1:A:4:ILE:HD13	1.68	0.75
1:E:179:THR:CG2	1:E:182:GLY:H	2.00	0.74
1:C:15:TYR:CE1	1:C:19:GLU:HG3	2.23	0.74
1:E:295:TYR:CZ	1:E:299:VAL:HG21	2.24	0.73
2:D:23:ILE:HD11	2:D:52:ASP:CG	2.14	0.72
1:C:80:GLN:HE21	1:C:113:ASN:HD21	1.38	0.72
1:C:149:ARG:NH1	1:C:158:GLU:OE1	2.25	0.70
2:B:72:ARG:HD3	2:B:74:ARG:NH1	2.08	0.69
1:A:-1:GLY:N	4:A:502:HOH:O	2.25	0.68
1:C:1:MET:CE	1:C:300:LYS:O	2.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:O	1:A:64:ARG:HD3	1.93	0.68
1:C:1:MET:SD	1:C:300:LYS:O	2.51	0.68
1:E:42:THR:HG23	1:E:44:ALA:N	2.08	0.68
2:D:51:GLU:HG3	2:D:59:TYR:OH	1.93	0.67
2:B:23:ILE:HA	2:B:26:VAL:CG1	2.25	0.67
1:E:203:PHE:C	1:E:204:ILE:HD12	2.21	0.66
1:A:149:ARG:NH1	1:A:158:GLU:OE1	2.26	0.66
2:B:42:ABA:HG3	2:B:49:GLN:HG2	1.76	0.65
2:B:47:GLY:O	2:B:48:LYS:HE2	1.98	0.64
2:F:59:TYR:HB2	2:F:61:ILE:CD1	2.28	0.64
1:A:107:GLN:OE1	4:A:501:HOH:O	2.16	0.63
2:B:23:ILE:CG1	2:B:52:ASP:HA	2.29	0.63
2:D:23:ILE:HD11	2:D:52:ASP:CB	2.29	0.63
1:C:29:GLY:N	1:C:50:ASN:HD21	1.89	0.63
2:F:27:LYS:HE3	2:F:52:ASP:OD1	1.99	0.62
1:C:1:MET:HG2	1:C:302:ASP:OD1	1.99	0.62
2:B:73:LEU:HD23	2:B:74:ARG:O	2.00	0.62
1:A:37:LYS:O	1:C:151:HIS:HE1	1.83	0.62
1:E:218:ILE:HD12	1:E:223:ARG:HA	1.80	0.62
1:A:1:MET:HE1	1:A:4:ILE:CD1	2.29	0.61
2:D:5:VAL:HG22	2:D:67:LEU:HD11	1.82	0.61
1:E:198:SER:OG	1:E:201:GLU:OE1	2.11	0.61
1:A:1:MET:CE	1:A:4:ILE:CD1	2.76	0.61
2:D:23:ILE:HD13	2:D:24:GLU:H	1.65	0.60
2:D:59:TYR:HB2	2:D:61:ILE:CD1	2.31	0.60
2:B:42:ABA:HG2	2:B:70:VAL:CG1	2.32	0.60
2:D:16:GLU:O	2:D:17:VAL:HB	2.02	0.60
1:A:1:MET:CE	1:A:77:PHE:CD2	2.85	0.59
1:C:264:ARG:O	1:C:268:ILE:HG12	2.01	0.59
1:E:179:THR:HG22	1:E:182:GLY:N	2.12	0.58
2:D:22:THR:HA	2:D:55:THR:HA	1.85	0.58
2:B:54:ARG:NE	2:B:58:ASP:HB2	2.17	0.58
2:D:10:GLY:O	2:D:12:THR:HG22	2.04	0.58
1:C:246:TYR:OH	2:D:68:HIS:HE1	1.87	0.58
2:B:23:ILE:HG13	2:B:52:ASP:HA	1.86	0.57
1:C:166:ARG:NH1	1:C:171:ARG:HH21	2.03	0.57
2:D:5:VAL:HG22	2:D:67:LEU:CD1	2.35	0.57
1:A:1:MET:HE2	1:A:77:PHE:CE2	2.40	0.57
1:A:1:MET:HE1	1:A:77:PHE:CD2	2.40	0.56
1:A:46:GLY:HA3	1:A:129:TYR:CD1	2.39	0.56
2:B:43:LEU:HD13	2:B:67:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ARG:HH11	1:C:171:ARG:NH2	2.03	0.56
1:C:204:ILE:HG21	1:C:257:ILE:HG21	1.88	0.56
1:A:157:SER:OG	1:A:160:GLU:HG3	2.05	0.56
1:A:-1:GLY:O	1:A:0:ALA:CB	2.54	0.56
1:E:50:ASN:HD22	1:E:53:ARG:HD2	1.72	0.55
1:C:29:GLY:H	1:C:50:ASN:ND2	1.90	0.55
1:A:57:ILE:HG23	1:A:281:ALA:HB1	1.89	0.55
1:A:206:HIS:O	1:A:207:SER:HB2	2.07	0.55
2:B:23:ILE:HA	2:B:26:VAL:HG12	1.89	0.55
2:B:72:ARG:HD3	2:B:74:ARG:HH11	1.72	0.54
2:D:23:ILE:HD13	2:D:24:GLU:N	2.23	0.53
2:D:23:ILE:HD12	2:D:52:ASP:HA	1.88	0.53
1:A:94:ARG:HD2	1:A:98:GLY:O	2.07	0.53
