



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2025 – 02:43 PM EDT

PDB ID : 9C42 / pdb_00009c42
Title : Structure of human MR1-ellagic acid in complex with human MAIT A-F7 TCR
Authors : Wang, C.J.H.; Le Nours, J.; Rossjohn, J.
Deposited on : 2024-06-02
Resolution : 2.69 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

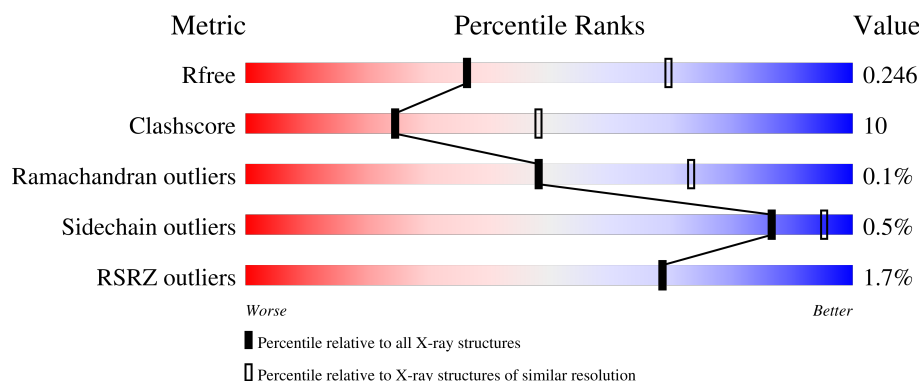
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	271	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>..</div> </div>
1	C	271	<div> <div>2%</div> <div>76%</div> <div>23%</div> <div>.</div> </div>
2	B	100	<div> <div>3%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	F	100	<div> <div>%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
3	D	204	<div> <div>3%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
3	G	204	 80% 18%
4	E	246	 80% 18%
4	H	246	 79% 20%

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
9	GOL	F	101	-	X	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12731 atoms, of which 45 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 Major histocompatibility complex class I-related gene protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	267	Total	C	N	O	S	0	5	0
			2148	1381	370	383	14			
1	C	266	Total	C	N	O	S	0	2	0
			2144	1380	370	382	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q95460
A	261	SER	CYS	conflict	UNP Q95460
C	0	MET	-	initiating methionine	UNP Q95460
C	261	SER	CYS	conflict	UNP Q95460

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	1	0
			755	486	125	141	3			
2	F	100	Total	C	N	O	S	0	0	0
			793	510	136	144	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called TRA@ protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	192	Total	C	N	O	S	0	2	0
			1411	909	221	271	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	201	Total	C	N	O	S	0	3	0
			1526	978	241	296	11			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	initiating methionine	UNP Q6P4G7
D	91	LYS	ARG	conflict	UNP Q6P4G7
D	93	SER	ALA	conflict	UNP Q6P4G7
D	94	ASN	SER	conflict	UNP Q6P4G7
D	95	TYR	ARG	conflict	UNP Q6P4G7
D	96	GLN	ARG	conflict	UNP Q6P4G7
D	?	-	GLY	deletion	UNP Q6P4G7
D	?	-	GLY	deletion	UNP Q6P4G7
D	?	-	GLY	deletion	UNP Q6P4G7
D	?	-	ASN	deletion	UNP Q6P4G7
D	?	-	LYS	deletion	UNP Q6P4G7
D	98	ILE	THR	conflict	UNP Q6P4G7
D	99	TRP	PHE	conflict	UNP Q6P4G7
D	101	ALA	THR	conflict	UNP Q6P4G7
D	104	LYS	GLN	conflict	UNP Q6P4G7
D	106	ILE	LYS	conflict	UNP Q6P4G7
D	107	ILE	VAL	conflict	UNP Q6P4G7
D	108	LYS	GLU	conflict	UNP Q6P4G7
D	109	PRO	LEU	conflict	UNP Q6P4G7
D	110	ASP	ASN	conflict	UNP Q6P4G7
D	157	CYS	THR	conflict	UNP Q6P4G7
G	0	MET	-	initiating methionine	UNP Q6P4G7
G	91	LYS	ARG	conflict	UNP Q6P4G7
G	93	SER	ALA	conflict	UNP Q6P4G7
G	94	ASN	SER	conflict	UNP Q6P4G7
G	95	TYR	ARG	conflict	UNP Q6P4G7
G	96	GLN	ARG	conflict	UNP Q6P4G7
G	?	-	GLY	deletion	UNP Q6P4G7
G	?	-	GLY	deletion	UNP Q6P4G7
G	?	-	GLY	deletion	UNP Q6P4G7
G	?	-	ASN	deletion	UNP Q6P4G7
G	?	-	LYS	deletion	UNP Q6P4G7
G	98	ILE	THR	conflict	UNP Q6P4G7
G	99	TRP	PHE	conflict	UNP Q6P4G7
G	101	ALA	THR	conflict	UNP Q6P4G7
G	104	LYS	GLN	conflict	UNP Q6P4G7

