



Full wwPDB X-ray Structure Validation Report i

Sep 11, 2023 – 04:56 pm BST

PDB ID : 8A9Q
Title : Computational design of stable mammalian serum albumins for bacterial expression
Authors : Khersonsky, O.; Dym, O.; Fleishman, J.S.
Deposited on : 2022-06-29
Resolution : 2.00 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

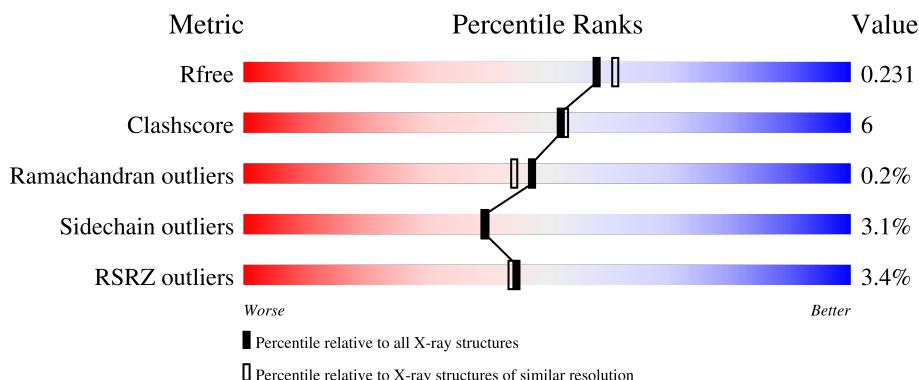
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

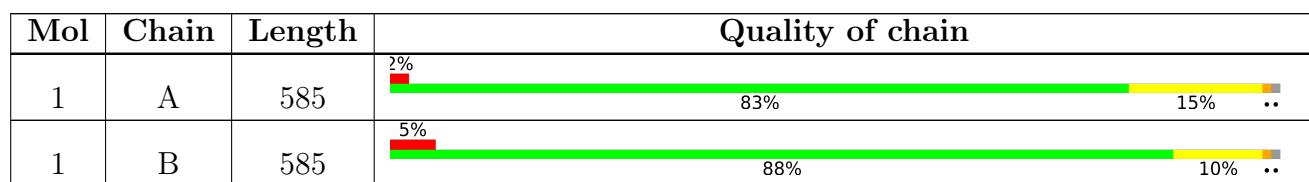
The reported resolution of this entry is 2.00 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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.



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9165 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 Albumin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	582	Total	C	N	O	S	0	0	1
			4458	2831	747	838	42			
1	B	582	Total	C	N	O	S	0	1	0
			4444	2826	746	829	43			

There are 32 discrepancies between the modelled and reference sequences:

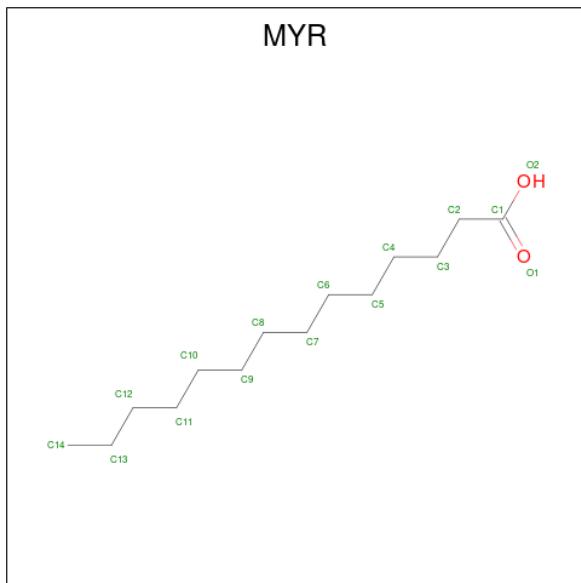
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	HIS	engineered mutation	UNP P02768
A	42	MET	LEU	engineered mutation	UNP P02768
A	120	PRO	VAL	engineered mutation	UNP P02768
A	156	TYR	PHE	engineered mutation	UNP P02768
A	187	GLU	ASP	engineered mutation	UNP P02768
A	198	HIS	LEU	engineered mutation	UNP P02768
A	202	ILE	SER	engineered mutation	UNP P02768
A	310	ILE	VAL	engineered mutation	UNP P02768
A	371	SER	ALA	engineered mutation	UNP P02768
A	381	ILE	VAL	engineered mutation	UNP P02768
A	409	ILE	VAL	engineered mutation	UNP P02768
A	427	ALA	SER	engineered mutation	UNP P02768
A	455	ILE	VAL	engineered mutation	UNP P02768
A	519	GLU	LYS	engineered mutation	UNP P02768
A	552	SER	ALA	engineered mutation	UNP P02768
A	576	ILE	VAL	engineered mutation	UNP P02768
B	39	LEU	HIS	engineered mutation	UNP P02768
B	42	MET	LEU	engineered mutation	UNP P02768
B	120	PRO	VAL	engineered mutation	UNP P02768
B	156	TYR	PHE	engineered mutation	UNP P02768
B	187	GLU	ASP	engineered mutation	UNP P02768
B	198	HIS	LEU	engineered mutation	UNP P02768
B	202	ILE	SER	engineered mutation	UNP P02768
B	310	ILE	VAL	engineered mutation	UNP P02768
B	371	SER	ALA	engineered mutation	UNP P02768