2:B:54:ARG:HE	2:B:58:ASP:HB2	1.74	0.53
1:E:214:VAL:O	1:E:218:ILE:HG12	2.08	0.53
1:C:67:HIS:HD2	1:C:126:GLU:OE2	1.93	0.52
1:C:80:GLN:HE21	1:C:113:ASN:ND2	2.04	0.52
1:A:247:ILE:HB	1:A:274:VAL:HG13	1.91	0.52
1:C:0:ALA:HB1	1:C:303:THR:OG1	2.10	0.52
2:B:22:THR:HG23	2:B:25:ASN:H	1.75	0.52
1:C:295:TYR:CZ	1:C:299:VAL:HG11	2.45	0.51
2:B:54:ARG:HG2	2:B:58:ASP:OD2	2.10	0.51
1:A:51:LEU:HD23	4:A:591:HOH:O	2.10	0.51
2:D:52:ASP:OD1	2:D:53:GLY:N	2.44	0.51
1:A:4:ILE:HD12	1:A:80:GLN:HG3	1.93	0.50
1:A:53:ARG:HB2	2:B:75:GLY:HA3	1.93	0.50
2:F:62:GLN:HG2	2:F:63:LYS:N	2.25	0.50
1:C:42:THR:O	1:E:36:HIS:HE1	1.95	0.50
1:A:38:THR:HG23	1:C:15:TYR:OH	2.12	0.50
1:C:21:LEU:O	1:C:64:ARG:HD3	2.11	0.50
2:D:37:PRO:HB2	2:D:40:GLN:OE1	2.12	0.50
2:B:42:ABA:HG2	2:B:70:VAL:HG12	1.93	0.49
2:D:16:GLU:O	2:D:17:VAL:CB	2.60	0.49
1:A:67:HIS:HD2	1:A:126:GLU:OE2	1.94	0.49
2:B:17:VAL:HG23	2:B:18:GLU:HB2	1.94	0.49
2:B:22:THR:HA	2:B:55:THR:HA	1.93	0.49
1:C:134:HIS:CE1	1:C:172:ILE:HG12	2.48	0.49
1:E:249:SER:HA	1:E:252:TRP:CE2	2.47	0.49
2:D:10:GLY:O	2:D:12:THR:CG2	2.60	0.49
2:B:17:VAL:HB	2:B:18:GLU:OE1	2.13	0.49
1:E:215:PRO:O	1:E:219:GLN:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:TYR:CE2	1:E:299:VAL:HG21	2.47	0.48
1:E:61:ARG:CG	1:E:61:ARG:HH11	2.26	0.48
1:A:1:MET:HE2	1:A:77:PHE:CD2	2.48	0.48
1:A:93:HIS:HE1	1:A:177:ASP:OD2	1.97	0.48
1:A:35:ASN:OD1	1:A:37:LYS:HB2	2.14	0.48
2:B:23:ILE:O	2:B:26:VAL:HG13	2.14	0.48
1:C:295:TYR:CZ	1:C:299:VAL:CG1	2.97	0.48
1:E:93:HIS:HE1	1:E:177:ASP:OD2	1.96	0.47
1:A:1:MET:HE3	1:A:4:ILE:CD1	2.41	0.47
1:A:205:GLY:O	1:A:261:ARG:NH2	2.48	0.47
2:B:31:GLN:CD	2:B:38:PRO:HD3	2.39	0.47
1:E:134:HIS:CE1	1:E:172:ILE:HG13	2.49	0.47
1:E:61:ARG:HH11	1:E:61:ARG:HG3	1.79	0.47
1:A:246:TYR:OH	2:B:68:HIS:HE1	1.97	0.46
1:E:258:GLU:O	1:E:259:SER:C	2.57	0.46
1:E:260:ASP:OD2	1:E:261:ARG:HG3	2.16	0.46
2:F:21:ASP:O	2:F:56:LEU:HD22	2.15	0.46
2:D:51:GLU:O	2:D:52:ASP:HB3	2.16	0.46
1:E:64:ARG:N	1:E:65:PRO:CD	2.79	0.46
1:C:1:MET:CG	1:C:302:ASP:OD1	2.62	0.46
1:C:166:ARG:NH1	1:C:171:ARG:NH2	2.63	0.46
1:C:249:SER:HA	1:C:252:TRP:CE2	2.51	0.46
1:A:-1:GLY:O	1:A:0:ALA:HB2	2.16	0.46
1:A:306:TRP:HA	1:A:309:GLN:CG	2.43	0.45
2:D:22:THR:HG23	2:D:24:GLU:HB3	1.99	0.45
1:E:295:TYR:CZ	1:E:299:VAL:CG2	2.95	0.45
2:D:6:LYS:HA	2:D:11:LYS:O	2.16	0.45
2:D:28:ALA:O	2:D:31:GLN:HB3	2.16	0.45
1:A:6:ASP:HB2	1:A:7:PRO:CD	2.47	0.45
1:C:258:GLU:O	1:C:259:SER:C	2.59	0.45
2:D:5:VAL:HG21	2:D:30:ILE:HD11	1.97	0.45
2:B:22:THR:O	2:B:26:VAL:HG12	2.16	0.45
1:C:295:TYR:CE1	1:C:299:VAL:CG1	3.00	0.45
1:E:204:ILE:HD12	1:E:204:ILE:N	2.31	0.45
1:E:223:ARG:NH2	1:E:270:GLY:HA3	2.32	0.45
1:A:1:MET:HE3	1:A:4:ILE:HG21	1.98	0.45
