



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:30 PM UTC

PDB ID : 7ESP / pdb_00007esp
Title : Structure and mutation analysis of the hexameric P4 from Pseudomonas aeruginosa phage phiYY
Authors : Zhang, C.Y.; Jin, T.C.
Deposited on : 2021-05-11
Resolution : 2.43 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

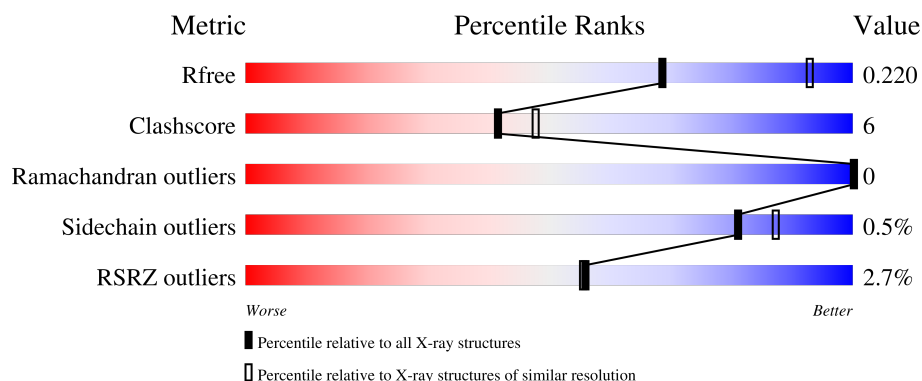
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	350	
1	B	350	
1	C	350	
1	D	350	
1	E	350	

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Mol	Chain	Length	Quality of chain
1	F	350	% 64% 9% 26%
1	G	350	3% 62% 13% 25%
1	H	350	2% 61% 12% 26%

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	TAR	F	401	-	X	X	-
2	TAR	H	401	-	-	X	-

2 Entry composition

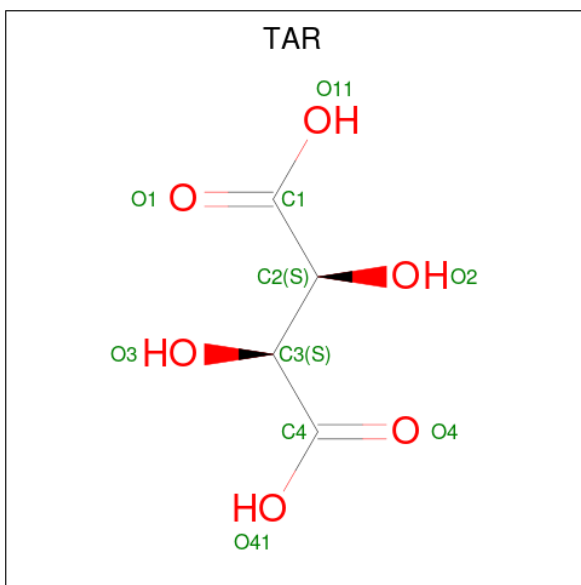
There are 4 unique types of molecules in this entry. The entry contains 15957 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Packaging NTPase.

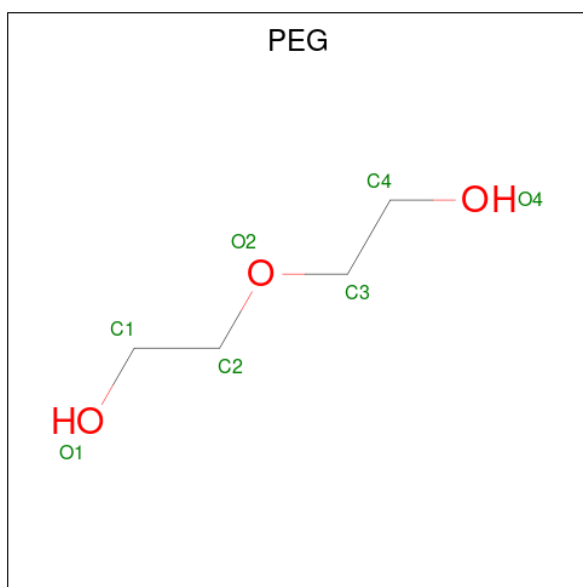
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			1968	1244	339	373	12			
1	B	260	Total	C	N	O	S	0	0	0
			1928	1217	332	367	12			
1	C	263	Total	C	N	O	S	0	0	0
			1951	1234	335	370	12			
1	D	259	Total	C	N	O	S	0	1	0
			1932	1222	332	366	12			
1	E	265	Total	C	N	O	S	0	0	0
			1964	1242	338	372	12			
1	F	258	Total	C	N	O	S	0	0	0
			1908	1206	326	364	12			
1	G	263	Total	C	N	O	S	0	0	0
			1949	1233	335	369	12			
1	H	258	Total	C	N	O	S	0	0	0
			1910	1207	327	364	12			

- Molecule 2 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		
2	C	1	Total	C	O	0	0
			10	4	6		
2	D	1	Total	C	O	0	0
			10	4	6		
2	E	1	Total	C	O	0	0
			10	4	6		
2	F	1	Total	C	O	0	0
			10	4	6		
2	G	1	Total	C	O	0	0
			10	4	6		
2	H	1	Total	C	O	0	0
			10	4	6		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			7	4	3		
3	D	1	Total	C	O	0	0
			7	4	3		
3	F	1	Total	C	O	0	0
			7	4	3		
3	H	1	Total	C	O	0	0
			7	4	3		

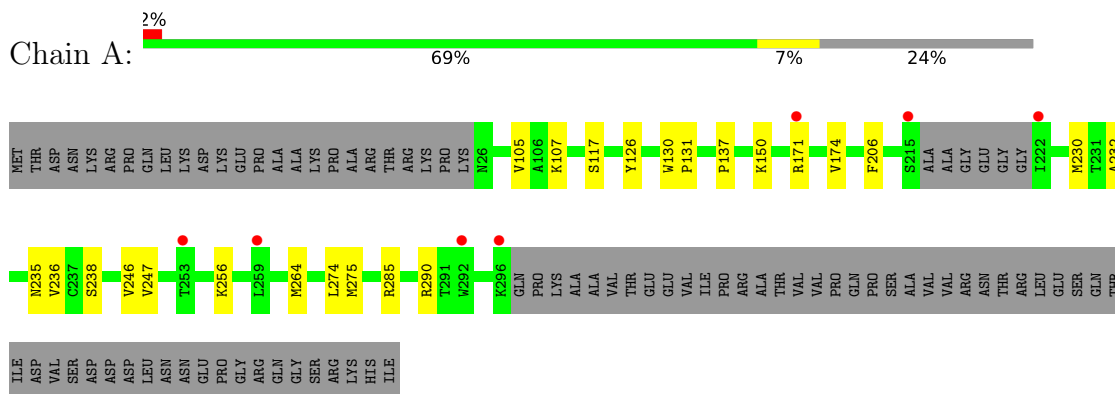
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	40	Total	O	0	0
			40	40		
4	C	34	Total	O	0	0
			34	34		
4	D	42	Total	O	0	0
			42	42		
4	E	56	Total	O	0	0
			56	56		
4	F	49	Total	O	0	0
			49	49		
4	G	24	Total	O	0	0
			24	24		
4	H	36	Total	O	0	0
			36	36		

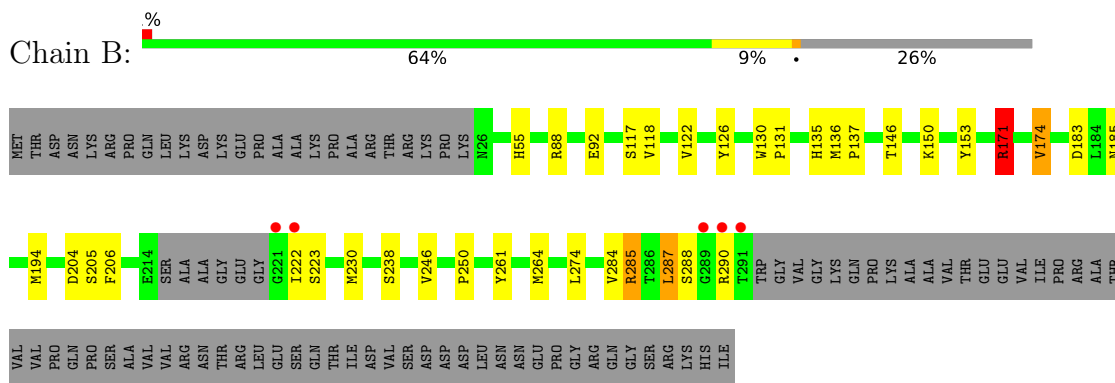
3 Residue-property plots [i](#)

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.

