



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 24, 2021 – 10:15 AM GMT

PDB ID : 7AQ1
Title : Crystal structure of human mature meprin beta in complex with the specific inhibitor MWT-S-270
Authors : Linnert, M.; Parthier, C.; Fritz, C.
Deposited on : 2020-10-20
Resolution : 2.41 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.17.1.dev1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.17.1.dev1

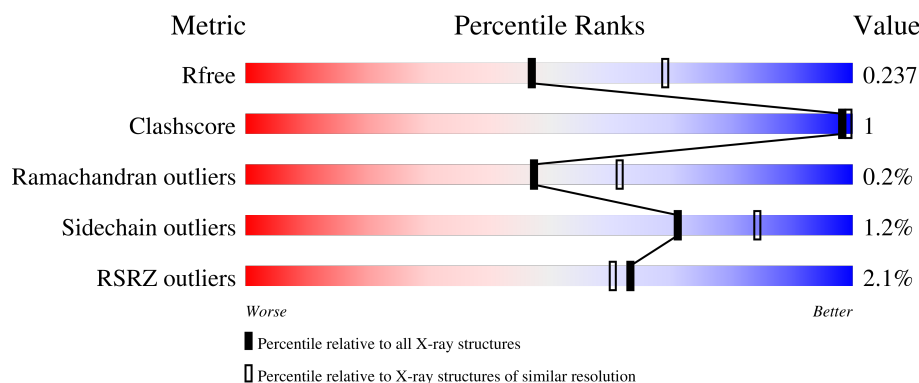
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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.



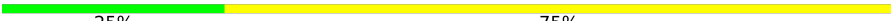
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	534	<div> <div>0%</div> <div>96%</div> <div>.</div> </div>
1	B	534	<div> <div>3%</div> <div>97%</div> <div>.</div> </div>
2	H	2	<div> <div>50%</div> <div>50%</div> </div>
2	K	2	<div> <div>100%</div> </div>
3	I	9	<div> <div>22%</div> <div>78%</div> </div>

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Mol	Chain	Length	Quality of chain
4	L	8	 A horizontal bar chart showing the quality of chain L. The bar is divided into two segments: a green segment on the left representing 25% and a yellow segment on the right representing 75%. The labels '25%' and '75%' are positioned below their respective segments.

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 17815 atoms, of which 8425 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 Meprin B subunit beta.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	533	Total	C	H	N	O	S	0	0	0
			8303	2685	4032	741	824	21			
1	B	533	Total	C	H	N	O	S	0	0	0
			8304	2685	4033	741	824	21			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			
2	K	2	Total	C	H	N	O	0	0	0
			53	16	25	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	9	Total	C	H	N	O	0	0	0
			193	58	88	2	45			

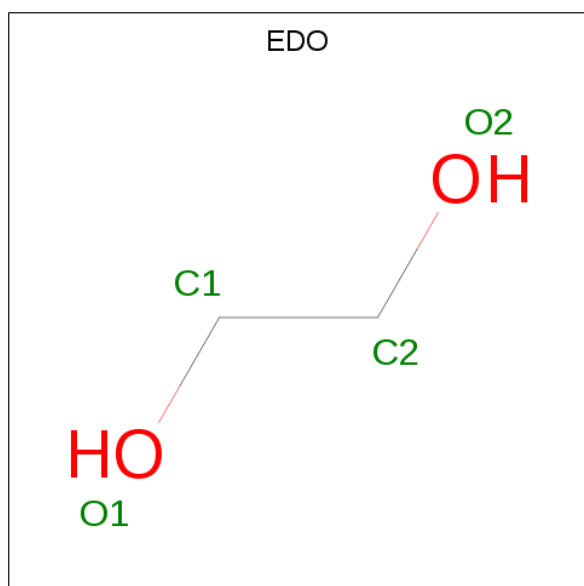
- Molecule 4 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	8	Total	C	H	N	O	0	0	0
			173	52	79	2	40			

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		
5	B	1	Total	Zn	0	0
			1	1		

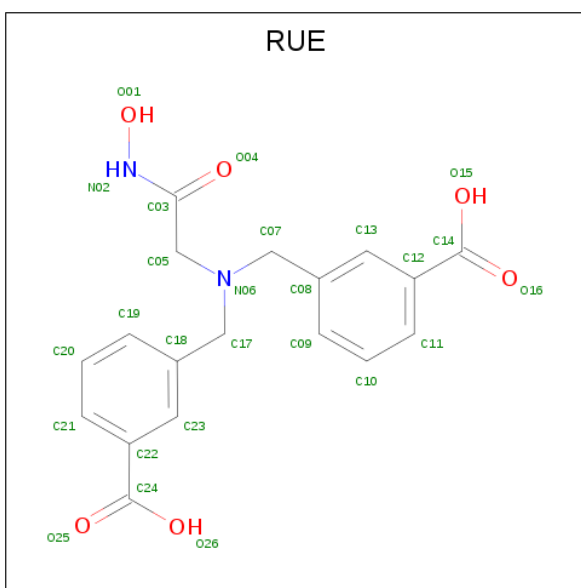
- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	A	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		
6	B	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 7 is 3-[[[(3-Carboxyphenyl)methyl]-[2-(hydroxyamino)-2-oxoethyl]amino]methyl]benzoic acid (three-letter code: RUE) (formula: C₁₈H₁₈N₂O₆) (labeled as "Ligand of Interest")

by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	H	N	O	0	1
			84	36	32	4	12		
7	B	1	Total	C	H	N	O	0	0
			42	18	16	2	6		