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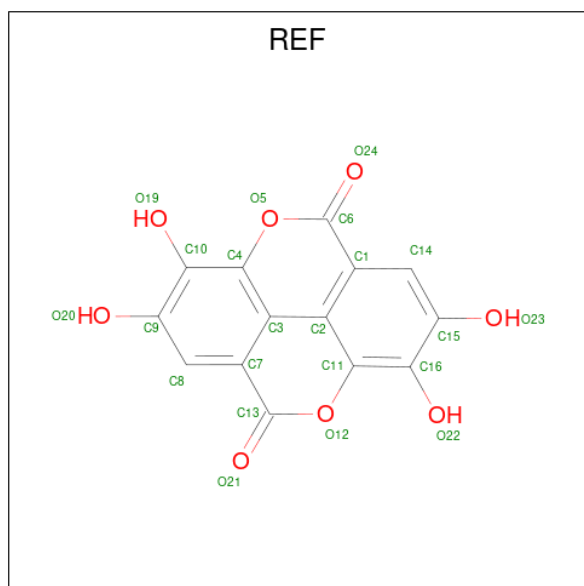
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Chain	Residue	Modelled	Actual	Comment	Reference
G	106	ILE	LYS	conflict	UNP Q6P4G7
G	107	ILE	VAL	conflict	UNP Q6P4G7
G	108	LYS	GLU	conflict	UNP Q6P4G7
G	109	PRO	LEU	conflict	UNP Q6P4G7
G	110	ASP	ASN	conflict	UNP Q6P4G7
G	157	CYS	THR	conflict	UNP Q6P4G7

- Molecule 4 is a protein called MAIT T-cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	242	Total	C	N	O	S	0	2	0
			1809	1147	311	341	10			
4	H	244	Total	C	N	O	S	0	4	0
			1875	1193	319	350	13			

- Molecule 5 is 2,3,7,8-tetrahydroxychromeno[5,4,3-cde]chromene-5,10-dione (CCD ID: REF) (formula: C₁₄H₆O₈) (labeled as "Ligand of Interest" by depositor).

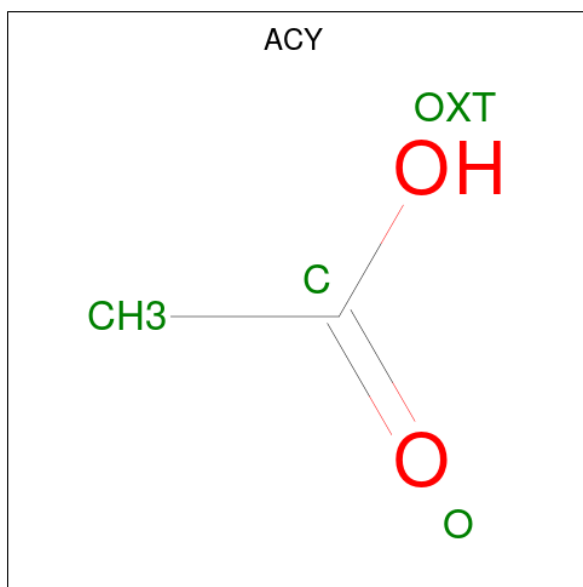


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			28	14	6	8		
5	C	1	Total	C	H	O	0	0
			28	14	6	8		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Na	0	0
			2	2		
6	H	1	Total	Na	0	0
			1	1		

- Molecule 7 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			7	2	3	2		
7	C	1	Total	C	H	O	0	0
			7	2	3	2		
7	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	E	1	Total	C	H	O	0	0
			14	3	8	3		
9	F	1	Total	C	H	O	0	0
			14	3	8	3		
9	F	1	Total	C	H	O	0	0
			14	3	8	3		

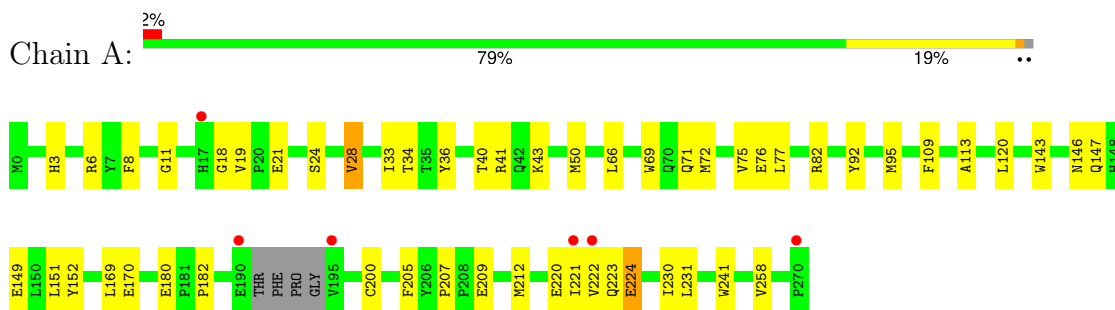
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	23	Total	O	0	0
			23	23		
10	B	7	Total	O	0	0
			7	7		
10	C	23	Total	O	0	0
			23	23		
10	D	20	Total	O	0	0
			20	20		
10	E	9	Total	O	0	0
			9	9		
10	F	11	Total	O	0	0
			11	11		
10	G	29	Total	O	0	0
			29	29		
10	H	25	Total	O	0	0
			25	25		