2:B:54:ARG:HD2	2:B:54:ARG:HA	1.77	0.44
2:D:17:VAL:HG13	2:D:18:GLU:H	1.83	0.44
1:E:5:LEU:HB2	1:E:10:LEU:HD21	1.98	0.44
1:E:6:ASP:OD1	1:E:6:ASP:C	2.61	0.44
2:F:59:TYR:CB	2:F:61:ILE:CD1	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:204:ILE:HG21	1:E:257:ILE:HG21	1.98	0.44
2:F:1:MET:HE2	2:F:18:GLU:HA	2.00	0.44
1:A:48:GLY:HA2	1:A:51:LEU:HG	2.00	0.43
1:E:126:GLU:O	1:E:127:ALA:C	2.59	0.43
2:D:40:GLN:OE1	2:D:40:GLN:N	2.52	0.43
2:D:67:LEU:HD23	2:D:67:LEU:N	2.34	0.43
2:F:61:ILE:HG12	2:F:67:LEU:HD11	1.99	0.43
3:C:401:A1H50:N12	2:D:49:GLN:HG2	2.34	0.43
2:F:51:GLU:OE1	2:F:54:ARG:NH1	2.52	0.43
1:A:37:LYS:O	1:C:151:HIS:CE1	2.68	0.43
1:C:126:GLU:O	1:C:127:ALA:C	2.60	0.42
1:E:252:TRP:N	1:E:253:PRO:CD	2.82	0.42
2:B:31:GLN:CG	2:B:36:ILE:O	2.67	0.42
1:C:252:TRP:N	1:C:253:PRO:CD	2.82	0.42
1:A:32:TRP:CE3	1:A:49:HIS:CE1	3.06	0.42
2:D:51:GLU:OE2	2:D:54:ARG:HB2	2.20	0.42
2:B:33:LYS:HD2	2:B:33:LYS:N	2.34	0.42
1:A:183:TYR:OH	1:A:220:LEU:HD21	2.20	0.42
2:B:31:GLN:HG2	2:B:36:ILE:O	2.20	0.42
1:E:52:GLN:HG3	1:E:66:ILE:HD11	2.02	0.42
1:E:29:GLY:N	1:E:50:ASN:HD21	2.03	0.41
1:E:249:SER:HA	1:E:252:TRP:CD2	2.55	0.41
2:D:54:ARG:HH22	2:F:58:ASP:HA	1.84	0.41
1:E:206:HIS:ND1	1:E:206:HIS:O	2.54	0.41
1:A:29:GLY:H	1:A:50:ASN:ND2	1.84	0.41
1:A:206:HIS:O	1:A:207:SER:CB	2.69	0.41
1:C:169:GLU:OE2	1:C:171:ARG:HG2	2.21	0.41
1:C:211:SER:OG	1:C:216:THR:OG1	2.39	0.41
1:A:252:TRP:N	1:A:253:PRO:CD	2.84	0.41
2:F:70:VAL:O	2:F:71:LEU:CB	2.48	0.41
1:A:166:ARG:NH1	1:A:171:ARG:NH1	2.69	0.41
1:C:179:THR:CG2	1:C:182:GLY:H	2.15	0.41
2:D:39:ASP:O	2:D:72:ARG:HD2	2.21	0.41
1:C:80:GLN:HA	1:C:109:LEU:HD21	2.03	0.41
1:A:64:ARG:N	1:A:65:PRO:CD	2.84	0.41
1:A:249:SER:HA	1:A:252:TRP:CE2	2.55	0.41
1:A:4:ILE:CG1	1:A:5:LEU:HD13	2.40	0.40
1:C:57:ILE:O	1:C:60:GLN:HB2	2.20	0.40
1:E:159:LYS:HD3	1:E:159:LYS:C	2.45	0.40
1:E:169:GLU:CD	1:E:171:ARG:HE	2.29	0.40
1:A:170:ASP:HA	4:A:556:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:176:PHE:CE1	1:E:186:HIS:HB3	2.56	0.40
2:B:36:ILE:HD12	2:B:36:ILE:N	2.37	0.40
2:B:31:GLN:HG3	2:B:38:PRO:HD3	2.04	0.40
1:E:42:THR:HG23	1:E:43:ARG:N	2.37	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	310/347 (89%)	302 (97%)	7 (2%)	1 (0%)	36	39
1	C	310/347 (89%)	303 (98%)	6 (2%)	1 (0%)	36	39
1	E	306/347 (88%)	298 (97%)	6 (2%)	2 (1%)	18	17
2	B	73/76 (96%)	68 (93%)	3 (4%)	2 (3%)	4	2
2	D	70/76 (92%)	61 (87%)	8 (11%)	1 (1%)	9	6
2	F	70/76 (92%)	67 (96%)	1 (1%)	2 (3%)	3	1
All	All	1139/1269 (90%)	1099 (96%)	31 (3%)	9 (1%)	16	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	0	ALA
2	B	17	VAL
1	C	259	SER
2	F	71	LEU
2	F	72	ARG
2	B	75	GLY
2	D	52	ASP
1	E	208	ARG
1	E	259	SER