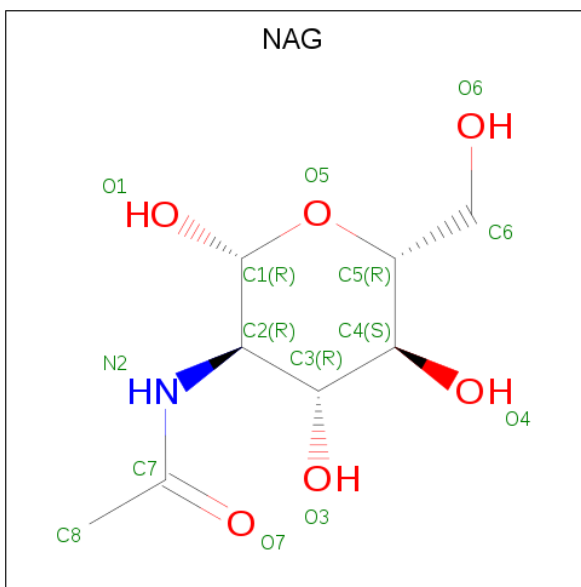
- Molecule 8 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Ca	0	0
			2	2		
8	B	2	Total	Ca	0	0
			2	2		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		
9	B	1	Total	Cl	0	0
			1	1		

- Molecule 10 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	A	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		
10	B	1	Total	C	H	N	O	0	0
			27	8	13	1	5		

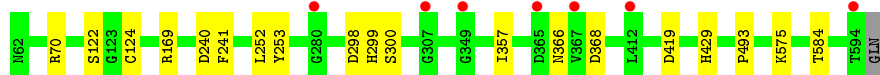
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	250	Total	O	0	0
			250	250		
11	B	167	Total	O	0	0
			167	167		

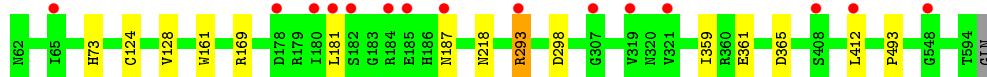
3 Residue-property plots [i](#)

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: Meprin B subunit beta



- Molecule 1: Meprin B subunit beta



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8
MAN9

- Molecule 4: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:

25%

75%

MAN1
MAN2
MAN3
MAN4
MAN5
MAN6
MAN7
MAN8

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.25Å 72.44Å 135.47Å 90.00° 118.43° 90.00°	Depositor
Resolution (Å)	44.97 – 2.41 44.97 – 2.41	Depositor EDS
% Data completeness (in resolution range)	99.2 (44.97-2.41) 99.7 (44.97-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.42Å)	Xtriage
Refinement program	PHENIX v1.14-3260	Depositor
R, R_{free}	0.199 , 0.236 0.198 , 0.237	Depositor DCC
R_{free} test set	2666 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17815	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: CA, CL, RUE, MAN, EDO, ZN, BMA, NAG

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	0.25	0/4379	0.45	0/5935
1	B	0.25	0/4379	0.45	0/5935
All	All	0.25	0/8758	0.45	0/11870

There are no bond length outliers.

There are no bond angle outliers.

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	4271	4032	4032	7	1
1	B	4271	4033	4033	4	1
2	H	28	25	25	1	0
2	K	28	25	25	0	0
3	I	105	88	88	0	0
4	L	94	79	79	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	12	18	18	0	0
6	B	8	12	12	0	0
7	A	52	32	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	26	16	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
9	A	1	0	0	0	0
9	B	1	0	0	0	0
10	A	42	39	39	0	0
10	B	28	26	26	0	0
11	A	250	0	0	0	0
11	B	167	0	0	0	0
All	All	9390	8425	8377	11	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 1.

All (11) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:VAL:HG21	1:B:161:TRP:CD1	2.45	0.51
1:A:253:TYR:HA	2:H:1:NAG:H82	1.94	0.50
1:A:357:ILE:N	1:A:357:ILE:HD12	2.30	0.46
1:A:429:HIS:CE1	1:A:584:THR:HG23	2.51	0.45
1:A:70:ARG:CZ	1:A:252:LEU:HD11	2.47	0.44
1:B:359:ILE:HG22	1:B:361:GLU:HG3	2.00	0.44
1:A:240:ASP:OD1	1:A:241:PHE:N	2.51	0.42
1:A:299:HIS:O	1:A:575:LYS:HE2	2.19	0.42
1:B:181:LEU:HD23	1:B:218:ASN:HB2	2.03	0.41
1:B:293:ARG:NH1	1:B:412:LEU:HD13	2.36	0.41
1:A:300:SER:OG	1:A:419:ASP:OD1	2.39	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:A:122:SER:H	1:B:365:ASP:OD1[2_555]	1.56	0.04

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	531/534 (99%)	521 (98%)	9 (2%)	1 (0%)	47	61
1	B	531/534 (99%)	518 (98%)	12 (2%)	1 (0%)	47	61
All	All	1062/1068 (99%)	1039 (98%)	21 (2%)	2 (0%)	47	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	493	PRO
1	A	493	PRO

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	473/474 (100%)	468 (99%)	5 (1%)	73	86
1	B	473/474 (100%)	467 (99%)	6 (1%)	69	83
All	All	946/948 (100%)	935 (99%)	11 (1%)	71	84

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	124	CYS
1	A	169	ARG
1	A	298	ASP
1	A	366	ASN

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Mol	Chain	Res	Type
1	A	368	ASP
1	B	73	HIS
1	B	124	CYS
1	B	169	ARG
1	B	187	ASN
1	B	293	ARG
1	B	298	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