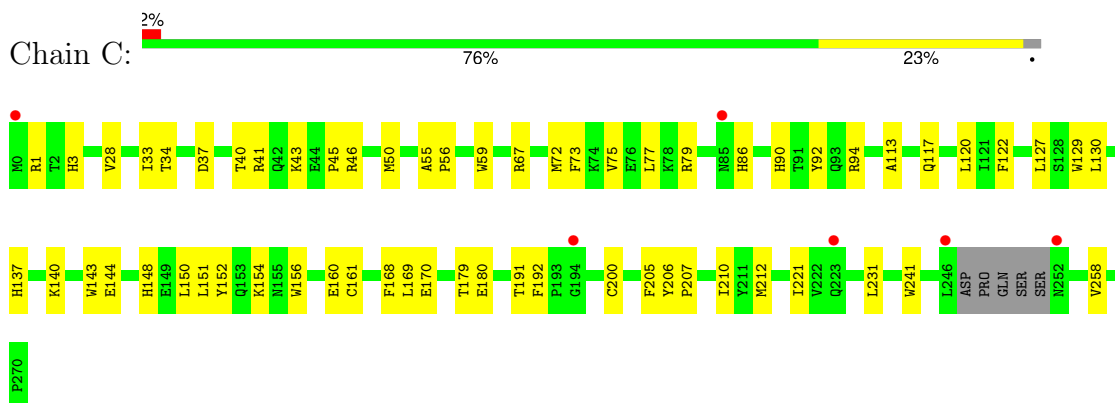
3 Residue-property plots

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.

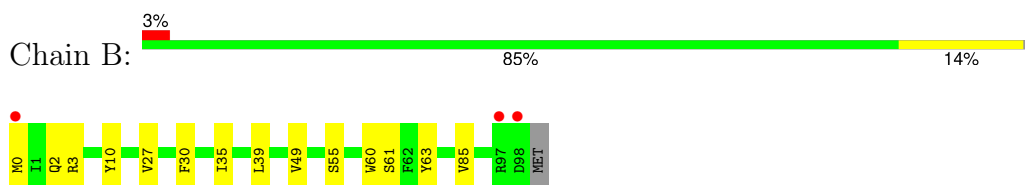
- Molecule 1: Major histocompatibility complex class I-related gene protein



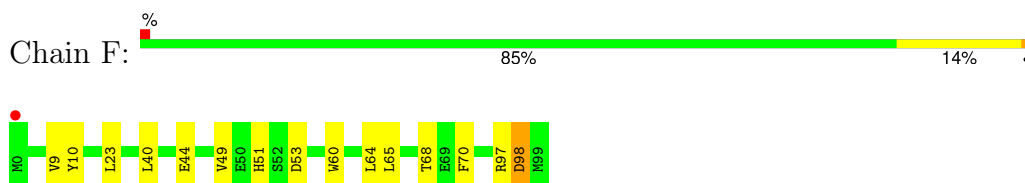
- Molecule 1: Major histocompatibility complex class I-related gene protein