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	261/295 (88%)	253 (97%)	8 (3%)	35	45
1	C	262/295 (89%)	253 (97%)	9 (3%)	32	41
1	E	260/295 (88%)	244 (94%)	16 (6%)	16	17
2	B	67/67 (100%)	61 (91%)	6 (9%)	9	8
2	D	64/67 (96%)	55 (86%)	9 (14%)	3	2
2	F	66/67 (98%)	63 (96%)	3 (4%)	24	30
All	All	980/1086 (90%)	929 (95%)	51 (5%)	21	24

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	57	ILE
1	A	80	GLN
1	A	163	LEU
1	A	210	VAL
1	A	274	VAL
1	A	282	LYS
1	A	309	GLN
2	B	13	ILE
2	B	17	VAL
2	B	23	ILE
2	B	26	VAL
2	B	31	GLN
2	B	62	GLN
1	C	1	MET
1	C	4	ILE
1	C	42	THR
1	C	47	THR
1	C	59	ASP
1	C	172	ILE
1	C	179	THR
1	C	210	VAL

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Mol	Chain	Res	Type
1	C	223	ARG
2	D	20	SER
2	D	23	ILE
2	D	32	ASP
2	D	54	ARG
2	D	55	THR
2	D	62	GLN
2	D	63	LYS
2	D	67	LEU
2	D	73	LEU
1	E	10	LEU
1	E	42	THR
1	E	57	ILE
1	E	60	GLN
1	E	128	SER
1	E	172	ILE
1	E	179	THR
1	E	210	VAL
1	E	211	SER
1	E	260	ASP
1	E	264	ARG
1	E	266	LEU
1	E	274	VAL
1	E	282	LYS
1	E	300	LYS
1	E	303	THR
2	F	62	GLN
2	F	70	VAL
2	F	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	67	HIS
1	A	80	GLN
1	A	93	HIS
1	A	143	GLN
1	A	189	HIS
1	A	206	HIS
2	B	25	ASN
2	B	49	GLN

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Mol	Chain	Res	Type
2	B	60	ASN
2	B	68	HIS
1	C	50	ASN
1	C	67	HIS
1	C	113	ASN
1	C	134	HIS
1	C	143	GLN
1	C	151	HIS
1	C	231	HIS
2	D	31	GLN
2	D	68	HIS
1	E	36	HIS
1	E	50	ASN
1	E	60	GLN
1	E	93	HIS
1	E	107	GLN
1	E	143	GLN
1	E	277	GLN
2	F	25	ASN
2	F	60	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	ABA	D	42	2,3	4,5,6	1.25	1 (25%)	1,5,7	9.60	1 (100%)
2	ABA	F	42	2,3	4,5,6	0.54	0	1,5,7	2.13	1 (100%)
2	ABA	B	42	2,3	4,5,6	0.77	0	1,5,7	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ABA	D	42	2,3	1/1/1/2	1/3/4/6	-
2	ABA	F	42	2,3	-	2/3/4/6	-
2	ABA	B	42	2,3	-	2/3/4/6	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	42	ABA	CB-CA	2.06	1.58	1.53

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	42	ABA	CB-CA-N	9.60	148.22	110.57
2	F	42	ABA	CB-CA-N	2.13	118.91	110.57

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	42	ABA	CA

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	42	ABA	N-CA-CB-CG
2	B	42	ABA	C-CA-CB-CG
2	D	42	ABA	C-CA-CB-CG
2	F	42	ABA	N-CA-CB-CG
2	F	42	ABA	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	42	ABA	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
3	A1H50	E	401	2,1	22,22,22	0.36	0	26,31,31	0.61	0
3	A1H50	A	401	2,1	22,22,22	0.38	0	26,31,31	0.87	0
3	A1H50	C	401	2,1	22,22,22	0.44	0	26,31,31	1.00	2 (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	A1H50	E	401	2,1	-	4/14/30/30	0/2/2/2
3	A1H50	A	401	2,1	-	5/14/30/30	0/2/2/2
3	A1H50	C	401	2,1	-	8/14/30/30	0/2/2/2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	401	A1H50	O26-S19-C21	2.53	113.78	106.76
3	C	401	A1H50	O18-S19-C21	-2.50	97.53	104.18

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1H50	O18-C17-C4-C3
3	A	401	A1H50	O18-C17-C4-O5
3	C	401	A1H50	O18-C17-C4-C3
3	C	401	A1H50	O18-C17-C4-O5
3	C	401	A1H50	C9-C8-O7-C6
3	C	401	A1H50	C22-C21-S19-O18
3	C	401	A1H50	C22-C21-S19-O26
3	E	401	A1H50	C22-C21-S19-O18
3	C	401	A1H50	O7-C8-C9-C10
3	A	401	A1H50	C22-C21-S19-O20
3	E	401	A1H50	C22-C21-S19-O26
3	C	401	A1H50	O7-C8-C9-N13
3	A	401	A1H50	C22-C21-S19-O18
3	E	401	A1H50	C17-O18-S19-O20
3	A	401	A1H50	C9-C8-O7-C6
3	C	401	A1H50	C22-C21-S19-O20
3	E	401	A1H50	O18-C17-C4-O5