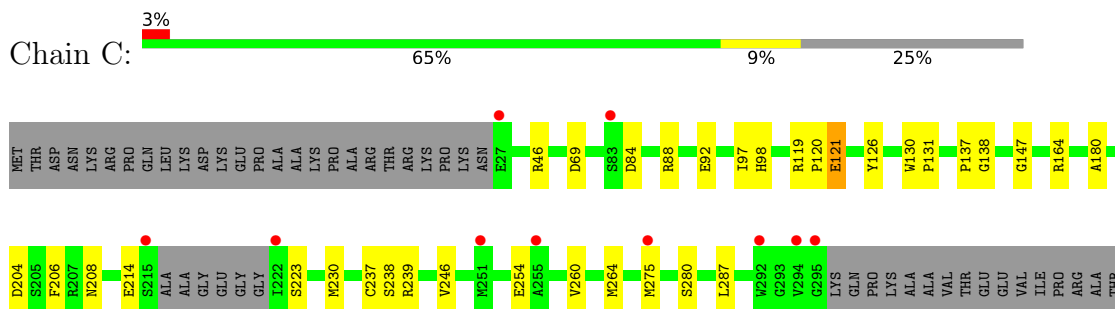
• Molecule 1: Packaging NTPase

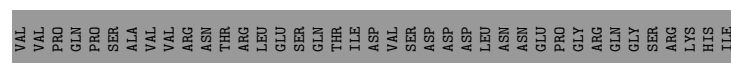


• Molecule 1: Packaging NTPase

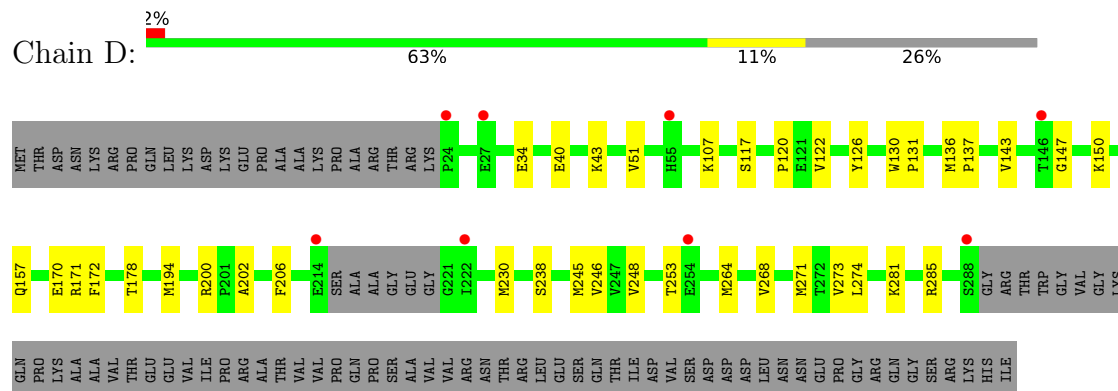


• Molecule 1: Packaging NTPase

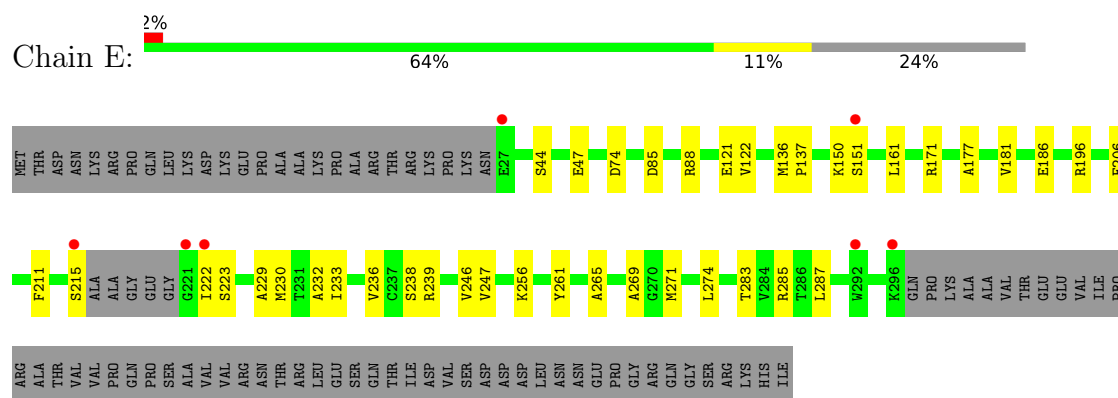




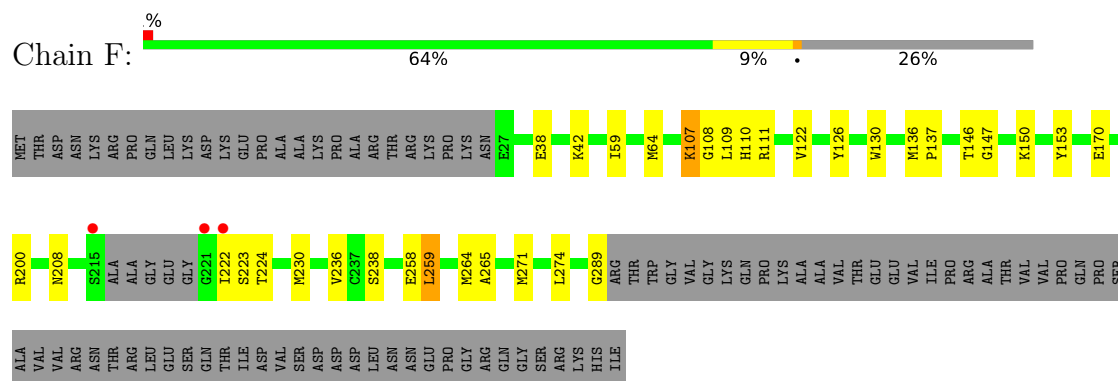
- Molecule 1: Packaging NTPase



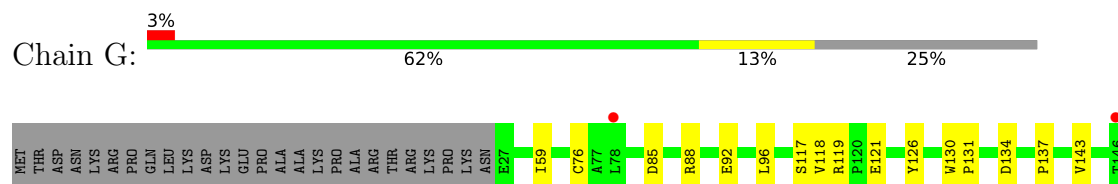
- Molecule 1: Packaging NTPase

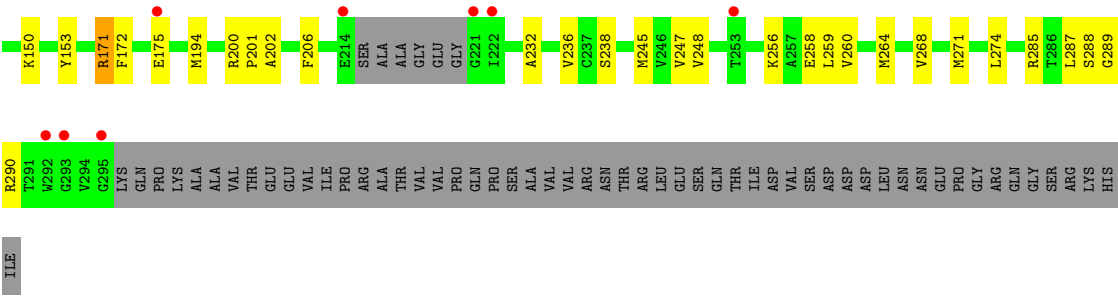


- Molecule 1: Packaging NTPase

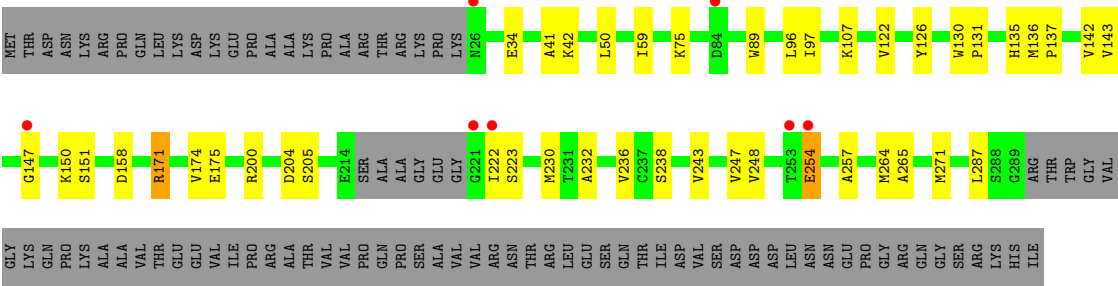


- Molecule 1: Packaging NTPase





● Molecule 1: Packaging NTPase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	240.13Å 240.13Å 152.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.97 – 2.43 40.97 – 2.43	Depositor EDS
% Data completeness (in resolution range)	97.8 (40.97-2.43) 97.8 (40.97-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.42Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.178 , 0.217 0.180 , 0.220	Depositor DCC
R_{free} test set	2004 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	56.6	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.012 for $-1/3^*h+1/3^*k+4/3^*l, -k, 2/3^*h+1/3^*k+1/3^*l$ 0.009 for $-2/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+4/3^*l, -1/3^*h+1/3^*k+1/3^*l$ 0.011 for $-h, 1/3^*h-1/3^*k-4/3^*l, -1/3^*h-2/3^*k+1/3^*l$ 0.064 for $-1/3^*h-2/3^*k+4/3^*l, -2/3^*h-1/3^*k-4/3^*l, 1/3^*h-1/3^*k-1/3^*l$ 0.043 for $-h, 2/3^*h+1/3^*k+4/3^*l, 1/3^*h+2/3^*k-1/3^*l$ 0.024 for $1/3^*h+2/3^*k-4/3^*l, -k, -2/3^*h-1/3^*k-1/3^*l$ 0.017 for $h, -h-k, -l$	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15957	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: PEG, TAR

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	0.47	0/2004	0.66	0/2730
1	B	0.62	4/1962 (0.2%)	0.67	2/2673 (0.1%)
1	C	0.47	3/1987 (0.2%)	0.61	1/2708 (0.0%)
1	D	0.51	0/1968	0.72	2/2681 (0.1%)
1	E	0.41	0/2000	0.64	0/2724
1	F	0.62	5/1942 (0.3%)	0.64	1/2646 (0.0%)
1	G	0.54	2/1985 (0.1%)	0.64	2/2705 (0.1%)
1	H	0.42	1/1944 (0.1%)	0.65	1/2649 (0.0%)
All	All	0.51	15/15792 (0.1%)	0.65	9/21516 (0.0%)

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	B	0	1
1	G	0	1
All	All	0	2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	108	GLY	C-O	-6.87	1.16	1.24
1	B	284	VAL	C-O	-6.84	1.17	1.24
1	B	174	VAL	N-CA	-6.56	1.40	1.46
1	B	285	ARG	C-O	-6.47	1.16	1.24
1	C	119	ARG	C-O	-6.05	1.16	1.24
1	F	111	ARG	C-O	-6.01	1.17	1.24
1	C	121	GLU	C-O	-5.88	1.16	1.23
1	F	109	LEU	C-O	-5.88	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	110	HIS	C-O	-5.70	1.17	1.24
1	C	120	PRO	C-O	-5.68	1.16	1.24
1	F	111	ARG	CZ-NH2	-5.39	1.26	1.33
1	G	172	PHE	C-O	-5.26	1.17	1.24
1	G	290	ARG	C-O	-5.09	1.17	1.24
1	B	285	ARG	CA-C	-5.07	1.46	1.52
1	H	171	ARG	CZ-NH1	5.05	1.39	1.32

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	253	THR	CA-C-N	-8.26	108.36	122.56
1	D	253	THR	C-N-CA	-8.26	108.36	122.56
1	C	254	GLU	CA-CB-CG	7.26	128.62	114.10
1	B	171	ARG	CD-NE-CZ	7.09	134.32	124.40
1	F	109	LEU	N-CA-C	6.60	118.47	111.28
1	G	171	ARG	NE-CZ-NH1	-6.19	115.31	121.50
1	H	254	GLU	CA-CB-CG	5.50	125.11	114.10
1	B	171	ARG	CB-CG-CD	5.47	123.87	111.30
1	G	289	GLY	N-CA-C	5.15	118.03	111.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	ARG	Sidechain
1	G	171	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	1968	0	1978	17	0
1	B	1928	0	1938	27	0
1	C	1951	0	1959	20	0
1	D	1932	0	1942	26	0
1	E	1964	0	1975	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1908	0	1917	27	0
1	G	1949	0	1957	27	1
1	H	1910	0	1918	38	1
2	A	10	0	4	1	0
2	B	10	0	4	1	0
2	C	10	0	4	1	0
2	D	10	0	4	2	0
2	E	10	0	4	1	0
2	F	10	0	4	4	0
2	G	10	0	4	0	0
2	H	10	0	4	6	0
3	B	7	0	10	1	0
3	D	7	0	10	1	0
3	F	7	0	10	0	0
3	H	7	0	10	0	0
4	A	58	0	0	0	0
4	B	40	0	0	1	0
4	C	34	0	0	0	0
4	D	42	0	0	2	0
4	E	56	0	0	0	0
4	F	49	0	0	0	0
4	G	24	0	0	0	0
4	H	36	0	0	0	0
All	All	15957	0	15656	200	1

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 6.