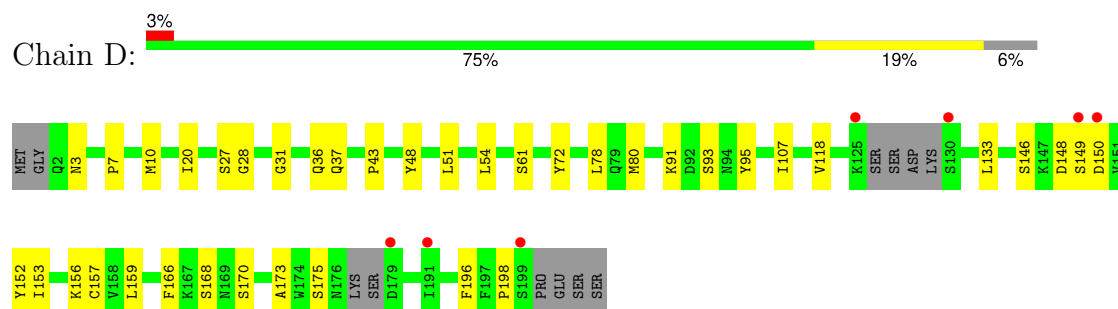
- Molecule 2: Beta-2-microglobulin



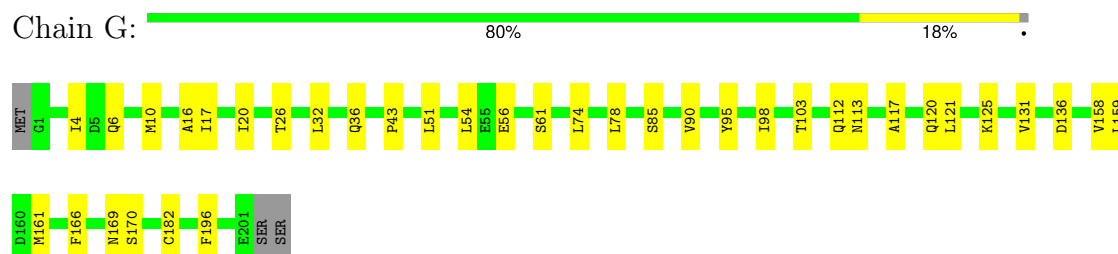
- Molecule 2: Beta-2-microglobulin



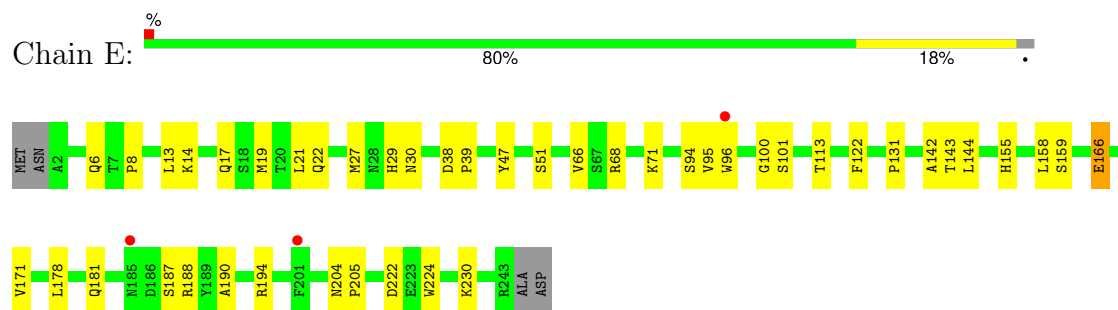
- Molecule 3: TRA@ protein



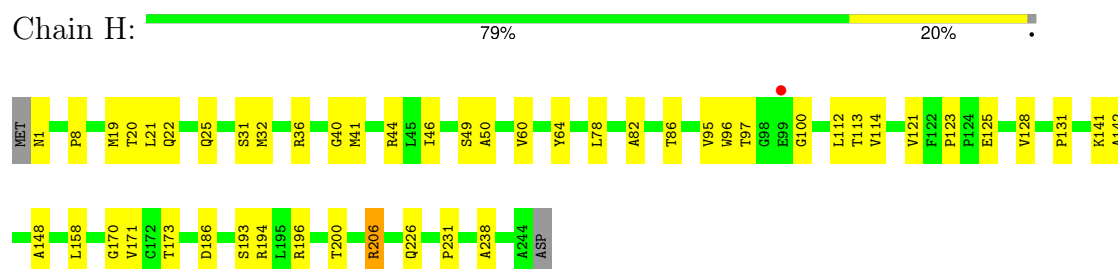
- Molecule 3: TRA@ protein



- Molecule 4: MAIT T-cell receptor beta chain



- Molecule 4: MAIT T-cell receptor beta chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	215.81Å 70.35Å 143.43Å 90.00° 104.09° 90.00°	Depositor
Resolution (Å)	47.78 – 2.69 47.78 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (47.78-2.69) 99.4 (47.78-2.69)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.194 , 0.246 0.197 , 0.246	Depositor DCC
R_{free} test set	2980 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.458	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 46.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12731	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: REF, NA, CL, ACY, GOL

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	0.46	0/2227	0.70	3/3032 (0.1%)
1	C	0.47	0/2216	0.68	0/3017
2	B	0.41	0/781	0.61	0/1071
2	F	0.43	0/816	0.61	0/1112
3	D	0.44	0/1449	0.66	0/1977
3	G	0.46	0/1570	0.74	0/2136
4	E	0.40	0/1865	0.65	2/2549 (0.1%)
4	H	0.44	0/1941	0.69	2/2647 (0.1%)
All	All	0.44	0/12865	0.68	7/17541 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	224	GLU	N-CA-C	-6.06	105.84	113.72
4	H	206	ARG	CD-NE-CZ	-5.82	116.25	124.40
4	E	166	GLU	CA-C-N	-5.66	115.81	123.10
4	E	166	GLU	C-N-CA	-5.66	115.81	123.10
1	A	28	VAL	N-CA-C	-5.33	99.49	107.37