21 monosaccharides 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	NAG	H	1	1,2	14,14,15	0.56	0	17,19,21	0.54	0
2	NAG	H	2	2	14,14,15	0.51	0	17,19,21	0.40	0
3	NAG	I	1	1,3	14,14,15	0.30	0	17,19,21	0.37	0
3	NAG	I	2	3	14,14,15	0.37	0	17,19,21	0.41	0
3	BMA	I	3	3	11,11,12	0.61	0	15,15,17	1.19	2 (13%)
3	MAN	I	4	3	11,11,12	0.88	0	15,15,17	0.89	1 (6%)
3	MAN	I	5	3	11,11,12	0.86	0	15,15,17	0.99	1 (6%)
3	MAN	I	6	3	11,11,12	0.76	0	15,15,17	1.37	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	I	7	3	11,11,12	0.69	0	15,15,17	1.22	2 (13%)
3	MAN	I	8	3	11,11,12	0.75	0	15,15,17	0.89	2 (13%)
3	MAN	I	9	3	11,11,12	0.82	0	15,15,17	1.22	1 (6%)
2	NAG	K	1	1,2	14,14,15	0.46	0	17,19,21	0.50	0
2	NAG	K	2	2	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	L	1	1,4	14,14,15	0.27	0	17,19,21	0.40	0
4	NAG	L	2	4	14,14,15	0.33	0	17,19,21	0.38	0
4	BMA	L	3	4	11,11,12	1.01	0	15,15,17	1.01	1 (6%)
4	MAN	L	4	4	11,11,12	0.78	0	15,15,17	1.02	2 (13%)
4	MAN	L	5	4	11,11,12	0.64	0	15,15,17	1.12	2 (13%)
4	MAN	L	6	4	11,11,12	0.54	0	15,15,17	1.11	2 (13%)
4	MAN	L	7	4	11,11,12	0.74	0	15,15,17	0.92	1 (6%)
4	MAN	L	8	4	11,11,12	0.85	0	15,15,17	1.02	2 (13%)

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	NAG	H	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
3	NAG	I	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	BMA	I	3	3	-	0/2/19/22	0/1/1/1
3	MAN	I	4	3	-	0/2/19/22	0/1/1/1
3	MAN	I	5	3	-	2/2/19/22	0/1/1/1
3	MAN	I	6	3	-	1/2/19/22	0/1/1/1
3	MAN	I	7	3	-	2/2/19/22	0/1/1/1
3	MAN	I	8	3	-	0/2/19/22	0/1/1/1
3	MAN	I	9	3	-	0/2/19/22	0/1/1/1
2	NAG	K	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	K	2	2	-	0/6/23/26	0/1/1/1
4	NAG	L	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	1/6/23/26	0/1/1/1
4	BMA	L	3	4	-	0/2/19/22	0/1/1/1
4	MAN	L	4	4	-	0/2/19/22	0/1/1/1
4	MAN	L	5	4	-	0/2/19/22	0/1/1/1
4	MAN	L	6	4	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	L	7	4	-	2/2/19/22	0/1/1/1
4	MAN	L	8	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	6	MAN	C1-O5-C5	4.21	117.89	112.19
3	I	7	MAN	C1-O5-C5	3.65	117.14	112.19
4	L	6	MAN	C1-O5-C5	3.06	116.34	112.19
3	I	9	MAN	C1-O5-C5	3.04	116.31	112.19
4	L	5	MAN	O2-C2-C3	-2.80	104.53	110.14
4	L	5	MAN	C1-O5-C5	2.50	115.58	112.19
3	I	3	BMA	C1-O5-C5	2.43	115.48	112.19
4	L	8	MAN	O2-C2-C3	-2.42	105.30	110.14
3	I	7	MAN	O2-C2-C3	-2.35	105.44	110.14
4	L	4	MAN	O2-C2-C3	-2.33	105.48	110.14
3	I	5	MAN	C1-O5-C5	2.31	115.32	112.19
3	I	4	MAN	O2-C2-C3	-2.28	105.57	110.14
3	I	6	MAN	O2-C2-C3	-2.27	105.59	110.14
4	L	7	MAN	O2-C2-C3	-2.21	105.70	110.14
4	L	8	MAN	C1-O5-C5	2.19	115.16	112.19
3	I	3	BMA	O2-C2-C3	-2.18	105.77	110.14
4	L	6	MAN	O2-C2-C3	-2.11	105.91	110.14
4	L	3	BMA	O2-C2-C3	-2.10	105.92	110.14
4	L	4	MAN	C1-O5-C5	2.08	115.00	112.19
3	I	8	MAN	C1-O5-C5	2.05	114.97	112.19
3	I	8	MAN	O2-C2-C3	-2.02	106.09	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	I	7	MAN	O5-C5-C6-O6
3	I	7	MAN	C4-C5-C6-O6
4	L	7	MAN	O5-C5-C6-O6
4	L	7	MAN	C4-C5-C6-O6
3	I	5	MAN	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
4	L	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	H	1	NAG	C4-C5-C6-O6
4	L	1	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
3	I	6	MAN	C4-C5-C6-O6
3	I	5	MAN	C4-C5-C6-O6
4	L	2	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0