All (200) 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:H:147:GLY:H	2:H:401:TAR:H2	1.29	0.97
1:E:137:PRO:HB2	1:E:238:SER:HA	1.59	0.84
1:C:230:MET:HE1	1:C:264:MET:HG2	1.62	0.80
1:H:230:MET:HE1	1:H:264:MET:HG2	1.65	0.78
1:G:143:VAL:HG21	1:G:271:MET:HE2	1.64	0.78
1:C:121:GLU:HG2	1:C:239:ARG:HG2	1.65	0.76
1:D:143:VAL:HG21	1:D:271:MET:HE2	1.68	0.76
1:F:147:GLY:H	2:F:401:TAR:H3	1.54	0.72
1:G:150:LYS:HD3	1:G:247:VAL:HG13	1.72	0.72
1:E:181:VAL:HB	1:E:186:GLU:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:401:TAR:O2	2:H:401:TAR:O4	2.03	0.70
1:E:150:LYS:HD2	1:E:247:VAL:HG13	1.76	0.68
1:G:248:VAL:HG11	1:G:264:MET:HE1	1.77	0.67
1:B:171:ARG:O	1:B:174:VAL:HG12	1.95	0.67
1:A:230:MET:HE1	1:A:264:MET:HG2	1.77	0.66
1:H:137:PRO:HB2	1:H:238:SER:HA	1.76	0.66
1:G:130:TRP:CE2	1:G:200:ARG:HD3	2.31	0.65
1:H:142:VAL:HG12	1:H:150:LYS:HG2	1.78	0.65
1:G:256:LYS:HA	1:G:256:LYS:HE2	1.79	0.64
1:C:137:PRO:HB2	1:C:238:SER:HA	1.80	0.64
1:D:273:VAL:CG1	1:D:281:LYS:HB3	2.29	0.63
1:H:222:ILE:HG13	1:H:223:SER:H	1.62	0.63
1:G:194:MET:HE2	1:G:201:PRO:HB3	1.80	0.63
1:B:171:ARG:O	1:B:174:VAL:CG1	2.48	0.62
1:D:273:VAL:HG12	1:D:281:LYS:HB3	1.82	0.61
1:C:214:GLU:HA	1:C:223:SER:HB2	1.83	0.61
1:A:150:LYS:NZ	2:A:401:TAR:O2	2.28	0.61
1:H:151:SER:HB3	2:H:401:TAR:O41	2.00	0.61
1:E:85:ASP:HB3	1:E:88:ARG:HB3	1.82	0.61
1:H:89:TRP:HZ3	1:H:97:ILE:HD11	1.67	0.60
1:D:137:PRO:HB2	1:D:238:SER:HA	1.84	0.59
1:F:259:LEU:O	1:F:259:LEU:HD22	2.02	0.59
1:B:131:PRO:HD2	1:B:135:HIS:CD2	2.36	0.59
1:B:250:PRO:HG3	1:B:261:TYR:HE1	1.68	0.59
1:C:260:VAL:HG12	1:C:264:MET:HE2	1.83	0.59
1:D:268:VAL:O	1:D:285:ARG:NH1	2.35	0.58
1:B:230:MET:HE1	1:B:264:MET:HG2	1.86	0.58
1:D:130:TRP:CE2	1:D:200:ARG:HD3	2.38	0.58
1:G:268:VAL:O	1:G:285:ARG:NH2	2.35	0.58
1:G:153:TYR:HB2	1:G:274:LEU:HD11	1.85	0.58
1:F:230:MET:HE1	1:F:264:MET:HG2	1.86	0.57
1:F:122:VAL:HG21	1:F:136:MET:HE1	1.86	0.57
1:B:88:ARG:O	1:B:92:GLU:HG3	2.05	0.56
1:E:136:MET:HE3	1:E:137:PRO:HD2	1.85	0.56
1:H:34:GLU:OE1	1:H:107:LYS:HD2	2.05	0.56
1:D:172:PHE:CE2	1:D:178:THR:HG22	2.40	0.55
1:F:59:ILE:HG12	1:F:236:VAL:HG21	1.88	0.55
1:H:143:VAL:HG12	1:H:248:VAL:HG13	1.89	0.55
1:H:147:GLY:N	2:H:401:TAR:H2	2.12	0.55
1:H:150:LYS:N	2:H:401:TAR:O4	2.38	0.55
1:H:222:ILE:HG13	1:H:223:SER:N	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:ARG:NH1	1:C:204:ASP:OD2	2.41	0.54
1:B:171:ARG:HD2	1:C:287:LEU:O	2.08	0.54
1:A:290:ARG:NH2	1:F:170:GLU:OE1	2.42	0.53
1:D:126:TYR:CE2	1:D:137:PRO:HD3	2.44	0.53
2:F:401:TAR:O11	2:F:401:TAR:O3	2.22	0.53
1:G:143:VAL:HG11	1:G:271:MET:HE3	1.91	0.53
1:A:290:ARG:HH21	1:F:170:GLU:CD	2.17	0.53
1:G:85:ASP:HB3	1:G:88:ARG:HB3	1.92	0.52
2:D:401:TAR:O1	2:D:401:TAR:O3	2.24	0.52
1:F:153:TYR:HB2	1:F:274:LEU:HD21	1.92	0.52
1:H:205:SER:HB3	1:H:247:VAL:HG23	1.93	0.51
1:D:194:MET:HE1	3:D:402:PEG:H32	1.92	0.51
1:A:206:PHE:CD2	1:A:246:VAL:HG11	2.46	0.50
1:B:126:TYR:CE1	1:B:137:PRO:HD3	2.46	0.50
1:D:40:GLU:HA	1:D:43:LYS:HE2	1.94	0.50
1:D:150:LYS:HA	1:D:274:LEU:HD12	1.94	0.50
1:B:222:ILE:HG13	1:B:223:SER:H	1.76	0.50
1:A:150:LYS:HD2	1:A:247:VAL:HG13	1.94	0.49
1:E:151:SER:H	2:E:401:TAR:H2	1.77	0.49
1:B:122:VAL:HG21	1:B:136:MET:HE1	1.93	0.49
1:D:172:PHE:CE2	1:D:178:THR:CG2	2.95	0.49
1:E:215:SER:HB3	1:E:223:SER:OG	2.13	0.49
1:H:204:ASP:HA	1:H:247:VAL:HG22	1.95	0.49
1:B:194:MET:HE1	3:B:402:PEG:H21	1.93	0.49
1:D:157:GLN:HG3	1:D:245:MET:HE1	1.94	0.49
1:G:119:ARG:NE	1:G:121:GLU:OE2	2.38	0.49
1:F:136:MET:HE3	1:F:137:PRO:HD2	1.94	0.49
1:C:130:TRP:CD1	1:C:131:PRO:HA	2.47	0.49
1:C:275:MET:HG3	1:C:280:SER:HB2	1.95	0.49
1:F:137:PRO:HB2	1:F:238:SER:HA	1.95	0.48
1:B:137:PRO:HB2	1:B:238:SER:HA	1.94	0.48
1:B:285:ARG:HA	1:B:290:ARG:HA	1.94	0.48
1:A:290:ARG:NH2	1:F:170:GLU:CD	2.71	0.48
1:H:131:PRO:HD2	1:H:135:HIS:CD2	2.49	0.48
1:C:126:TYR:CE2	1:C:137:PRO:HD3	2.48	0.48
1:A:232:ALA:O	1:A:236:VAL:HG23	2.14	0.47
1:C:84:ASP:OD1	1:C:84:ASP:N	2.44	0.47
1:F:107:LYS:HD3	1:F:107:LYS:HA	1.50	0.47
1:F:150:LYS:HA	1:F:274:LEU:HD22	1.94	0.47
1:D:147:GLY:H	2:D:401:TAR:H3	1.79	0.47
1:D:206:PHE:HB2	1:D:248:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:ILE:HG12	1:G:236:VAL:HG21	1.95	0.47
1:F:38:GLU:O	1:F:42:LYS:HG3	2.14	0.47
1:H:174:VAL:HG13	1:H:175:GLU:HG3	1.97	0.47
1:B:55:HIS:HB3	4:B:504:HOH:O	2.13	0.47
1:E:44:SER:OG	1:E:47:GLU:HG3	2.13	0.47
1:F:265:ALA:HB2	1:F:271:MET:HE2	1.97	0.47
1:D:122:VAL:HG21	1:D:136:MET:HE1	1.96	0.47
1:G:232:ALA:O	1:G:236:VAL:HG23	2.15	0.47
1:B:146:THR:HA	2:B:401:TAR:O41	2.15	0.47
1:B:174:VAL:O	1:B:174:VAL:HG22	2.15	0.47
1:H:130:TRP:CG	1:H:131:PRO:HA	2.49	0.46
1:D:34:GLU:OE2	1:D:107:LYS:HD3	2.15	0.46
1:H:150:LYS:HE2	2:H:401:TAR:O2	2.15	0.46
1:B:183:ASP:OD2	1:B:185:ASN:HB2	2.15	0.46
1:C:138:GLY:HA2	1:C:237:CYS:HB2	1.97	0.46
1:H:254:GLU:OE1	1:H:257:ALA:HB3	2.16	0.46
1:E:229:ALA:O	1:E:233:ILE:HG13	2.16	0.46
1:A:126:TYR:CE2	1:A:137:PRO:HD3	2.50	0.46
1:E:230:MET:HE3	1:E:230:MET:HB2	1.80	0.45
1:G:150:LYS:HD3	1:G:247:VAL:CG1	2.44	0.45
1:D:206:PHE:CD2	1:D:246:VAL:HG11	2.51	0.45
1:F:222:ILE:HG13	1:F:223:SER:N	2.30	0.45
1:F:259:LEU:HD23	1:F:259:LEU:HA	1.80	0.45
2:F:401:TAR:O4	2:F:401:TAR:O2	2.32	0.45
1:H:222:ILE:CG1	1:H:223:SER:H	2.29	0.45
1:B:55:HIS:CD2	1:B:55:HIS:H	2.34	0.45
1:H:265:ALA:HB2	1:H:271:MET:HE2	1.97	0.45
1:E:206:PHE:CD2	1:E:246:VAL:HG11	2.51	0.45
1:C:208:ASN:ND2	1:D:117:SER:HB2	2.32	0.45
1:G:134:ASP:HB3	1:G:287:LEU:HB2	1.99	0.45
1:D:171:ARG:HG3	1:E:287:LEU:O	2.17	0.45
1:E:269:ALA:O	1:E:285:ARG:HD2	2.17	0.45
1:E:122:VAL:HG22	1:E:137:PRO:HG2	1.99	0.45
1:C:46:ARG:NH2	1:C:69:ASP:OD2	2.44	0.45
1:E:261:TYR:O	1:E:271:MET:HE1	2.16	0.45
1:H:130:TRP:CD1	1:H:131:PRO:HA	2.52	0.45
1:F:259:LEU:HD22	1:F:259:LEU:C	2.42	0.44
1:A:117:SER:HB2	1:F:208:ASN:HD21	1.82	0.44
1:H:158:ASP:HB3	1:H:200:ARG:NH1	2.32	0.44
1:H:131:PRO:HD3	1:H:243:VAL:HG11	1.98	0.44
1:C:180:ALA:HB1	1:D:120:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:126:TYR:CE2	1:H:137:PRO:HD3	2.52	0.44
1:G:206:PHE:HB2	1:G:248:VAL:HG22	1.98	0.44
1:H:89:TRP:CZ3	1:H:97:ILE:HD11	2.50	0.44
1:H:265:ALA:HB2	1:H:271:MET:CE	2.46	0.44
1:G:130:TRP:CD1	1:G:131:PRO:HA	2.53	0.44
1:G:85:ASP:HB3	1:G:88:ARG:CB	2.47	0.44
1:A:275:MET:HB2	1:A:275:MET:HE3	1.71	0.43
1:B:153:TYR:HB2	1:B:274:LEU:HD11	2.00	0.43
1:B:171:ARG:O	1:B:171:ARG:HG3	2.17	0.43
1:H:171:ARG:O	1:H:174:VAL:HG12	2.17	0.43
1:E:222:ILE:HG13	1:E:223:SER:H	1.82	0.43
1:C:88:ARG:O	1:C:92:GLU:HG3	2.18	0.43
1:F:130:TRP:CE2	1:F:200:ARG:HD3	2.53	0.43
1:G:126:TYR:CE2	1:G:137:PRO:HD3	2.53	0.43
1:F:265:ALA:HB2	1:F:271:MET:CE	2.48	0.43
1:H:158:ASP:HB3	1:H:200:ARG:HH11	1.83	0.43
1:F:146:THR:HA	2:F:401:TAR:H3	2.01	0.43
1:F:64:MET:HE3	1:F:64:MET:HB2	1.86	0.43
1:D:130:TRP:CD1	1:D:131:PRO:HA	2.53	0.43
1:E:74:ASP:OD1	1:E:196:ARG:NH2	2.52	0.43
1:E:256:LYS:HA	1:E:256:LYS:HE2	2.00	0.43
1:G:260:VAL:O	1:G:264:MET:HG3	2.18	0.43
1:A:235:ASN:HA	1:A:238:SER:HB3	2.01	0.42
1:E:232:ALA:O	1:E:236:VAL:HG23	2.19	0.42
1:G:76:CYS:SG	1:G:96:LEU:HD13	2.59	0.42
1:G:117:SER:OG	1:G:118:VAL:N	2.52	0.42
1:B:117:SER:OG	1:B:118:VAL:N	2.51	0.42
1:D:230:MET:HE1	1:D:264:MET:HG2	2.01	0.42
1:H:42:LYS:HB3	1:H:42:LYS:HE2	1.71	0.42
1:E:211:PHE:CD1	1:F:224:THR:HB	2.55	0.42
1:G:137:PRO:HB2	1:G:238:SER:HA	2.02	0.42
1:E:150:LYS:HA	1:E:274:LEU:HD12	2.00	0.42
1:F:126:TYR:CE2	1:F:137:PRO:HD3	2.54	0.42
1:B:150:LYS:HE2	1:B:150:LYS:HB2	1.72	0.42
1:C:97:ILE:HG13	1:C:98:HIS:N	2.35	0.42
1:G:92:GLU:N	1:G:92:GLU:OE1	2.53	0.42
1:D:51:VAL:HG13	4:D:537:HOH:O	2.20	0.41
1:E:265:ALA:HB1	1:E:283:THR:HG21	2.02	0.41
1:G:258:GLU:HG3	1:G:259:LEU:N	2.35	0.41
1:H:287:LEU:HD23	1:H:287:LEU:HA	1.69	0.41
1:B:150:LYS:HA	1:B:274:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:122:VAL:HG21	1:H:136:MET:HE1	2.01	0.41
1:B:287:LEU:HD13	1:B:287:LEU:HA	1.73	0.41
1:A:274:LEU:HA	1:A:274:LEU:HD23	1.81	0.41
1:D:202:ALA:HA	1:D:245:MET:O	2.21	0.41
1:H:130:TRP:CD2	1:H:200:ARG:HD2	2.55	0.41
1:A:256:LYS:HA	1:A:256:LYS:HE2	2.02	0.41
1:H:75:LYS:HE3	1:H:96:LEU:HD21	2.02	0.41
1:A:130:TRP:CD1	1:A:131:PRO:HA	2.55	0.41
1:E:161:LEU:HD12	1:E:177:ALA:C	2.46	0.41
1:B:206:PHE:CD2	1:B:246:VAL:HG11	2.56	0.41
1:C:147:GLY:HA2	2:C:401:TAR:H3	2.02	0.41
1:C:275:MET:HE2	1:C:275:MET:HB2	2.00	0.41
1:G:202:ALA:HA	1:G:245:MET:O	2.21	0.41
1:G:287:LEU:HA	1:G:287:LEU:HD23	1.87	0.41
1:H:232:ALA:O	1:H:236:VAL:HG23	2.21	0.41
1:C:206:PHE:CD2	1:C:246:VAL:HG11	2.56	0.41
1:D:170:GLU:HG3	4:D:501:HOH:O	2.20	0.41
1:E:121:GLU:HG2	1:E:239:ARG:HG2	2.01	0.41
1:H:59:ILE:HG12	1:H:236:VAL:HG21	2.03	0.41
1:A:285:ARG:HD3	1:F:170:GLU:HG2	2.02	0.40
1:B:130:TRP:CD1	1:B:131:PRO:HA	2.56	0.40
1:B:204:ASP:OD1	1:B:205:SER:HB3	2.22	0.40
1:A:105:VAL:O	1:A:107:LYS:NZ	2.48	0.40
1:E:171:ARG:HD3	1:F:289:GLY:HA3	2.03	0.40
1:H:41:ALA:HB1	1:H:50:LEU:HD12	2.03	0.40
1:H:205:SER:CB	1:H:247:VAL:HG23	2.52	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:SER:CA	1:H:171:ARG:NH2[2_655]	2.05	0.15