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	2148	0	1987	42	0
1	C	2144	0	1995	51	0
2	B	755	0	654	11	0
2	F	793	0	728	12	0
3	D	1411	0	1221	25	0
3	G	1526	0	1401	40	0
4	E	1809	0	1627	38	0
4	H	1875	0	1738	44	0
5	A	22	6	3	3	0
5	C	22	6	3	1	0
6	A	2	0	0	0	0
6	H	1	0	0	0	0
7	A	4	3	3	0	0
7	C	4	3	3	1	0
7	D	4	3	3	1	0
8	C	1	0	0	0	0
9	E	6	8	8	0	0
9	F	12	16	15	3	0
10	A	23	0	0	1	0
10	B	7	0	0	1	0
10	C	23	0	0	0	0
10	D	20	0	0	1	0
10	E	9	0	0	0	0
10	F	11	0	0	0	0
10	G	29	0	0	0	0
10	H	25	0	0	2	0
All	All	12686	45	11389	232	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 10.

The worst 5 of 232 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)
3:G:120:GLN:NE2	3:G:182:CYS:SG	2.31	1.02
3:G:10:MET:HE1	3:G:20:ILE:HG12	1.45	0.98
1:A:212:MET:HG2	1:A:258:VAL:HG22	1.50	0.93
3:G:121:LEU:HD12	3:G:131:VAL:HG12	1.52	0.89
1:C:34:THR:HB	1:C:43:LYS:HE2	1.54	0.88

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	268/271 (99%)	259 (97%)	9 (3%)	0	100	100
1	C	264/271 (97%)	256 (97%)	8 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	95 (97%)	2 (2%)	1 (1%)	13	33
3	D	188/204 (92%)	179 (95%)	9 (5%)	0	100	100
3	G	202/204 (99%)	193 (96%)	9 (4%)	0	100	100
4	E	242/246 (98%)	230 (95%)	12 (5%)	0	100	100
4	H	247/246 (100%)	240 (97%)	7 (3%)	0	100	100
All	All	1607/1642 (98%)	1548 (96%)	58 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	98	ASP

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	213/241 (88%)	213 (100%)	0	100	100
1	C	214/241 (89%)	213 (100%)	1 (0%)	86	95
2	B	74/95 (78%)	74 (100%)	0	100	100
2	F	81/95 (85%)	80 (99%)	1 (1%)	67	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	129/181 (71%)	127 (98%)	2 (2%)	58	82
3	G	154/181 (85%)	153 (99%)	1 (1%)	84	94
4	E	177/212 (84%)	176 (99%)	1 (1%)	84	94
4	H	192/212 (91%)	192 (100%)	0	100	100
All	All	1234/1458 (85%)	1228 (100%)	6 (0%)	86	95

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	E	166	GLU
2	F	64	LEU
3	G	6	GLN
3	D	3	ASN
1	C	73	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
4	H	65	ASN
4	H	168	HIS
4	H	214	GLN
4	H	155	HIS
4	E	30	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	F	102	-	5,5,5	0.67	0	5,5,5	1.48	2 (40%)
7	ACY	C	303	-	3,3,3	2.04	1 (33%)	3,3,3	1.86	1 (33%)
7	ACY	A	304	-	3,3,3	1.70	0	3,3,3	2.20	1 (33%)
5	REF	C	301	-	25,25,25	1.07	1 (4%)	32,40,40	1.02	2 (6%)
9	GOL	F	101	-	5,5,5	1.64	2 (40%)	5,5,5	1.79	2 (40%)
9	GOL	E	301	-	5,5,5	1.06	0	5,5,5	1.48	1 (20%)
5	REF	A	301	-	25,25,25	0.96	1 (4%)	32,40,40	1.05	2 (6%)
7	ACY	D	301	-	3,3,3	1.93	1 (33%)	3,3,3	2.03	1 (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
9	GOL	F	102	-	-	2/4/4/4	-
5	REF	C	301	-	-	-	0/4/4/4
9	GOL	F	101	-	-	2/4/4/4	-
9	GOL	E	301	-	-	2/4/4/4	-
5	REF	A	301	-	-	-	0/4/4/4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	F	101	GOL	O1-C1	-2.75	1.30	1.42
7	C	303	ACY	CH3-C	2.66	1.59	1.49
7	D	301	ACY	CH3-C	2.45	1.58	1.49
9	F	101	GOL	O2-C2	-2.20	1.37	1.43
5	A	301	REF	C11-C2	-2.03	1.39	1.43

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	101	GOL	C3-C2-C1	-3.05	100.61	111.80
7	A	304	ACY	O-C-CH3	-3.02	110.15	122.53
9	E	301	GOL	C3-C2-C1	-3.01	100.77	111.80
5	C	301	REF	O12-C11-C16	2.95	118.64	115.05
7	D	301	ACY	O-C-CH3	-2.80	111.04	122.53