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Chain	Residue	Modelled	Actual	Comment	Reference
B	381	ILE	VAL	engineered mutation	UNP P02768
B	409	ILE	VAL	engineered mutation	UNP P02768
B	427	ALA	SER	engineered mutation	UNP P02768
B	455	ILE	VAL	engineered mutation	UNP P02768
B	519	GLU	LYS	engineered mutation	UNP P02768
B	552	SER	ALA	engineered mutation	UNP P02768
B	576	ILE	VAL	engineered mutation	UNP P02768

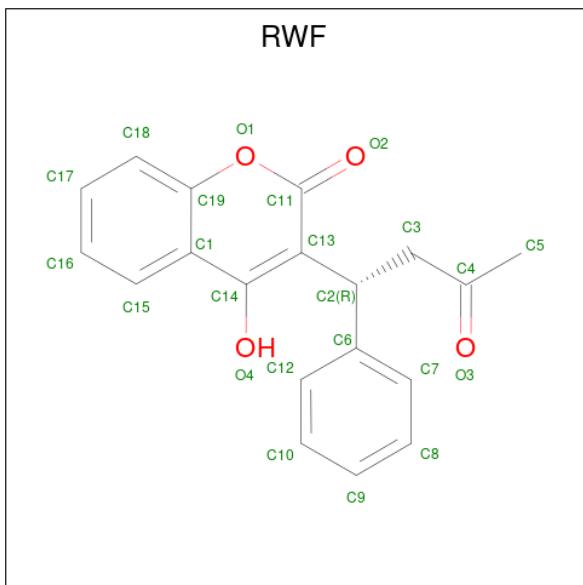
- Molecule 2 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	A	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0
2	B	1	Total C O 16 14 2	0	0

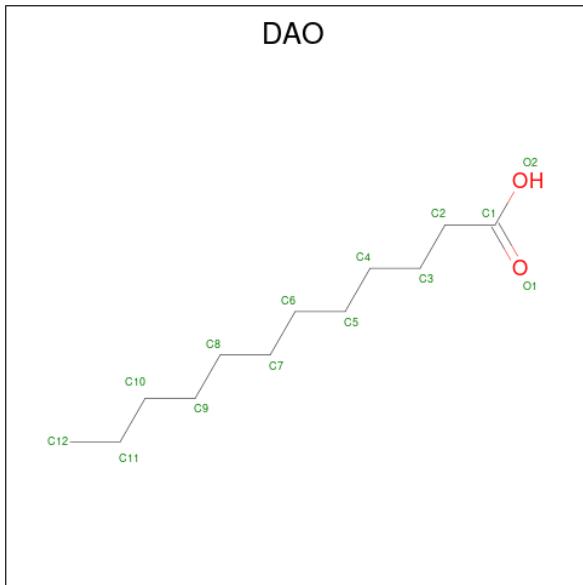
- Molecule 3 is R-WARFARIN (three-letter code: RWF) (formula: C₁₉H₁₆O₄) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 23	C 19	O 4	0	0
3	B	1	Total 23	C 19	O 4	0	0