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	261/350 (75%)	252 (97%)	9 (3%)	0	100	100
1	B	256/350 (73%)	248 (97%)	8 (3%)	0	100	100
1	C	259/350 (74%)	249 (96%)	10 (4%)	0	100	100
1	D	256/350 (73%)	246 (96%)	10 (4%)	0	100	100
1	E	261/350 (75%)	252 (97%)	9 (3%)	0	100	100
1	F	254/350 (73%)	247 (97%)	7 (3%)	0	100	100
1	G	259/350 (74%)	248 (96%)	11 (4%)	0	100	100
1	H	254/350 (73%)	244 (96%)	10 (4%)	0	100	100
All	All	2060/2800 (74%)	1986 (96%)	74 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/278 (74%)	205 (99%)	2 (1%)	68	77
1	B	203/278 (73%)	201 (99%)	2 (1%)	68	77
1	C	205/278 (74%)	205 (100%)	0	100	100
1	D	204/278 (73%)	204 (100%)	0	100	100
1	E	206/278 (74%)	206 (100%)	0	100	100
1	F	201/278 (72%)	198 (98%)	3 (2%)	57	69
1	G	204/278 (73%)	203 (100%)	1 (0%)	81	87
1	H	201/278 (72%)	201 (100%)	0	100	100
All	All	1631/2224 (73%)	1623 (100%)	8 (0%)	81	87

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	ARG
1	A	174	VAL
1	B	287	LEU
1	B	288	SER
1	F	107	LYS
1	F	258	GLU
1	F	259	LEU
1	G	175	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	C	93	ASN
1	C	98	HIS
1	C	133	GLN
1	C	282	GLN
1	F	133	GLN
1	G	133	GLN
1	G	282	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](#)

12 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	TAR	E	401	-	9,9,9	1.17	0	12,12,12	1.97	4 (33%)
3	PEG	D	402	-	6,6,6	0.50	0	5,5,5	0.44	0
3	PEG	H	402	-	6,6,6	0.49	0	5,5,5	0.39	0
2	TAR	B	401	-	9,9,9	1.29	0	12,12,12	1.67	2 (16%)
3	PEG	B	402	-	6,6,6	0.51	0	5,5,5	0.55	0
2	TAR	C	401	-	9,9,9	1.09	0	12,12,12	1.62	2 (16%)
2	TAR	H	401	-	9,9,9	1.04	0	12,12,12	1.64	2 (16%)
2	TAR	A	401	-	9,9,9	1.34	1 (11%)	12,12,12	1.74	4 (33%)
2	TAR	F	401	-	9,9,9	1.13	0	12,12,12	1.83	5 (41%)
2	TAR	G	401	-	9,9,9	1.15	0	12,12,12	1.38	3 (25%)
3	PEG	F	402	-	6,6,6	0.48	0	5,5,5	0.32	0
2	TAR	D	401	-	9,9,9	1.02	0	12,12,12	1.92	4 (33%)

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	TAR	E	401	-	-	4/12/12/12	-
3	PEG	D	402	-	-	1/4/4/4	-
3	PEG	H	402	-	-	2/4/4/4	-
2	TAR	B	401	-	-	4/12/12/12	-
3	PEG	B	402	-	-	2/4/4/4	-
2	TAR	C	401	-	-	6/12/12/12	-
2	TAR	H	401	-	-	10/12/12/12	-
2	TAR	A	401	-	-	7/12/12/12	-
2	TAR	F	401	-	-	12/12/12/12	-
2	TAR	G	401	-	-	10/12/12/12	-
3	PEG	F	402	-	-	3/4/4/4	-
2	TAR	D	401	-	-	6/12/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	TAR	C3-C4	2.17	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	TAR	O2-C2-C3	-3.45	103.14	110.17
2	A	401	TAR	O2-C2-C1	-3.42	103.38	110.69
2	D	401	TAR	O41-C4-C3	3.42	122.82	113.31
2	B	401	TAR	O2-C2-C1	-3.36	103.51	110.69
2	E	401	TAR	C2-C3-C4	-3.19	102.74	109.82
2	F	401	TAR	O41-C4-C3	3.13	122.01	113.31
2	C	401	TAR	O11-C1-C2	3.03	121.72	113.31
2	F	401	TAR	O11-C1-C2	2.89	121.34	113.31
2	C	401	TAR	O41-C4-C3	2.87	121.28	113.31
2	G	401	TAR	O41-C4-C3	2.72	120.88	113.31
2	H	401	TAR	O41-C4-C3	2.68	120.77	113.31
2	D	401	TAR	O11-C1-C2	2.63	120.61	113.31
2	E	401	TAR	O11-C1-C2	2.56	120.44	113.31
2	H	401	TAR	O11-C1-C2	2.55	120.39	113.31
2	A	401	TAR	O41-C4-O4	-2.50	118.41	124.08
2	F	401	TAR	O2-C2-C1	-2.45	105.45	110.69
2	F	401	TAR	O41-C4-O4	-2.45	118.52	124.08
2	D	401	TAR	O3-C3-C2	-2.44	105.19	110.17
2	E	401	TAR	O41-C4-C3	2.43	120.08	113.31
2	A	401	TAR	C2-C3-C4	2.32	114.97	109.82
2	D	401	TAR	C3-C2-C1	-2.31	104.70	109.82
2	A	401	TAR	O41-C4-C3	2.28	119.65	113.31
2	G	401	TAR	O41-C4-O4	-2.26	118.95	124.08
2	F	401	TAR	O11-C1-O1	-2.19	119.11	124.08
2	G	401	TAR	O11-C1-C2	2.11	119.17	113.31
2	B	401	TAR	O41-C4-C3	2.09	119.13	113.31

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	TAR	O1-C1-C2-C3
2	D	401	TAR	O11-C1-C2-C3
2	F	401	TAR	C2-C3-C4-O41
2	H	401	TAR	C1-C2-C3-C4
2	H	401	TAR	O2-C2-C3-O3
2	F	401	TAR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
2	B	401	TAR	O1-C1-C2-O2
2	D	401	TAR	O1-C1-C2-O2
2	D	401	TAR	O11-C1-C2-O2
2	E	401	TAR	O1-C1-C2-O2
2	E	401	TAR	O11-C1-C2-O2
2	F	401	TAR	O1-C1-C2-O2
2	F	401	TAR	O11-C1-C2-O2
2	H	401	TAR	O1-C1-C2-O2
2	H	401	TAR	O11-C1-C2-O2
2	A	401	TAR	C2-C3-C4-O4
2	A	401	TAR	C2-C3-C4-O41
2	F	401	TAR	O1-C1-C2-C3
2	F	401	TAR	O11-C1-C2-C3
2	F	401	TAR	C2-C3-C4-O4
2	F	401	TAR	O2-C2-C3-C4
2	H	401	TAR	C1-C2-C3-O3
2	F	401	TAR	O2-C2-C3-O3
2	F	401	TAR	C1-C2-C3-O3
2	A	401	TAR	O3-C3-C4-O4
2	A	401	TAR	O3-C3-C4-O41
2	B	401	TAR	O11-C1-C2-O2
2	B	401	TAR	O3-C3-C4-O4
2	B	401	TAR	O3-C3-C4-O41
2	G	401	TAR	O1-C1-C2-O2
2	G	401	TAR	O11-C1-C2-O2
2	H	401	TAR	O2-C2-C3-C4
2	F	401	TAR	O3-C3-C4-O4
2	F	401	TAR	O3-C3-C4-O41
2	C	401	TAR	C2-C3-C4-O41
2	H	401	TAR	O11-C1-C2-C3
2	C	401	TAR	C2-C3-C4-O4
2	H	401	TAR	O1-C1-C2-C3
3	H	402	PEG	O2-C3-C4-O4
2	G	401	TAR	C2-C3-C4-O4
3	H	402	PEG	O1-C1-C2-O2
2	C	401	TAR	O1-C1-C2-C3
2	G	401	TAR	C2-C3-C4-O41
2	G	401	TAR	O2-C2-C3-O3
2	C	401	TAR	O11-C1-C2-C3
2	G	401	TAR	O2-C2-C3-C4
3	B	402	PEG	O1-C1-C2-O2
3	F	402	PEG	O2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
2	D	401	TAR	C2-C3-C4-O4
2	D	401	TAR	C2-C3-C4-O41
2	G	401	TAR	C1-C2-C3-O3
3	F	402	PEG	C1-C2-O2-C3
2	A	401	TAR	O11-C1-C2-C3
3	F	402	PEG	C4-C3-O2-C2
2	A	401	TAR	O1-C1-C2-C3
2	E	401	TAR	C2-C3-C4-O4
2	G	401	TAR	O3-C3-C4-O4
2	E	401	TAR	C2-C3-C4-O41
2	C	401	TAR	O3-C3-C4-O41
2	C	401	TAR	O3-C3-C4-O4
3	B	402	PEG	C4-C3-O2-C2
2	H	401	TAR	C2-C3-C4-O4
2	G	401	TAR	C1-C2-C3-C4
2	H	401	TAR	C2-C3-C4-O41
2	A	401	TAR	O1-C1-C2-O2
2	G	401	TAR	O3-C3-C4-O41
3	D	402	PEG	C1-C2-O2-C3

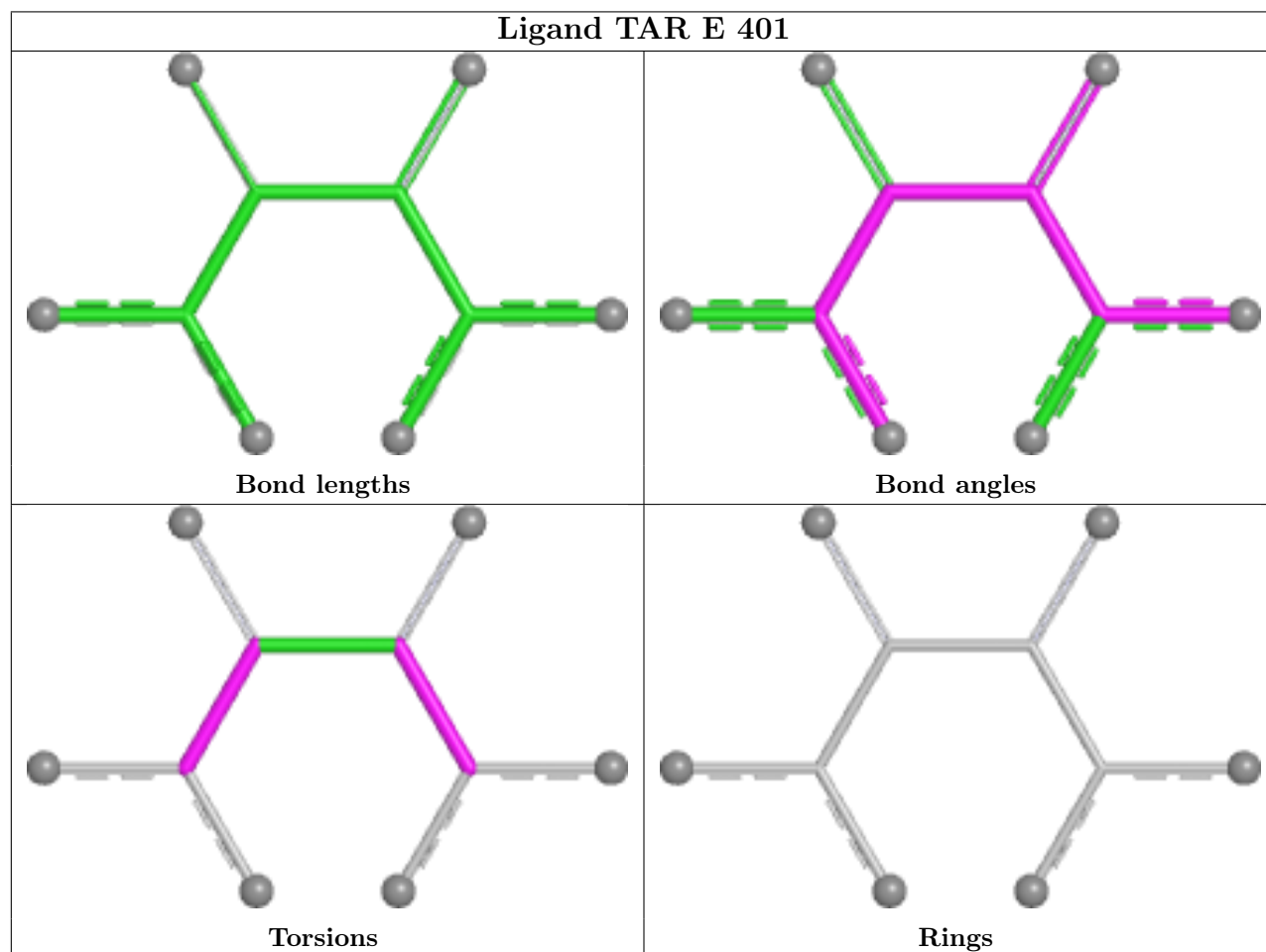
There are no ring outliers.