5.6 Ligand geometry

Of 21 ligands modelled in this entry, 8 are monoatomic - leaving 13 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	$\# Z > 2$
7	RUE	A	605[B]	5	23,27,27	0.63	0	30,36,36	1.13	3 (10%)
6	EDO	B	603	-	3,3,3	0.49	0	2,2,2	0.24	0
7	RUE	A	605[A]	5	23,27,27	0.63	0	30,36,36	0.97	2 (6%)
7	RUE	B	604	5	23,27,27	0.63	0	30,36,36	1.62	5 (16%)
10	NAG	B	608	1	14,14,15	0.26	0	17,19,21	0.52	0
10	NAG	A	611	1	14,14,15	0.36	0	17,19,21	0.72	1 (5%)
10	NAG	A	609	1	14,14,15	0.40	0	17,19,21	0.43	0
6	EDO	A	602	-	3,3,3	0.50	0	2,2,2	0.30	0
10	NAG	B	609	1	14,14,15	0.48	0	17,19,21	0.49	0
6	EDO	A	604	-	3,3,3	0.44	0	2,2,2	0.36	0
6	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.31	0
6	EDO	B	602	-	3,3,3	0.47	0	2,2,2	0.49	0
10	NAG	A	610	1	14,14,15	0.26	0	17,19,21	0.54	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
7	RUE	A	605[B]	5	-	6/14/22/22	0/2/2/2
6	EDO	B	603	-	-	0/1/1/1	-
7	RUE	A	605[A]	5	-	5/14/22/22	0/2/2/2
7	RUE	B	604	5	-	3/14/22/22	0/2/2/2
10	NAG	B	608	1	-	0/6/23/26	0/1/1/1
10	NAG	A	611	1	-	1/6/23/26	0/1/1/1
10	NAG	A	609	1	-	2/6/23/26	0/1/1/1
6	EDO	A	602	-	-	0/1/1/1	-
10	NAG	B	609	1	-	2/6/23/26	0/1/1/1
6	EDO	A	604	-	-	0/1/1/1	-
6	EDO	A	603	-	-	0/1/1/1	-
6	EDO	B	602	-	-	0/1/1/1	-
10	NAG	A	610	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	604	RUE	C18-C17-N06	3.93	120.75	113.12
7	B	604	RUE	C17-N06-C05	3.54	119.60	112.02
7	B	604	RUE	O04-C03-N02	-3.32	119.19	123.27
7	B	604	RUE	C05-C03-N02	2.84	121.49	115.25
10	A	611	NAG	C1-O5-C5	2.56	115.67	112.19
7	B	604	RUE	C03-C05-N06	-2.54	107.46	113.36
7	A	605[B]	RUE	C07-N06-C05	2.53	117.43	112.02
7	A	605[B]	RUE	O04-C03-N02	-2.46	120.25	123.27
7	A	605[B]	RUE	C17-N06-C05	2.42	117.19	112.02
7	A	605[A]	RUE	O04-C03-N02	-2.34	120.40	123.27
7	A	605[A]	RUE	C07-N06-C05	2.25	116.83	112.02

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	605[A]	RUE	C03-C05-N06-C07
7	A	605[B]	RUE	C03-C05-N06-C07