- Molecule 4 is LAURIC ACID (three-letter code: DAO) (formula: C₁₂H₂₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total 14	C 12	O 2	0	0

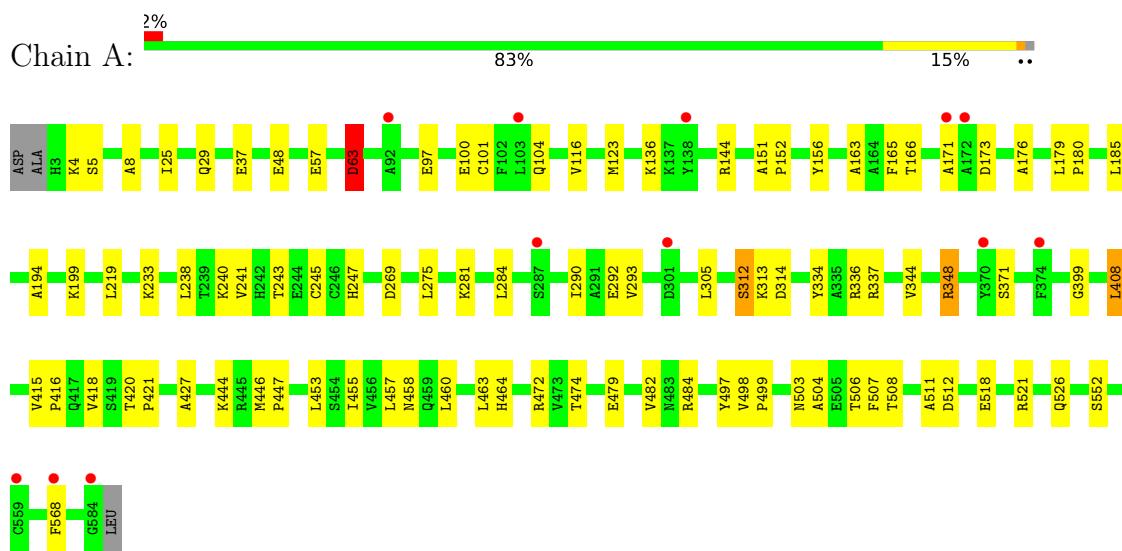
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	52	Total O 52 52	0	0
5	B	39	Total O 39 39	0	0

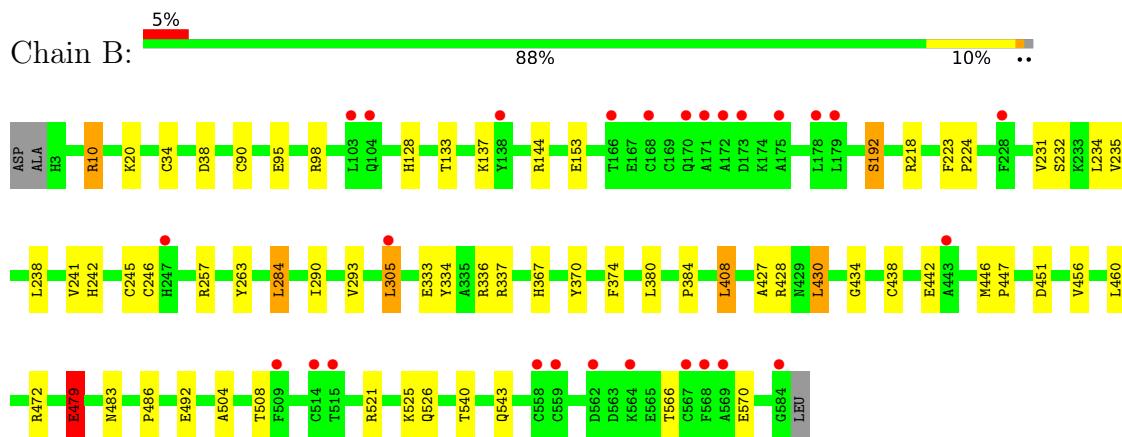
3 Residue-property plots [\(i\)](#)