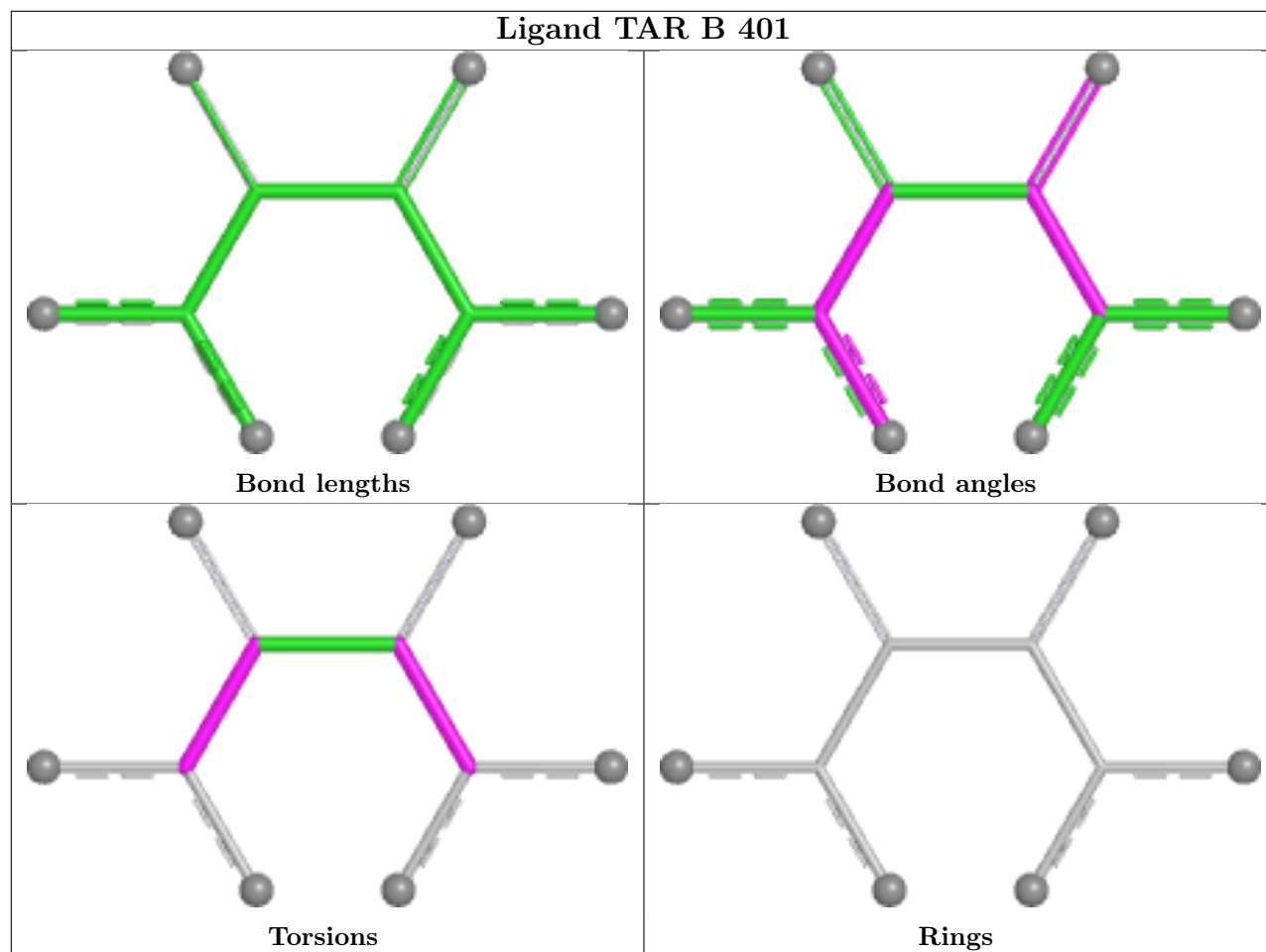
9 monomers are involved in 18 short contacts:

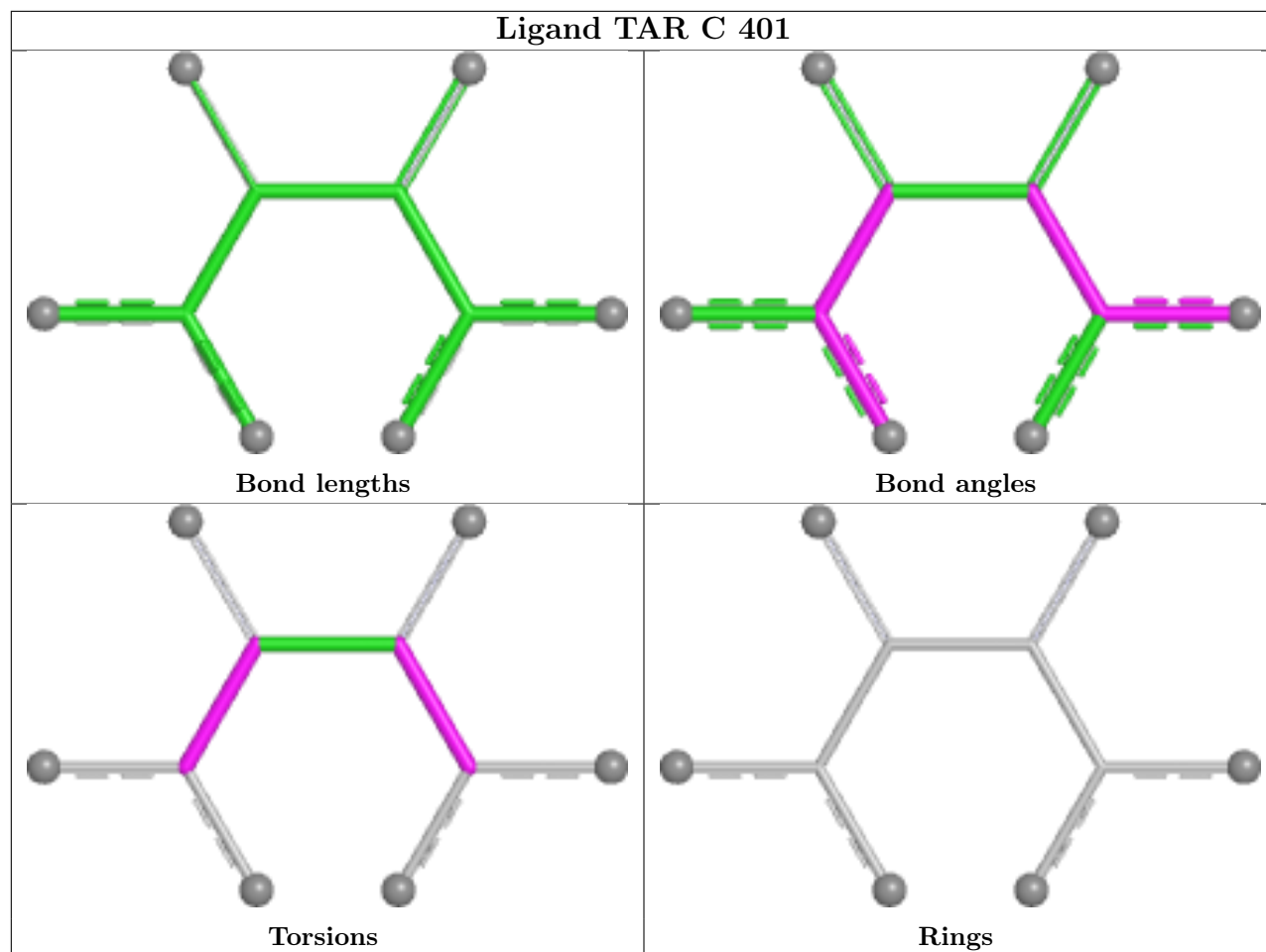
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	401	TAR	1	0
3	D	402	PEG	1	0
2	B	401	TAR	1	0
3	B	402	PEG	1	0
2	C	401	TAR	1	0
2	H	401	TAR	6	0
2	A	401	TAR	1	0
2	F	401	TAR	4	0
2	D	401	TAR	2	0

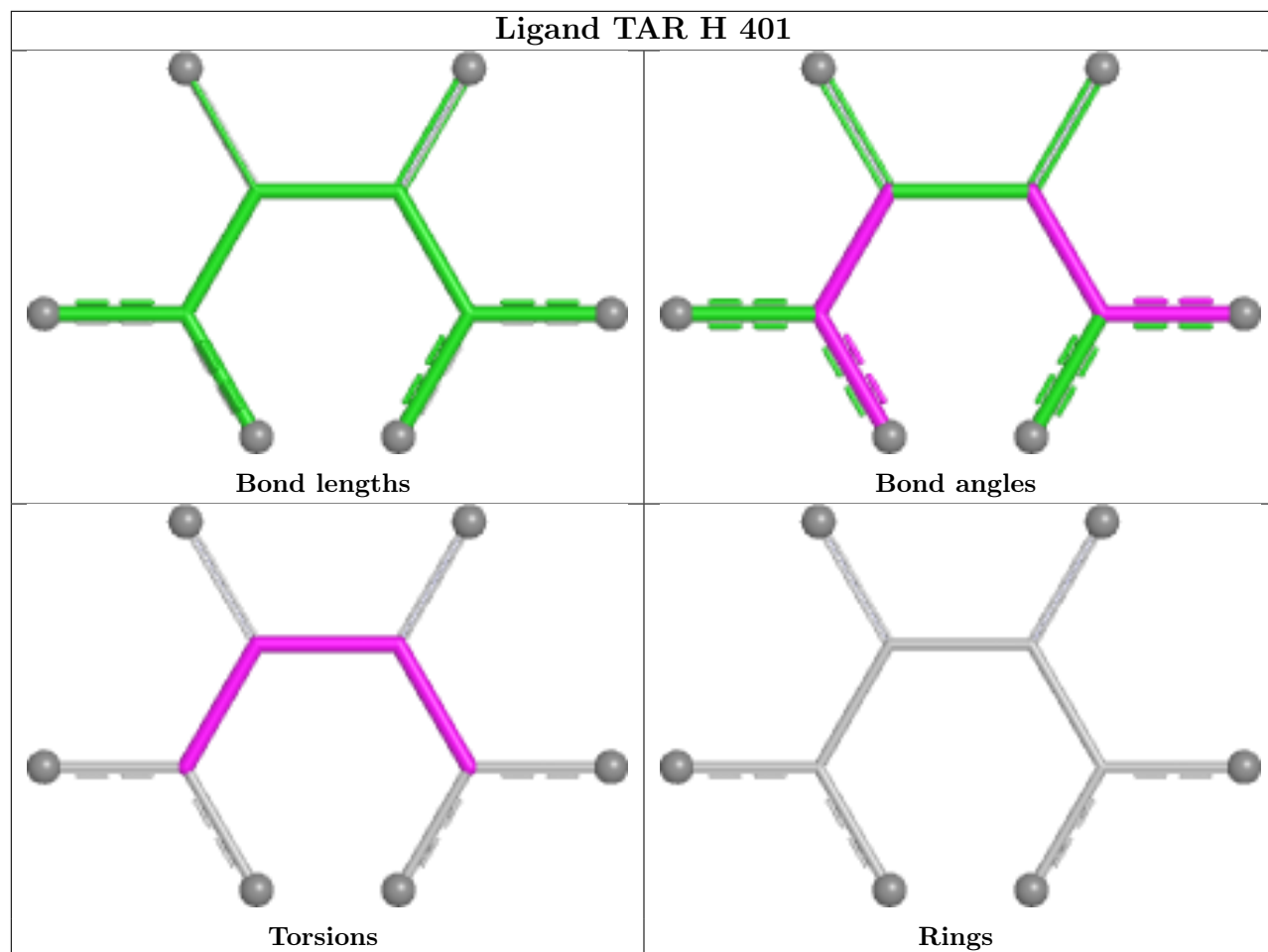
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