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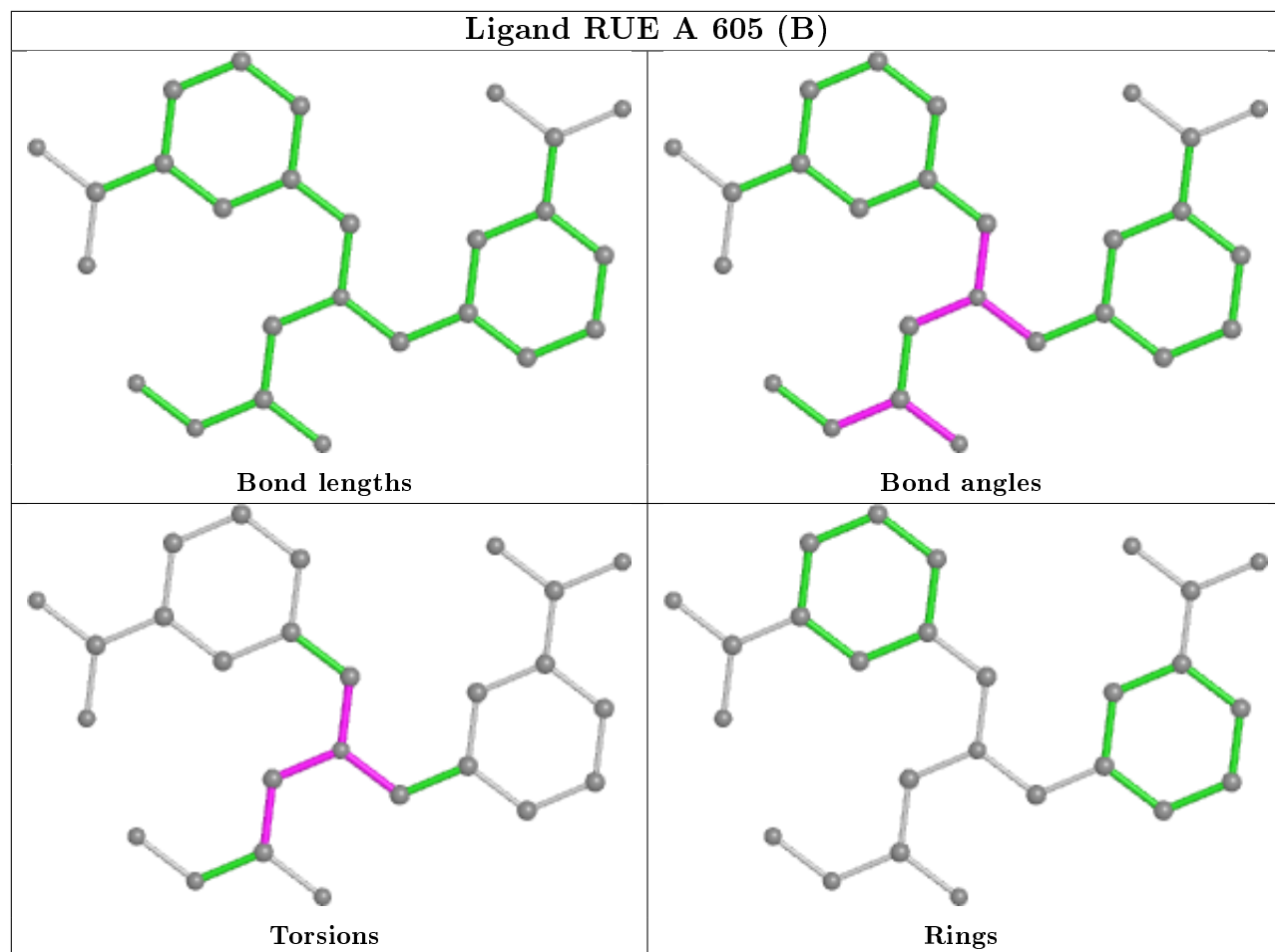
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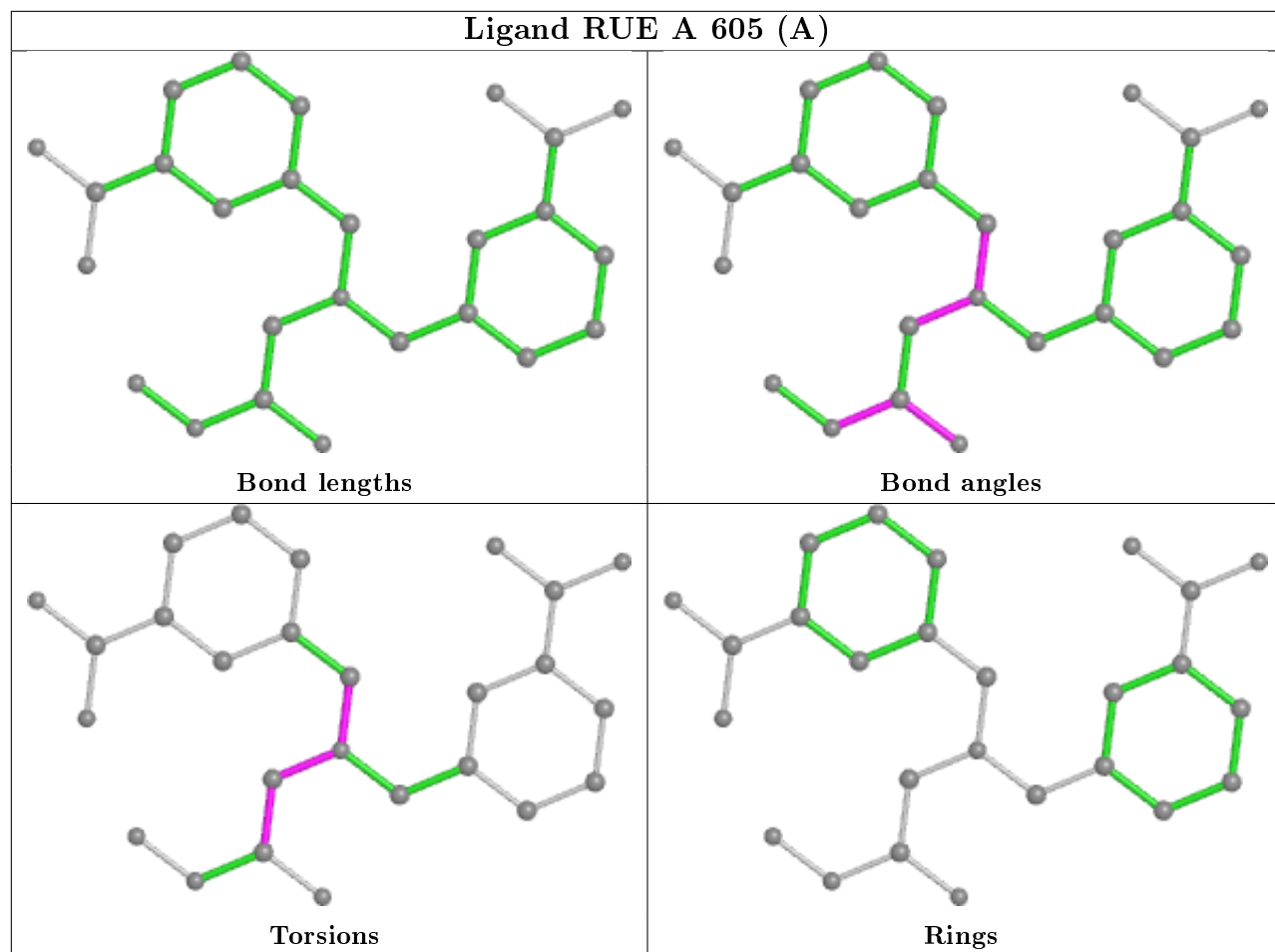
Mol	Chain	Res	Type	Atoms
10	A	610	NAG	O5-C5-C6-O6
10	A	610	NAG	C4-C5-C6-O6
7	A	605[B]	RUE	C08-C07-N06-C05
10	A	610	NAG	C8-C7-N2-C2
10	A	610	NAG	O7-C7-N2-C2
7	A	605[A]	RUE	C08-C07-N06-C17
7	A	605[B]	RUE	C08-C07-N06-C17
10	A	609	NAG	C4-C5-C6-O6
7	A	605[B]	RUE	N02-C03-C05-N06
7	A	605[B]	RUE	O04-C03-C05-N06
7	A	605[A]	RUE	N02-C03-C05-N06
7	A	605[A]	RUE	C08-C07-N06-C05
10	A	609	NAG	O5-C5-C6-O6
7	A	605[A]	RUE	O04-C03-C05-N06
10	B	609	NAG	O5-C5-C6-O6
7	A	605[B]	RUE	C18-C17-N06-C05
10	B	609	NAG	C4-C5-C6-O6
7	B	604	RUE	N02-C03-C05-N06
7	B	604	RUE	C03-C05-N06-C07
10	A	611	NAG	C4-C5-C6-O6
7	B	604	RUE	O04-C03-C05-N06