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

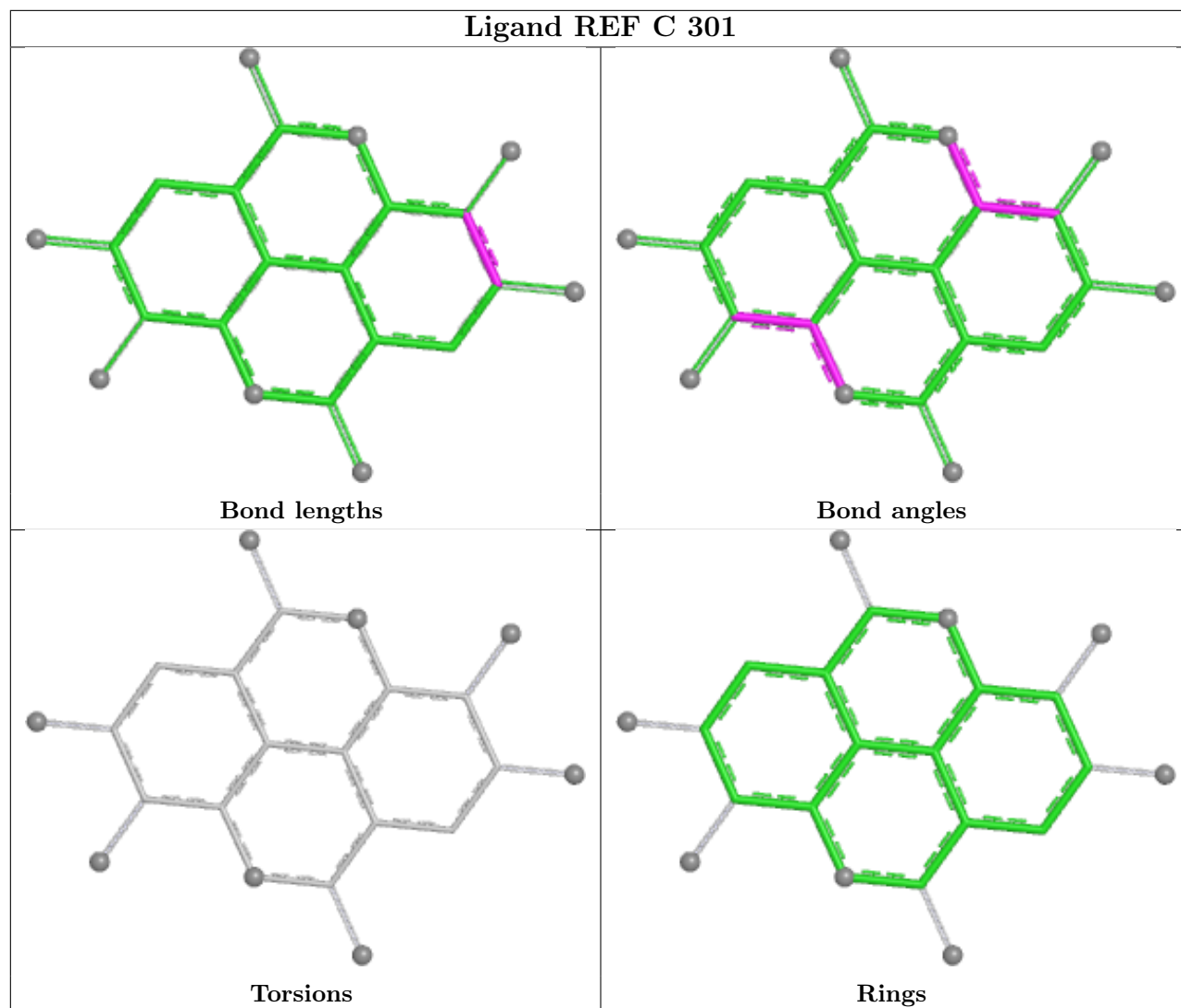
Mol	Chain	Res	Type	Atoms
9	E	301	GOL	C1-C2-C3-O3
9	E	301	GOL	O2-C2-C3-O3
9	F	101	GOL	O1-C1-C2-C3
9	F	102	GOL	O1-C1-C2-C3
9	F	102	GOL	O1-C1-C2-O2