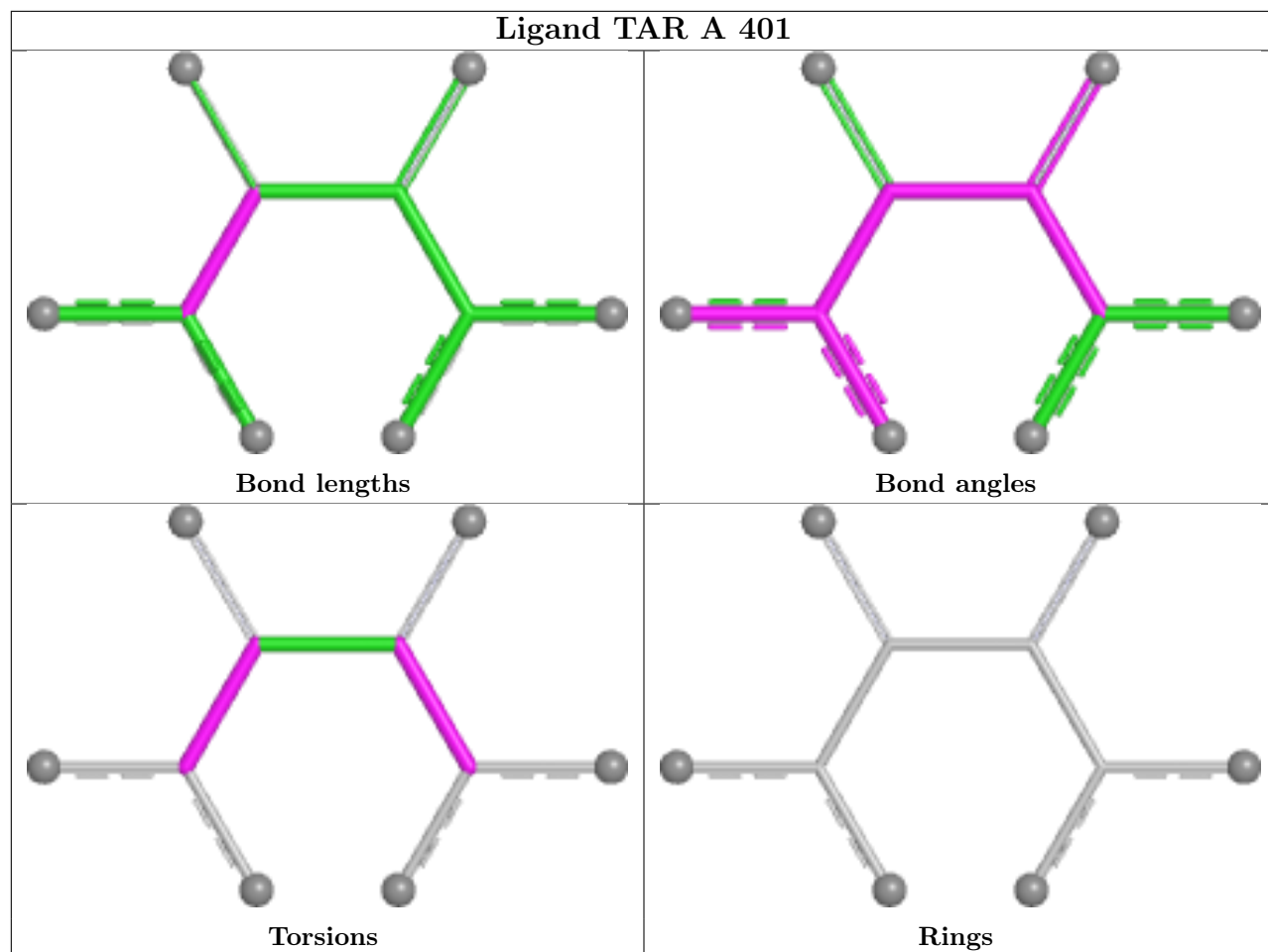
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