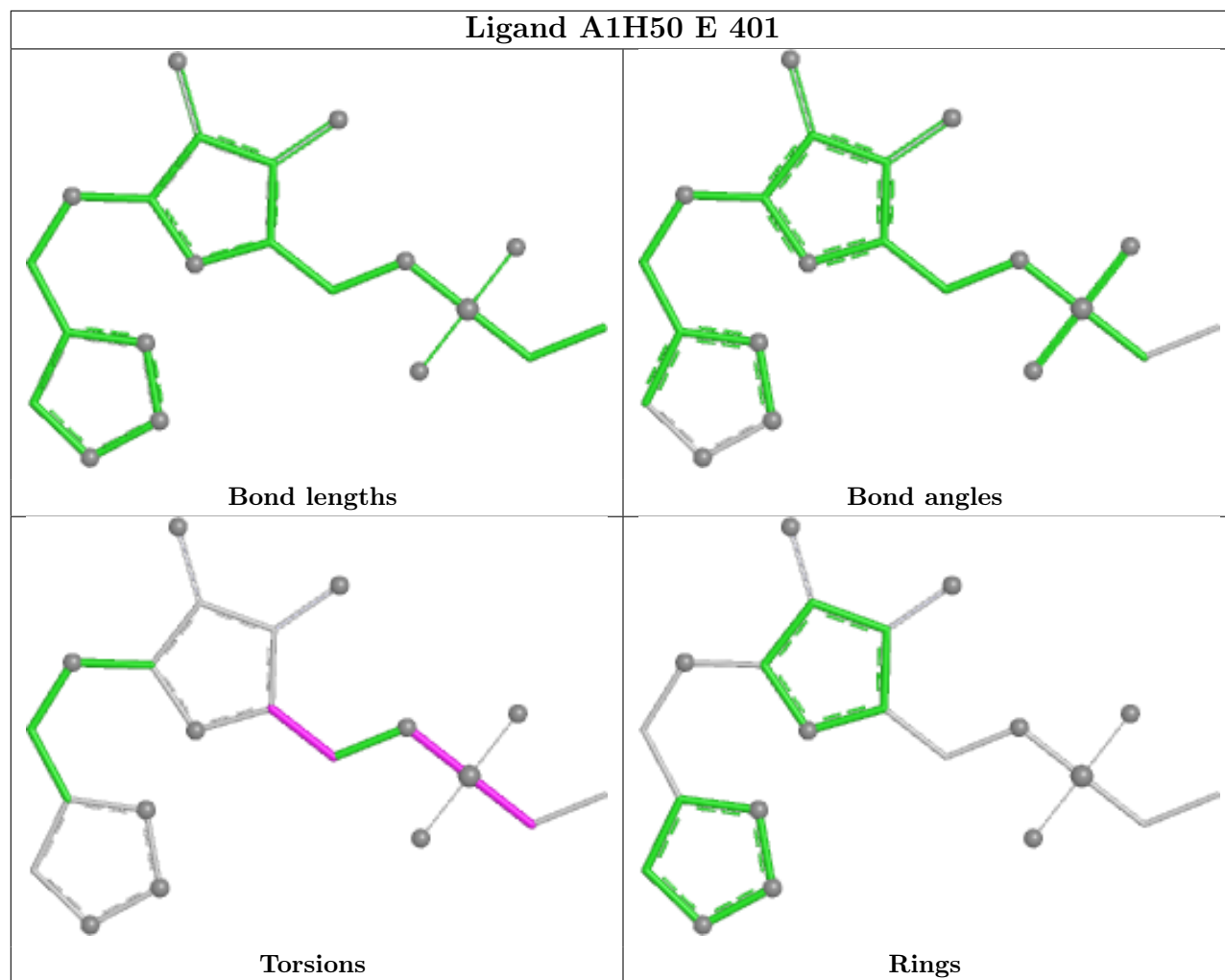
There are no ring outliers.

1 monomer is involved in 1 short contact:

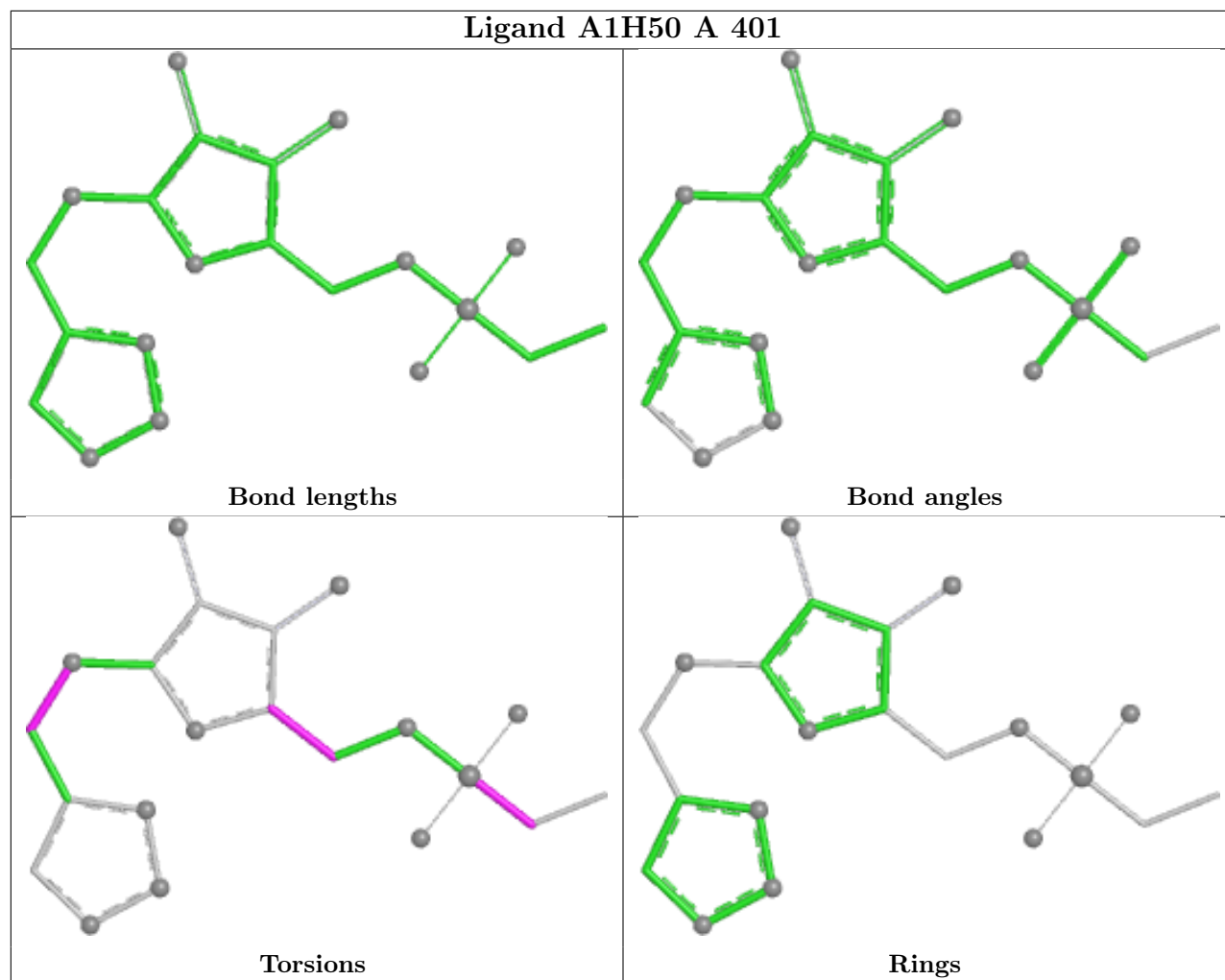
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	A1H50	1	0

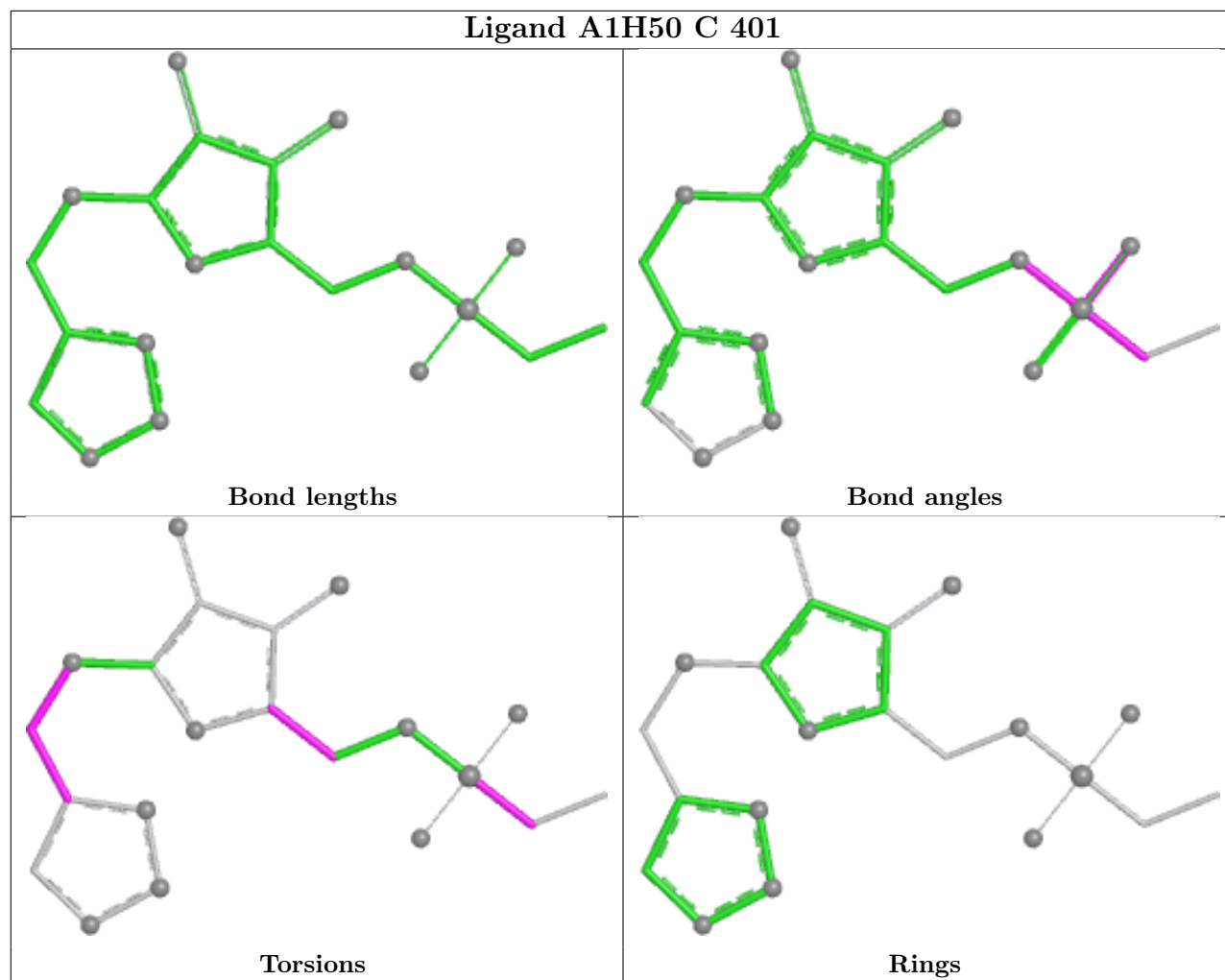
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand A1H50 E 401