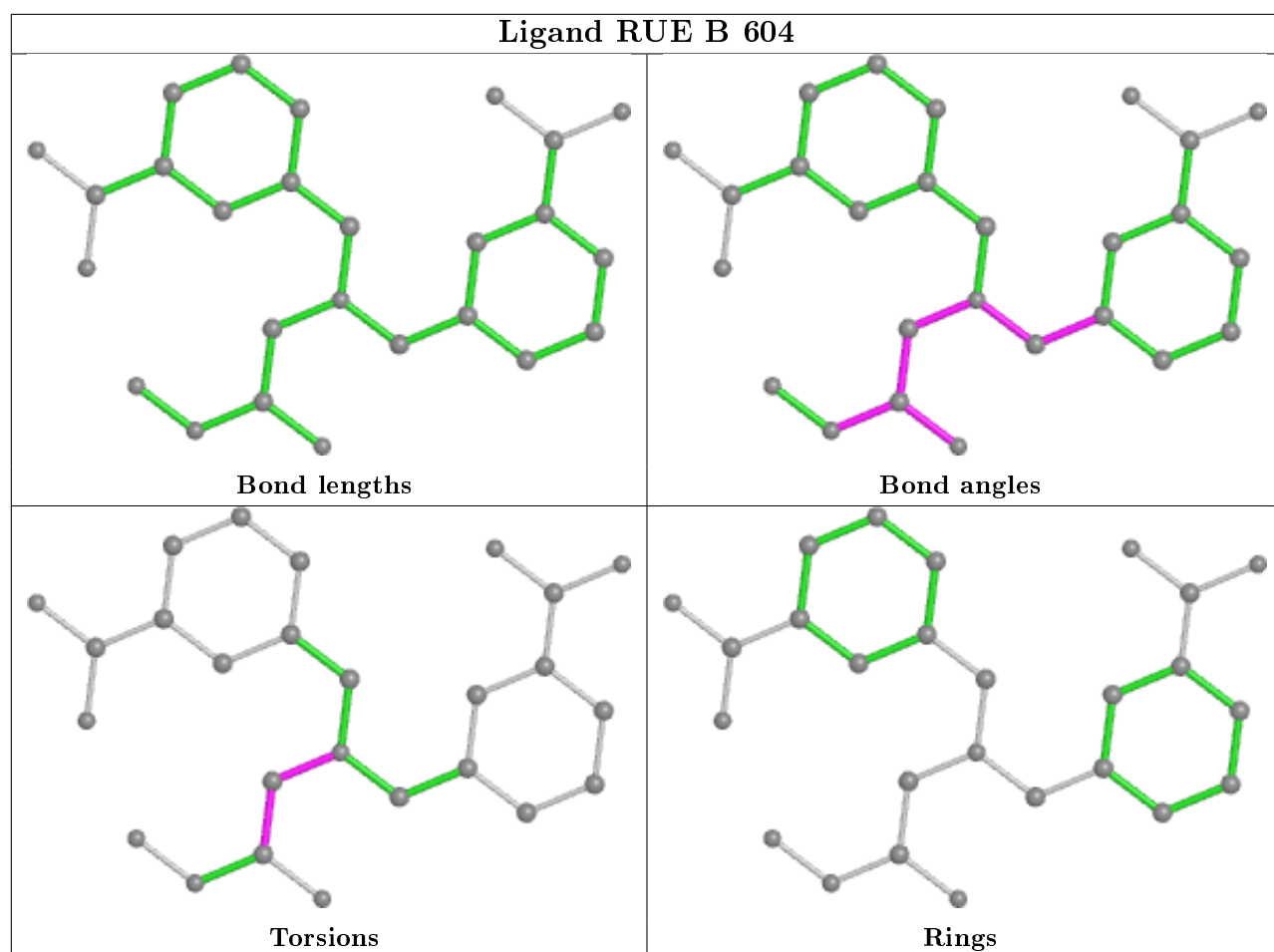
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	533/534 (99%)	-0.02	7 (1%) 77 75	31, 44, 73, 120	0
1	B	533/534 (99%)	0.12	15 (2%) 53 50	34, 53, 83, 138	0
All	All	1066/1068 (99%)	0.05	22 (2%) 63 60	31, 49, 79, 138	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	184	ARG	3.9
1	A	365	ASP	3.6
1	A	367	VAL	3.5
1	B	187	ASN	3.5
1	B	182	SER	3.3
1	B	307	GLY	2.8
1	B	293	ARG	2.7
1	A	412	LEU	2.7
1	B	185	GLU	2.7
1	A	280	GLY	2.6
1	B	319	VAL	2.5
1	B	178	ASP	2.5
1	B	548	GLY	2.4
1	B	412	LEU	2.4
1	A	594	THR	2.2
1	B	181	LEU	2.2
1	B	180	ILE	2.1
1	B	321	VAL	2.1
1	B	408	SER	2.1
1	B	65	ILE	2.1
1	A	307	GLY	2.1
1	A	349	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