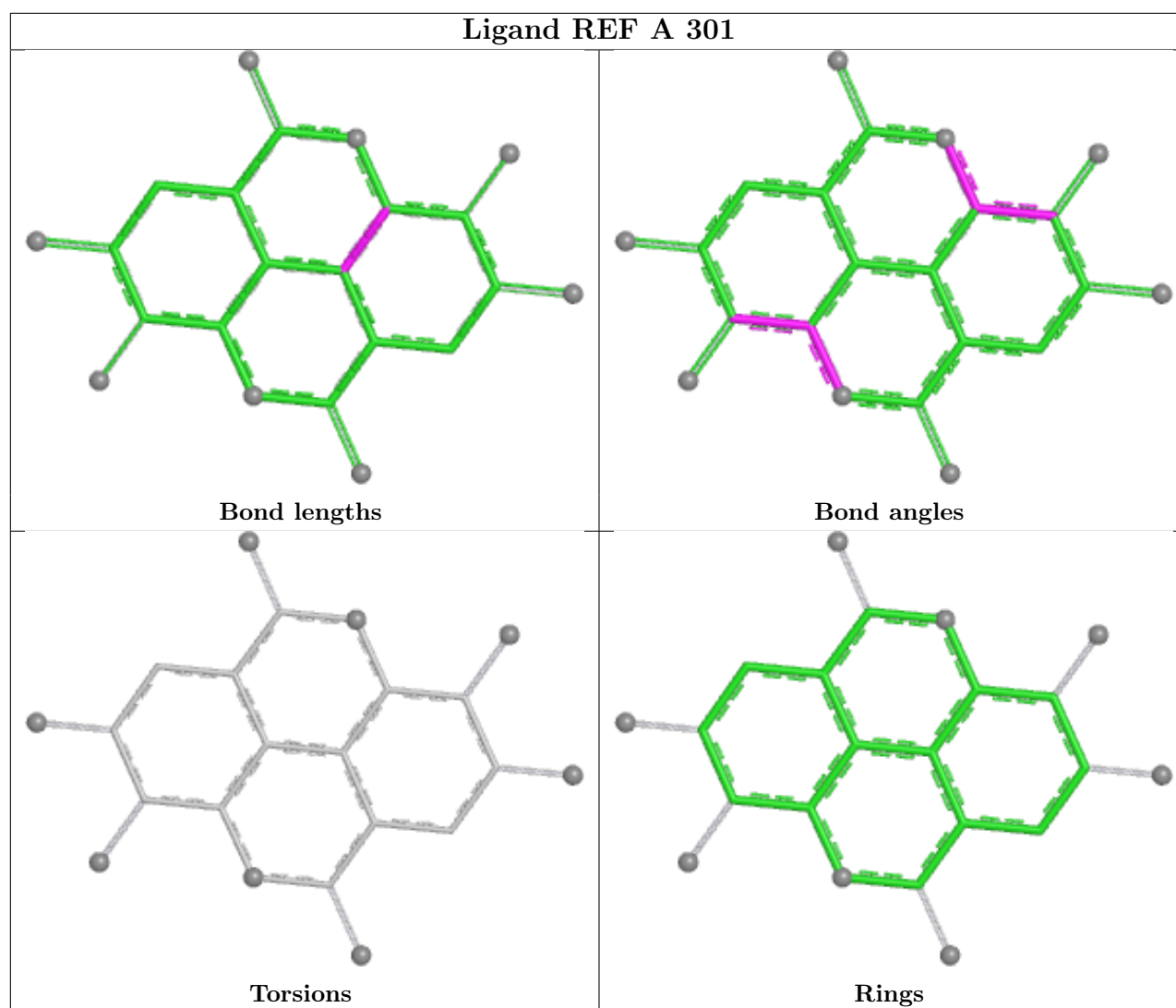
There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	102	GOL	3	0
7	C	303	ACY	1	0
5	C	301	REF	1	0
5	A	301	REF	3	0
7	D	301	ACY	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.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	267/271 (98%)	-0.17	6 (2%) 62 61	22, 44, 81, 105	5 (1%)
1	C	266/271 (98%)	-0.17	6 (2%) 61 60	25, 44, 66, 87	3 (1%)
2	B	99/100 (99%)	0.14	3 (3%) 52 50	31, 61, 93, 100	1 (1%)
2	F	100/100 (100%)	-0.29	1 (1%) 79 79	29, 46, 66, 88	1 (1%)
3	D	192/204 (94%)	0.12	7 (3%) 46 45	26, 54, 85, 108	4 (2%)
3	G	201/204 (98%)	-0.22	0 100 100	24, 43, 70, 90	5 (2%)
4	E	242/246 (98%)	0.01	3 (1%) 76 76	26, 56, 81, 97	2 (0%)
4	H	244/246 (99%)	-0.18	1 (0%) 89 88	18, 46, 66, 78	4 (1%)
All	All	1611/1642 (98%)	-0.10	27 (1%) 69 68	18, 47, 79, 108	25 (1%)

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	ILE	4.8
1	C	252	ASN	4.5
1	C	223	GLN	4.3
1	A	195	VAL	3.6
2	B	98	ASP	3.3

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 monosaccharides in this entry.