Ligand A1H50 A 401





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	312/347 (89%)	-0.34	3 (0%) 79 79	29, 45, 80, 100	0
1	C	312/347 (89%)	-0.22	4 (1%) 75 75	34, 52, 87, 115	0
1	E	308/347 (88%)	-0.03	6 (1%) 66 65	33, 63, 101, 116	0
2	B	75/76 (98%)	1.12	12 (16%) 5 4	50, 112, 139, 152	2 (2%)
2	D	72/76 (94%)	1.52	19 (26%) 1 1	66, 122, 147, 163	0
2	F	72/76 (94%)	0.60	2 (2%) 55 54	63, 82, 107, 119	0
All	All	1151/1269 (90%)	0.05	46 (3%) 42 41	29, 58, 124, 163	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	73	LEU	7.7
2	F	73	LEU	5.7
2	B	17	VAL	4.3
2	D	4	PHE	3.5
2	D	61	ILE	3.5
1	E	3	SER	3.5
2	D	19	PRO	3.3
2	D	56	LEU	3.1
2	B	53	GLY	3.0
1	A	310	VAL	2.9
2	D	15	LEU	2.8
2	D	71	LEU	2.8
2	B	75	GLY	2.8
1	A	36	HIS	2.7
2	B	59	TYR	2.7
2	B	47	GLY	2.7
1	E	206	HIS	2.6
2	B	20	SER	2.6
2	B	74	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	302	ASP	2.5
1	E	256	GLY	2.5
2	D	23	ILE	2.5
2	D	59	TYR	2.4
1	E	310	VAL	2.4
2	B	46	ALA	2.4
2	D	43	LEU	2.4
2	B	76	GLY	2.4
2	D	50	LEU	2.4
2	D	26	VAL	2.3
2	D	17	VAL	2.3
1	C	0	ALA	2.3
2	D	28	ALA	2.3
2	D	53	GLY	2.3
2	B	61	ILE	2.2
1	C	1	MET	2.2
2	D	30	ILE	2.1
2	D	22	THR	2.1
2	D	52	ASP	2.1
1	A	40	TYR	2.1
2	F	72	ARG	2.1
2	D	75	GLY	2.1
1	C	57	ILE	2.1
1	C	311	LYS	2.0
1	E	210	VAL	2.0
2	B	4	PHE	2.0
2	D	12	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	ABA	D	42	6/7	0.69	0.15	100,116,120,129	0
2	ABA	B	42	6/7	0.88	0.11	66,90,95,97	0
2	ABA	F	42	6/7	0.92	0.12	62,74,92,95	0

6.3 Carbohydrates [i](#)

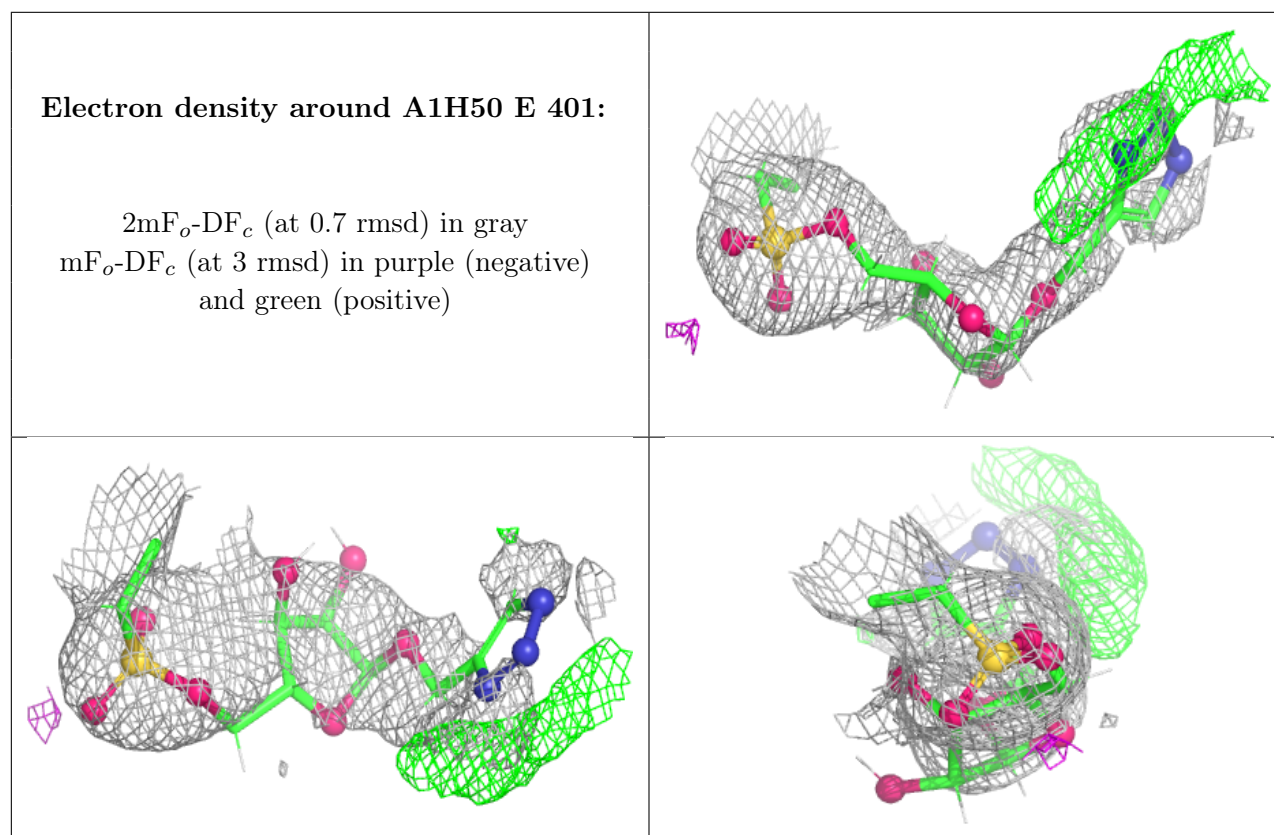
There are no oligosaccharides in this entry.