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	NAG	H	2	14/15	0.71	0.39	74,91,111,113	0
2	NAG	K	2	14/15	0.78	0.29	76,91,108,116	0
4	MAN	L	4	11/12	0.82	0.26	68,81,99,107	0
4	MAN	L	7	11/12	0.82	0.31	75,90,103,109	0
4	MAN	L	8	11/12	0.83	0.34	83,97,114,117	0
2	NAG	H	1	14/15	0.84	0.32	57,77,94,101	0
3	MAN	I	9	11/12	0.85	0.28	79,92,106,115	0
3	MAN	I	8	11/12	0.88	0.24	67,77,92,92	0
3	MAN	I	7	11/12	0.88	0.37	69,86,104,106	0
4	NAG	L	2	14/15	0.88	0.22	54,69,85,94	0
3	MAN	I	5	11/12	0.89	0.18	56,62,74,85	0
4	MAN	L	5	11/12	0.89	0.32	65,79,95,107	0
3	MAN	I	4	11/12	0.90	0.17	53,67,80,86	0
4	BMA	L	3	11/12	0.90	0.21	71,78,94,107	0
3	BMA	I	3	11/12	0.91	0.17	57,69,80,87	0
4	MAN	L	6	11/12	0.93	0.29	62,70,83,89	0
3	MAN	I	6	11/12	0.93	0.20	47,65,78,81	0
2	NAG	K	1	14/15	0.93	0.22	64,82,96,101	0
3	NAG	I	1	14/15	0.94	0.11	43,58,77,77	0
4	NAG	L	1	14/15	0.94	0.18	58,81,91,98	0
3	NAG	I	2	14/15	0.94	0.15	43,61,74,83	0

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
10	NAG	B	608	14/15	0.72	0.33	66,90,112,116	0

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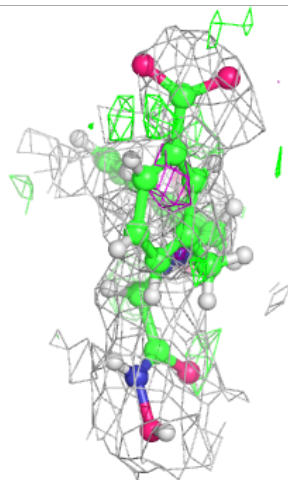
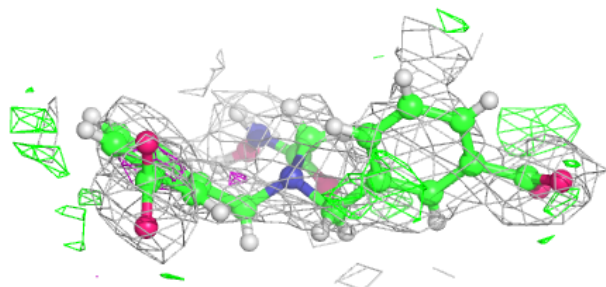
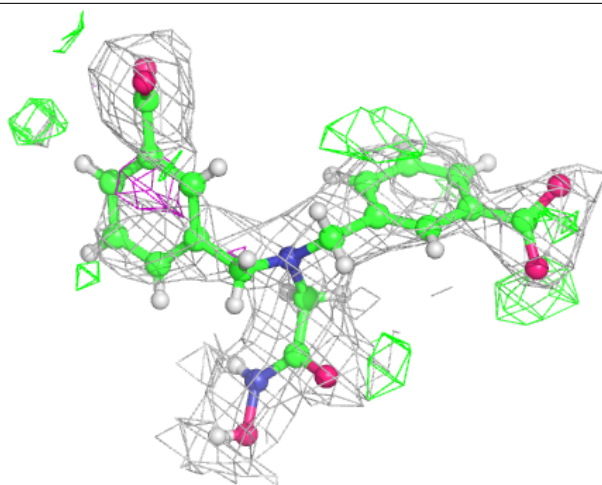
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	NAG	A	611	14/15	0.85	0.38	72,87,105,115	0
10	NAG	A	609	14/15	0.87	0.22	55,66,80,85	0
7	RUE	A	605[A]	26/26	0.87	0.25	42,62,75,86	42
7	RUE	A	605[B]	26/26	0.87	0.25	42,62,75,85	42
6	EDO	B	602	4/4	0.88	0.20	42,51,52,53	0
7	RUE	B	604	26/26	0.89	0.24	46,63,77,86	42
10	NAG	B	609	14/15	0.90	0.28	64,79,93,98	0
6	EDO	A	602	4/4	0.93	0.17	32,39,42,47	0
6	EDO	B	603	4/4	0.93	0.20	44,56,67,67	0
10	NAG	A	610	14/15	0.93	0.25	56,71,81,93	0
6	EDO	A	603	4/4	0.94	0.14	49,59,65,66	0
8	CA	B	606	1/1	0.95	0.03	69,69,69,69	0
6	EDO	A	604	4/4	0.95	0.31	32,41,49,51	0
8	CA	A	607	1/1	0.97	0.05	67,67,67,67	0
9	CL	B	607	1/1	0.98	0.28	48,48,48,48	0
8	CA	B	605	1/1	0.99	0.11	39,39,39,39	0
5	ZN	B	601	1/1	0.99	0.12	43,43,43,43	0
9	CL	A	608	1/1	0.99	0.17	28,28,28,28	1
5	ZN	A	601	1/1	1.00	0.14	40,40,40,40	0
8	CA	A	606	1/1	1.00	0.14	42,42,42,42	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.