6.4 Ligands

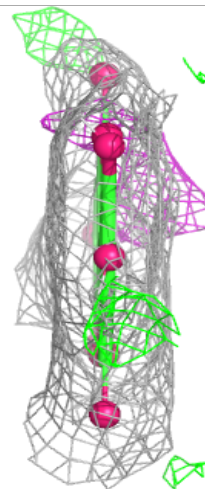
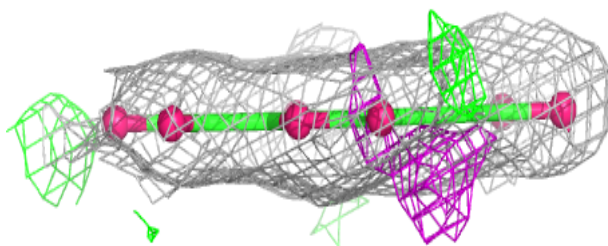
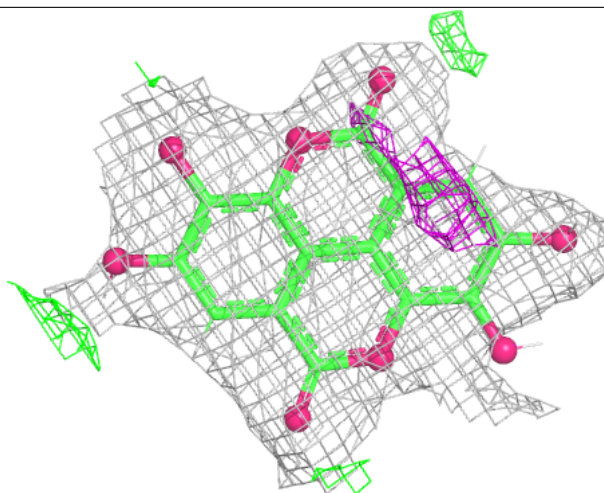
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	REF	C	301	22/22	0.82	0.12	49,57,65,69	0
7	ACY	A	304	4/4	0.83	0.13	42,49,50,55	0
7	ACY	D	301	4/4	0.84	0.17	48,53,63,63	0
7	ACY	C	303	4/4	0.87	0.13	40,47,49,52	0
6	NA	A	302	1/1	0.88	0.33	65,65,65,65	0
5	REF	A	301	22/22	0.88	0.12	35,42,52,59	28
9	GOL	E	301	6/6	0.88	0.14	56,67,82,82	0
9	GOL	F	101	6/6	0.90	0.14	38,46,51,54	0
6	NA	A	303	1/1	0.91	0.08	30,30,30,30	0
8	CL	C	302	1/1	0.91	0.08	62,62,62,62	0
9	GOL	F	102	6/6	0.94	0.08	29,37,43,46	0
6	NA	H	301	1/1	0.96	0.23	60,60,60,60	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.

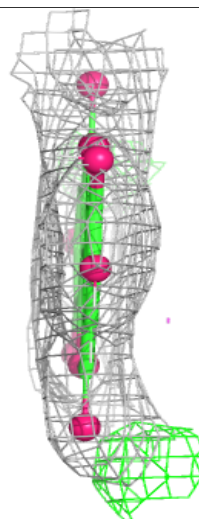
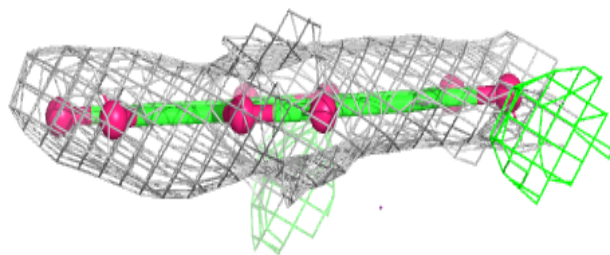
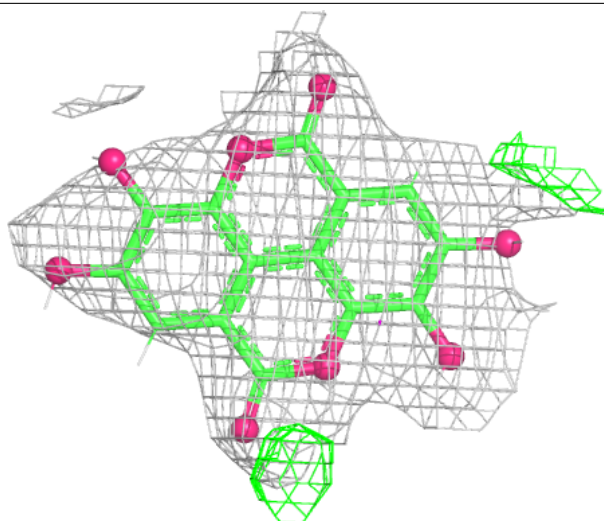
Electron density around REF C 301:

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



Electron density around REF A 301:

$2mF_o-DF_c$ (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.