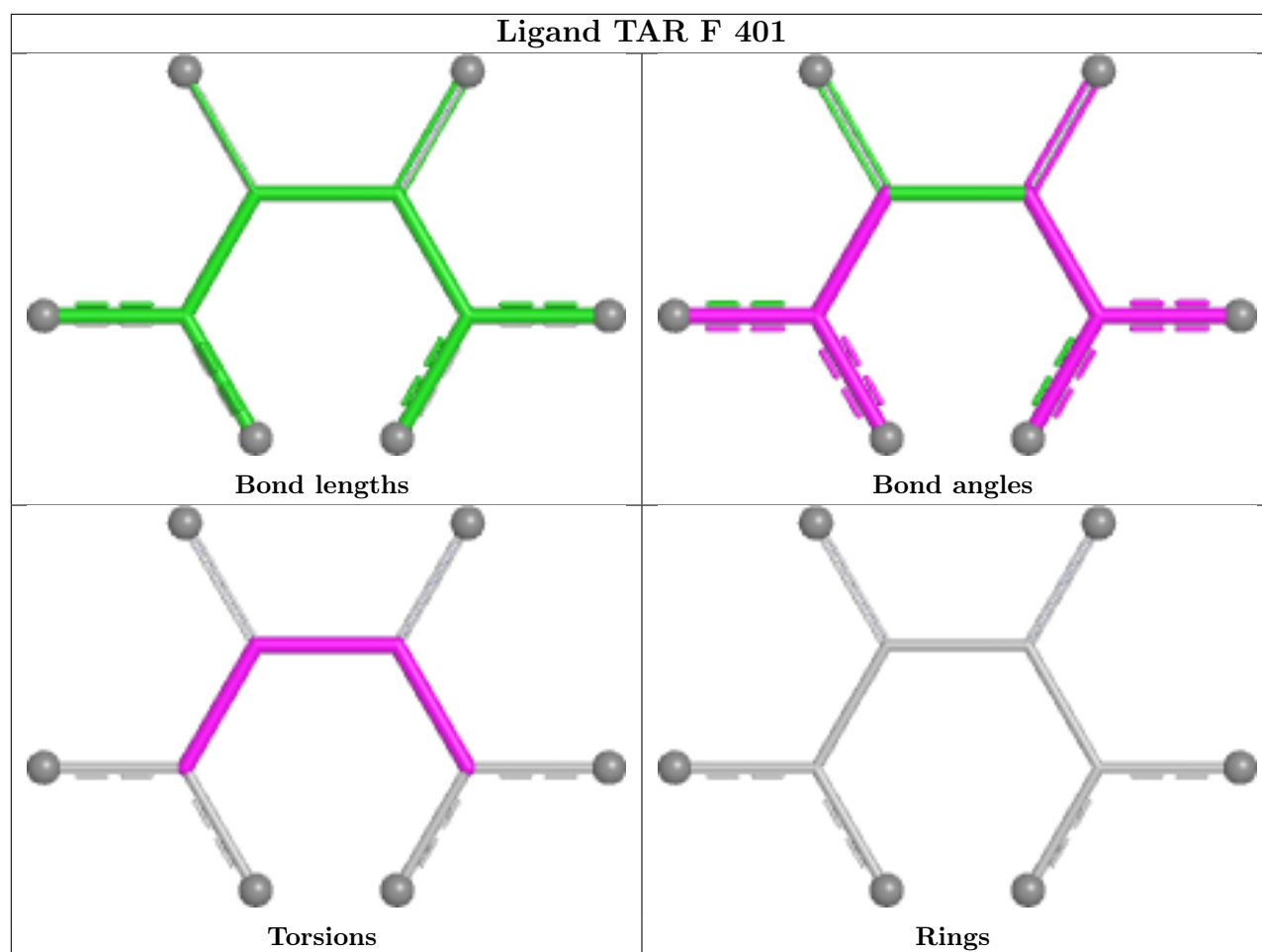


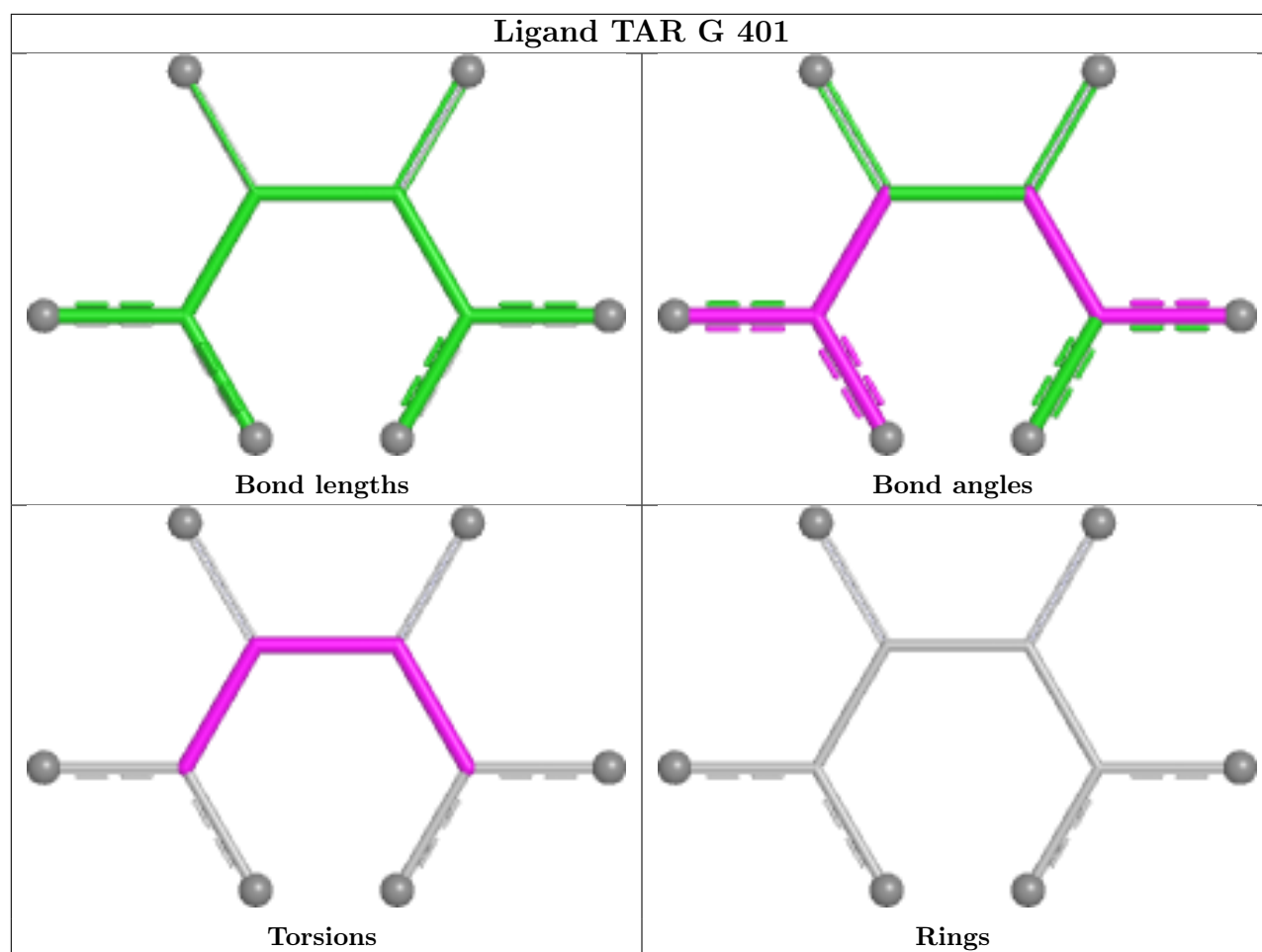


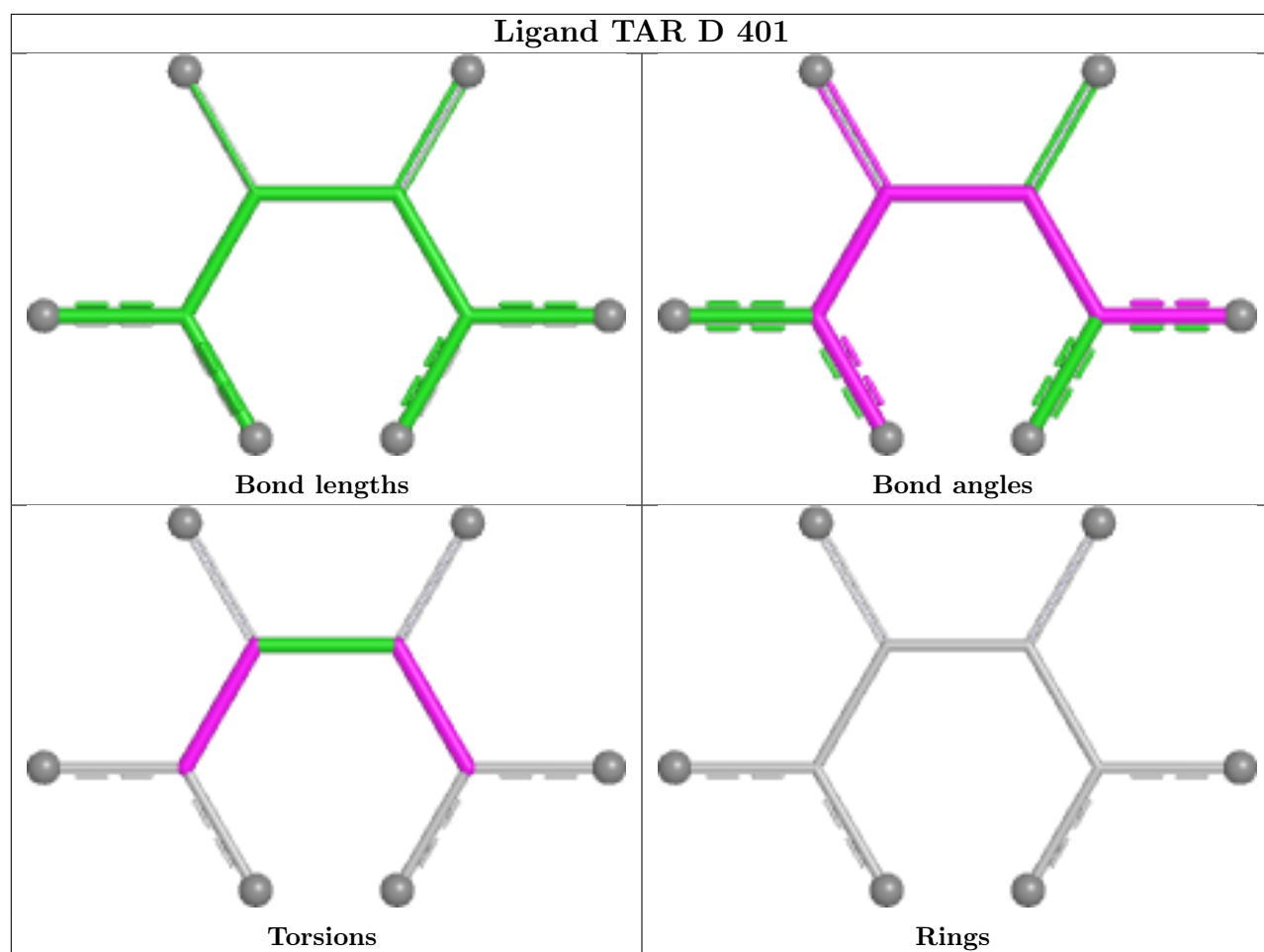












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	265/350 (75%)	-0.01	7 (2%) 57 57	42, 55, 81, 102	0
1	B	260/350 (74%)	0.03	5 (1%) 66 67	43, 58, 84, 102	0
1	C	263/350 (75%)	0.25	10 (3%) 44 42	47, 62, 91, 104	0
1	D	259/350 (74%)	0.07	8 (3%) 51 50	29, 56, 85, 100	1 (0%)
1	E	265/350 (75%)	0.03	7 (2%) 57 57	42, 55, 83, 99	0
1	F	258/350 (73%)	-0.01	3 (1%) 76 78	41, 55, 81, 97	0
1	G	263/350 (75%)	0.30	10 (3%) 44 42	46, 64, 91, 106	0
1	H	258/350 (73%)	0.16	7 (2%) 56 55	48, 60, 89, 101	0
All	All	2091/2800 (74%)	0.10	57 (2%) 56 55	29, 58, 87, 106	1 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	24	PRO	6.0
1	C	292	TRP	5.7
1	H	222	ILE	4.3
1	C	215	SER	4.1
1	C	295	GLY	4.0
1	C	294	VAL	4.0
1	G	292	TRP	3.8
1	E	221	GLY	3.8
1	C	222	ILE	3.7
1	G	221	GLY	3.3
1	E	222	ILE	3.2
1	B	289	GLY	3.2
1	E	215	SER	3.1
1	D	288	SER	3.1
1	D	55[A]	HIS	3.1
1	G	295	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	175	GLU	3.0
1	G	146	THR	3.0
1	A	259	LEU	3.0
1	A	296	LYS	2.9
1	B	222	ILE	2.9
1	E	296	LYS	2.9
1	D	222	ILE	2.9
1	B	290	ARG	2.9
1	A	292	TRP	2.8
1	D	27	GLU	2.8
1	G	222	ILE	2.8
1	G	253	THR	2.8
1	A	215	SER	2.8
1	G	214	GLU	2.7
1	E	27	GLU	2.7
1	H	26	ASN	2.6
1	A	171	ARG	2.5
1	B	221	GLY	2.5
1	C	83	SER	2.5
1	H	221	GLY	2.5
1	B	291	THR	2.4
1	H	253	THR	2.4
1	C	255	ALA	2.3
1	F	221	GLY	2.3
1	A	222	ILE	2.3
1	E	292	TRP	2.3
1	D	214	GLU	2.3
1	G	293	GLY	2.2
1	H	147	GLY	2.2
1	F	215	SER	2.2
1	A	253	THR	2.2
1	C	275	MET	2.2
1	E	151	SER	2.2
1	G	78	LEU	2.2
1	H	84	ASP	2.2
1	H	254	GLU	2.1
1	C	251	MET	2.1
1	C	27	GLU	2.1
1	D	146	THR	2.0
1	F	222	ILE	2.0
1	D	254	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

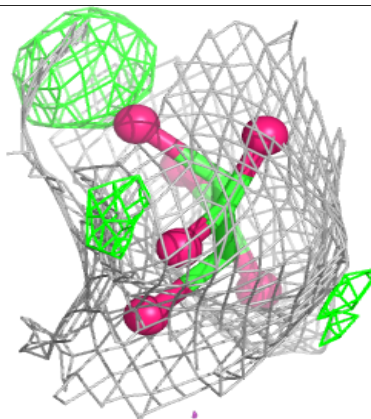
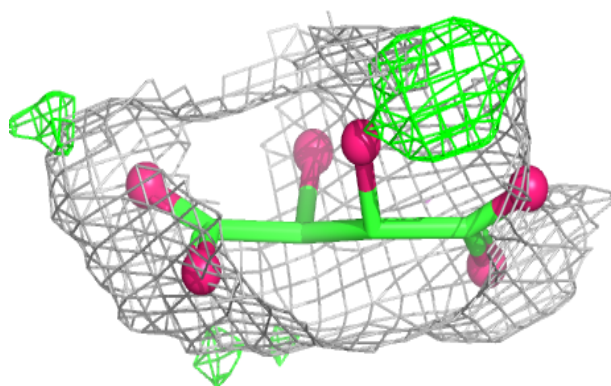
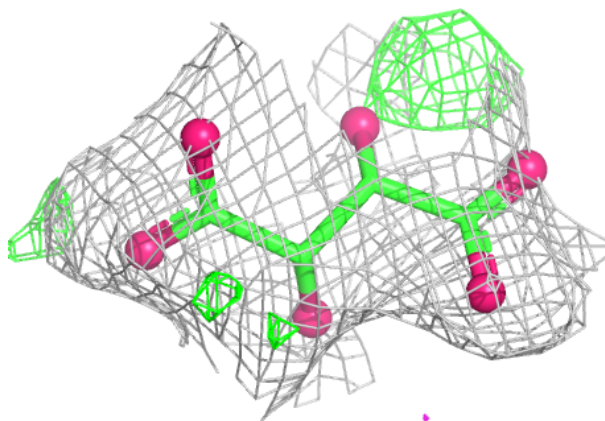
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TAR	C	401	10/10	0.69	0.15	82,94,98,100	0
2	TAR	D	401	10/10	0.78	0.15	75,85,87,90	0
2	TAR	G	401	10/10	0.78	0.14	83,92,100,100	0
2	TAR	F	401	10/10	0.79	0.15	74,82,91,93	0
2	TAR	E	401	10/10	0.82	0.14	70,83,88,95	0
2	TAR	H	401	10/10	0.83	0.12	81,90,94,104	0
2	TAR	A	401	10/10	0.85	0.13	73,79,91,91	0
3	PEG	H	402	7/7	0.86	0.17	65,71,77,79	0
2	TAR	B	401	10/10	0.87	0.12	76,84,89,90	0
3	PEG	F	402	7/7	0.89	0.17	70,72,74,78	0
3	PEG	B	402	7/7	0.90	0.15	60,69,71,72	0
3	PEG	D	402	7/7	0.93	0.12	60,64,69,76	0

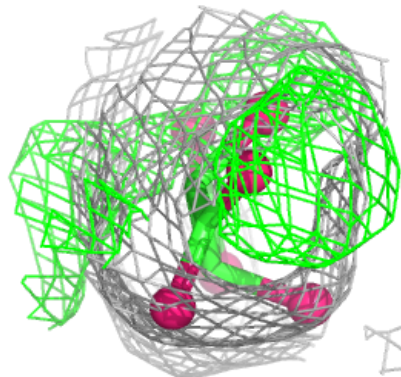
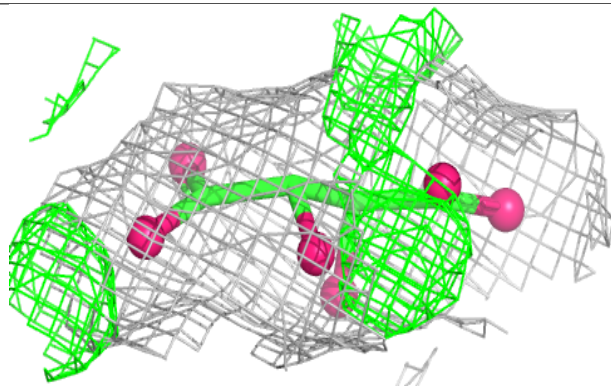
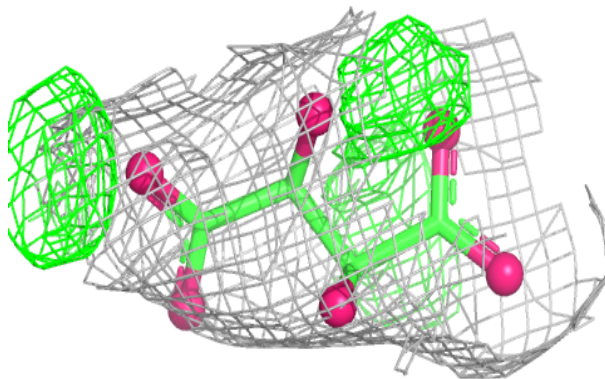
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TAR 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)

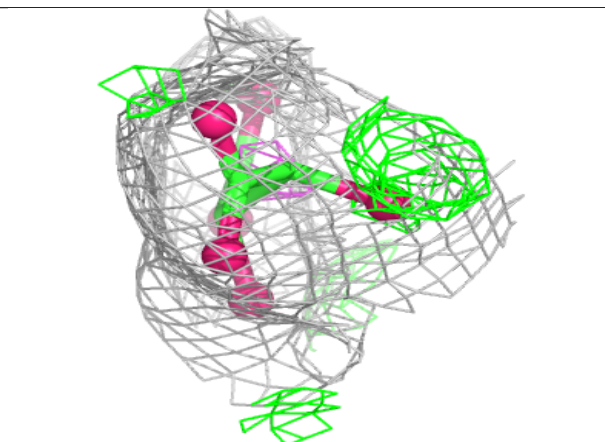
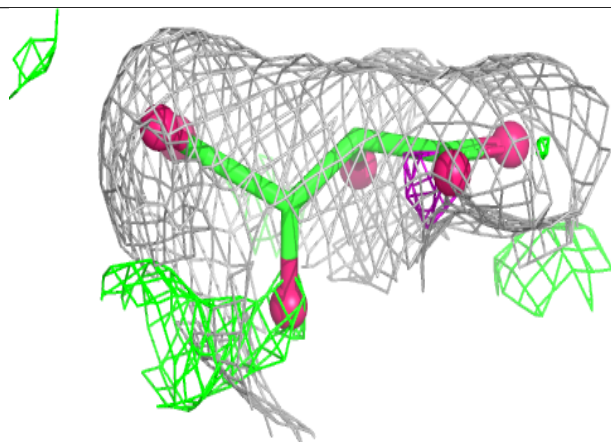
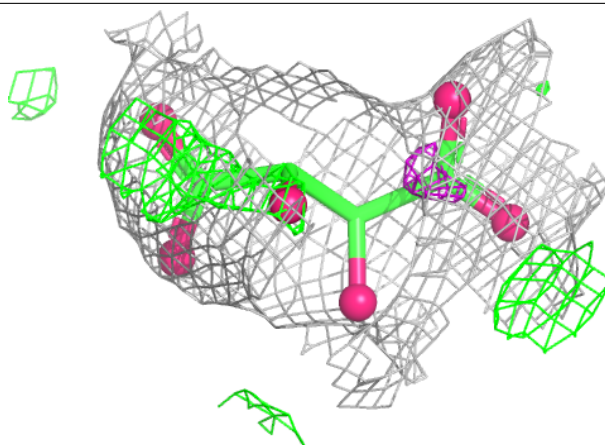
**Electron density around TAR D 401:**