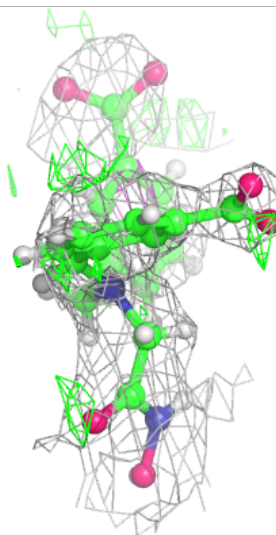
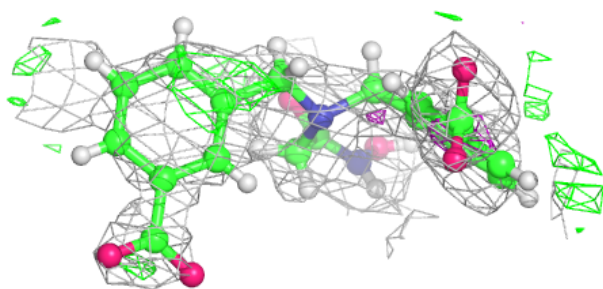
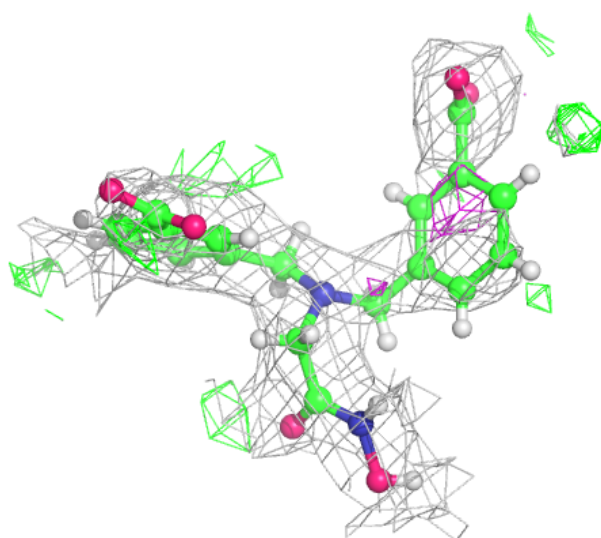
Electron density around RUE A 605 (A):

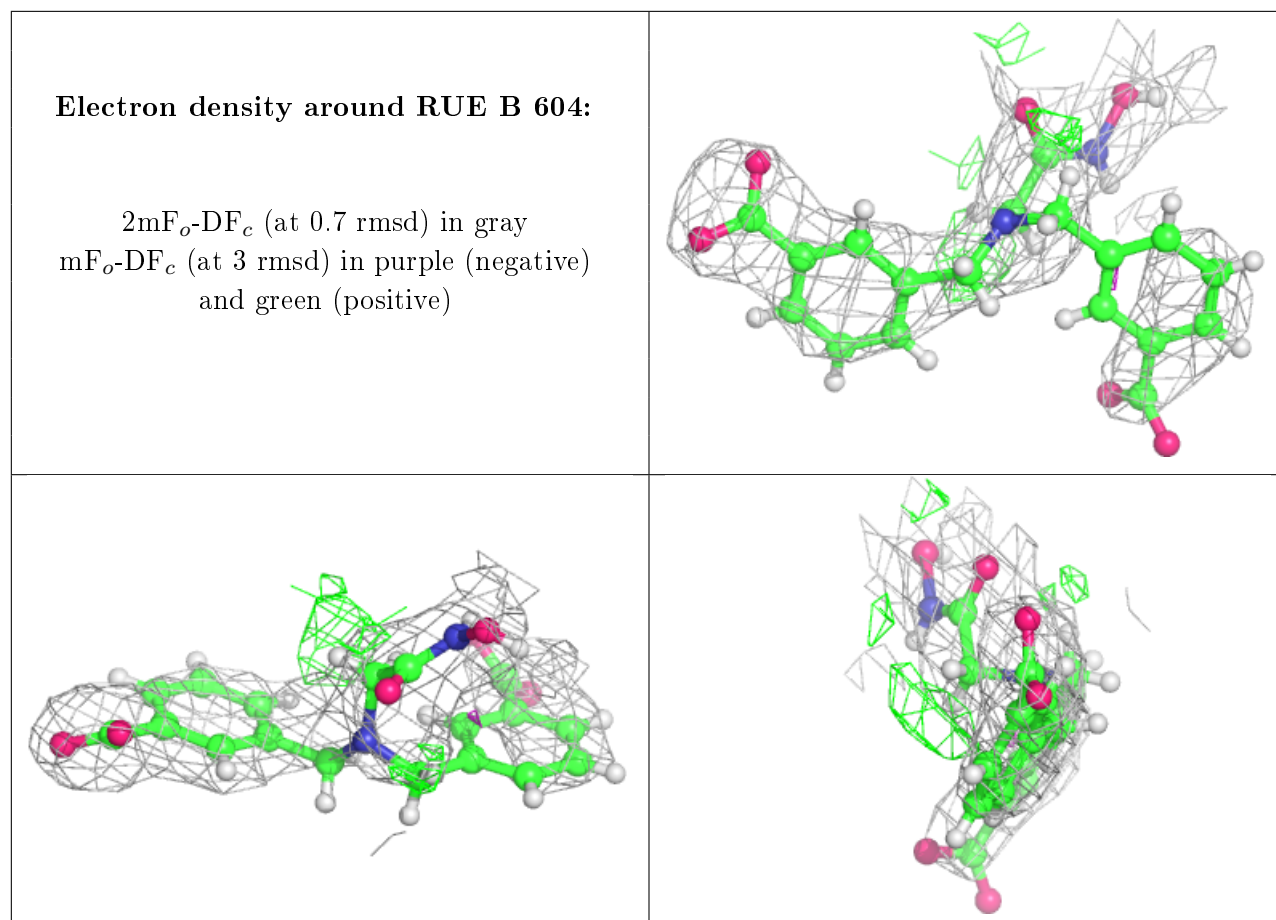
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RUE A 605 (B):

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.