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.

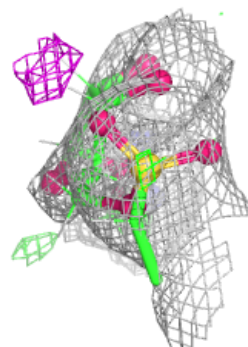
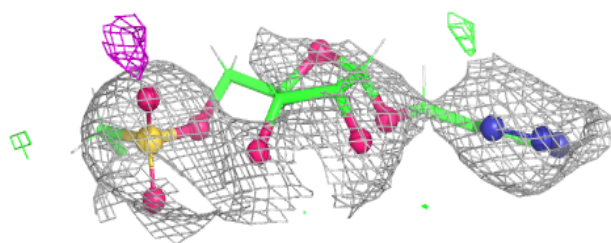
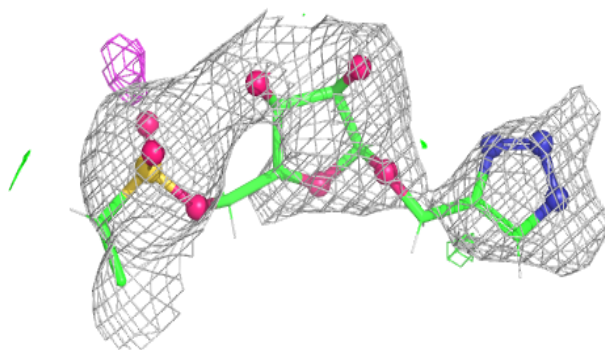
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	A1H50	E	401	21/21	0.78	0.15	30,118,138,147	2
3	A1H50	C	401	21/21	0.84	0.14	30,111,118,125	2
3	A1H50	A	401	21/21	0.86	0.12	30,110,127,132	2

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.

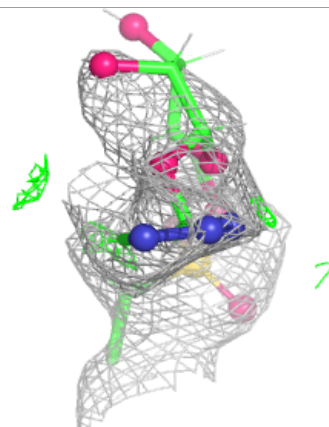
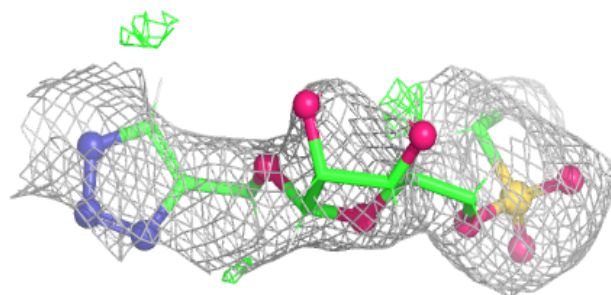
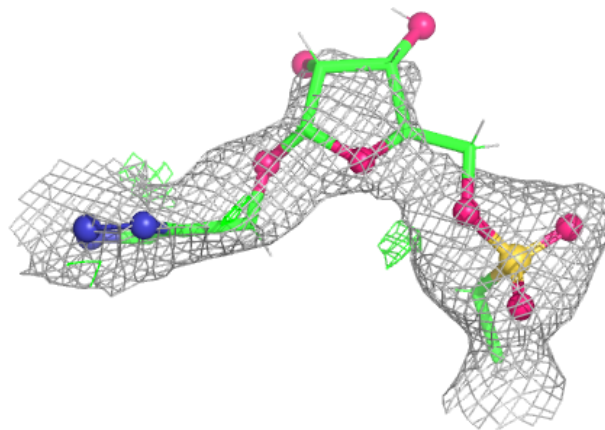


Electron density around A1H50 C 401:

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

**Electron density around A1H50 A 401:**

$2mF_o-DF_c$ (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.