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

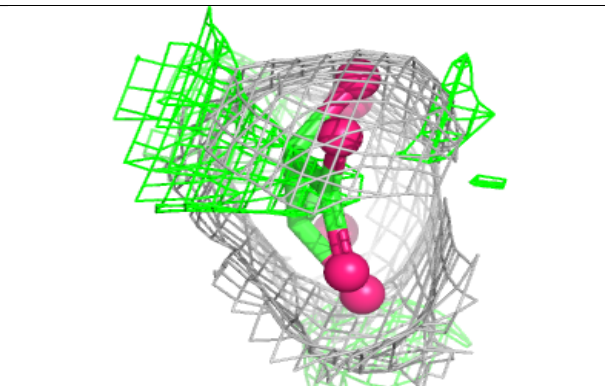
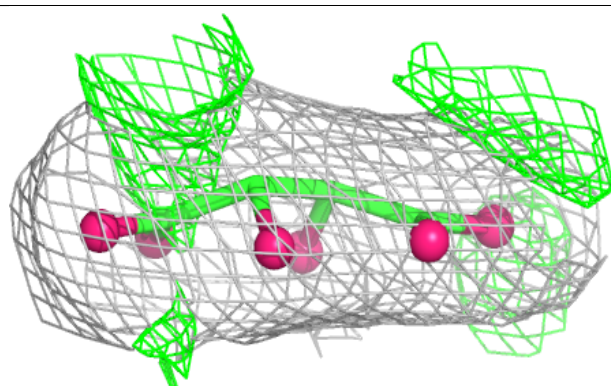
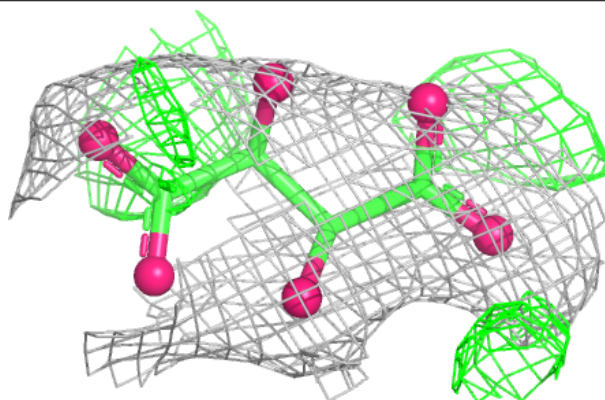


Electron density around TAR G 401:

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

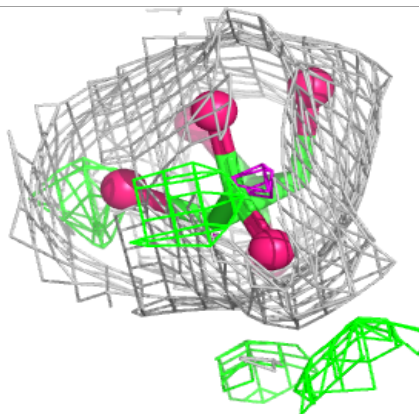
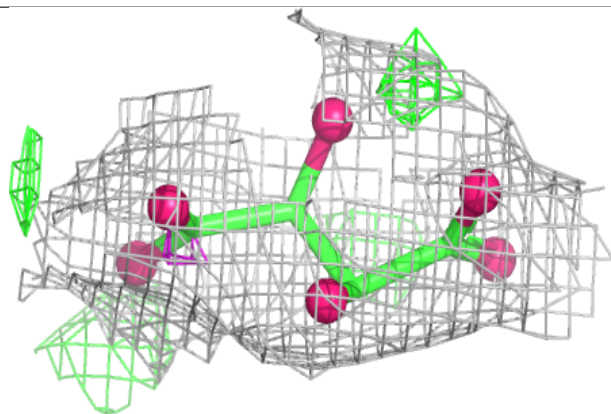
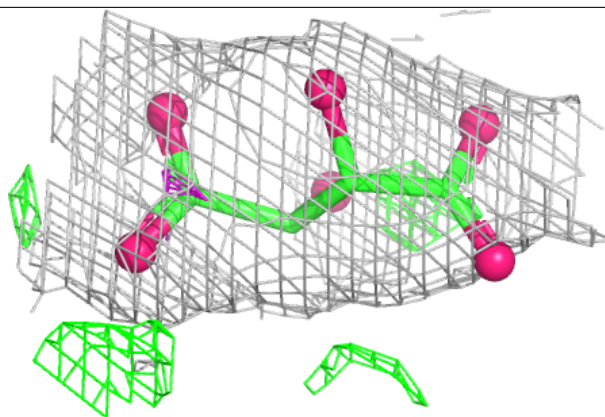
**Electron density around TAR F 401:**

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



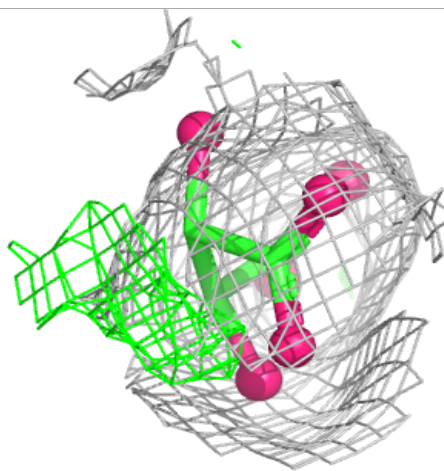
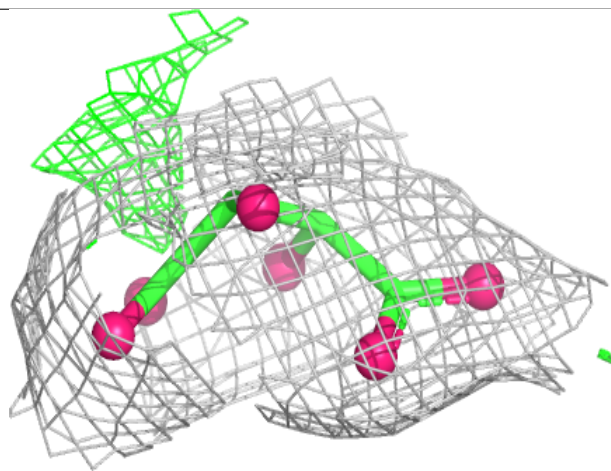
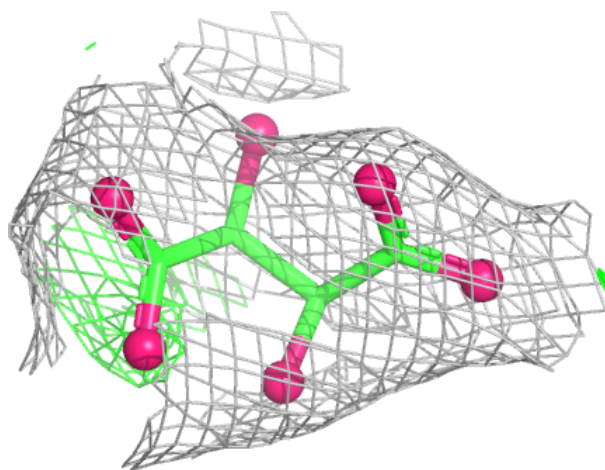
Electron density around TAR E 401:

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



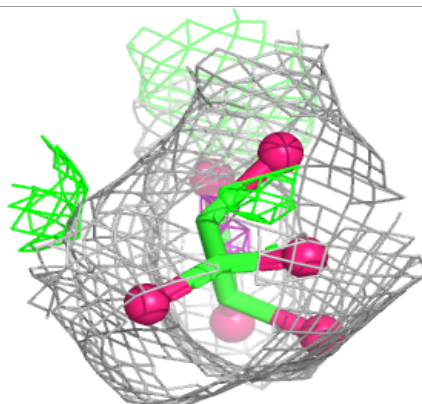
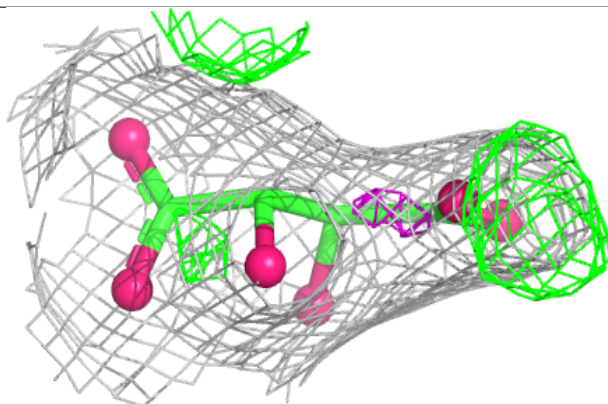
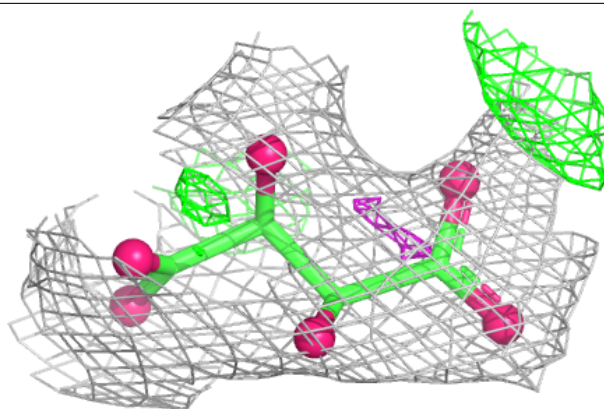
Electron density around TAR H 401:

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

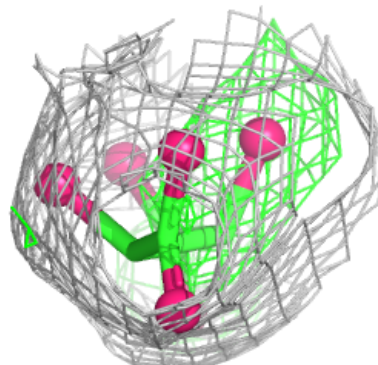
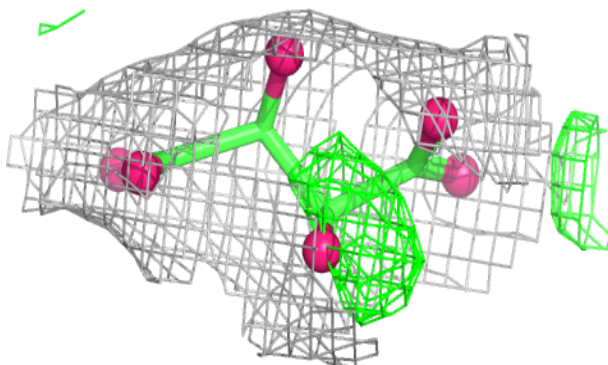
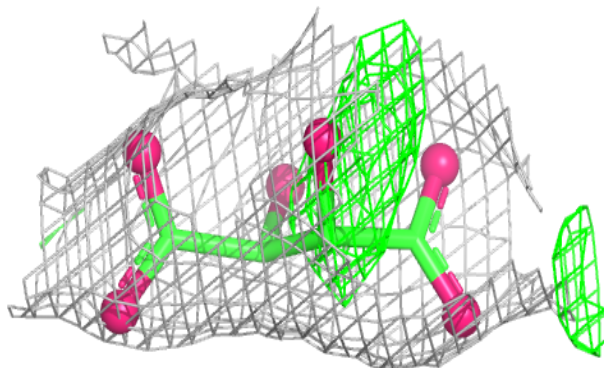


Electron density around TAR A 401:

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

**Electron density around TAR B 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.