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: Albumin



- Molecule 1: Albumin



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	38.26Å 92.13Å 95.55Å 74.35° 89.29° 79.98°	Depositor
Resolution (Å)	46.02 – 2.00 46.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (46.02-2.00) 89.0 (46.18-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ ¹	1.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15.2	Depositor
R , R_{free}	0.220 , 0.271 0.235 , 0.231	Depositor DCC
R_{free} test set	3600 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.290	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.1	EDS
L-test for twinning ²	$< L > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.076 for h,h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9165	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MYR, DAO, RWF

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	0.84	1/4548 (0.0%)	1.01	8/6165 (0.1%)
1	B	0.83	0/4535	1.03	6/6152 (0.1%)
All	All	0.83	1/9083 (0.0%)	1.02	14/12317 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	LYS	C-O	5.12	1.33	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336	ARG	NE-CZ-NH2	-13.89	113.35	120.30
1	B	336	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	B	144	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	B	144	ARG	NE-CZ-NH2	-10.41	115.09	120.30
1	A	336	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	472	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	144	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	472	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	A	348	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	336	ARG	NE-CZ-NH1	5.72	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	428	ARG	NE-CZ-NH2	5.63	123.12	120.30
1	B	428	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	63	ASP	CB-CA-C	5.25	120.90	110.40
1	A	199	LYS	CB-CA-C	5.04	120.48	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	SER	Peptide
1	A	399	GLY	Peptide

5.2 Too-close contacts [\(i\)](#)

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	4458	0	4226	52	0
1	B	4444	0	4201	40	0
2	A	64	0	108	11	0
2	B	48	0	81	1	0
3	A	23	0	16	1	0
3	B	23	0	16	2	0
4	B	14	0	23	2	0
5	A	52	0	0	0	0
5	B	39	0	0	1	0
All	All	9165	0	8671	98	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 6.

All (98) 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:A:241:VAL:O	1:A:245:CYS:SG	2.09	1.09
1:A:312:SER:OG	1:A:313:LYS:O	1.83	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:ALA:O	1:B:508:THR:HG23	1.77	0.84
1:A:504:ALA:O	1:A:508:THR:HG23	1.81	0.80
1:B:305:LEU:HD11	1:B:333:GLU:HB3	1.64	0.80
1:A:415:VAL:HG12	1:A:418:VAL:HG23	1.63	0.79
1:A:552:SER:OG	2:A:603:MYR:O2	2.02	0.77
1:A:460:LEU:HD11	2:A:602:MYR:H132	1.72	0.72
1:A:453:LEU:HD11	2:A:601:MYR:H81	1.71	0.72
1:A:408:LEU:HD13	1:A:427:ALA:CB	2.21	0.70
1:B:408:LEU:HD13	1:B:427:ALA:CB	2.21	0.70
1:A:116:VAL:HG21	1:B:128:HIS:CG	2.27	0.69
1:B:238:LEU:HD21	3:B:605:RWF:C12	2.23	0.68
1:A:101:CYS:HA	1:A:104:GLN:OE1	1.97	0.63
1:B:218:ARG:NE	5:B:701:HOH:O	2.31	0.63
1:A:503:ASN:O	1:A:506:THR:OG1	2.15	0.63
2:B:602:MYR:H92	4:B:603:DAO:H22	1.82	0.61
1:A:313:LYS:O	1:A:314:ASP:HB2	2.00	0.61
2:A:602:MYR:H132	2:A:602:MYR:H91	1.83	0.60
1:B:540:THR:OG1	1:B:543:GLN:HG3	2.00	0.60
1:B:472:ARG:NH2	1:B:492:GLU:O	2.35	0.59
1:A:418:VAL:HG21	2:A:602:MYR:C14	2.32	0.59
1:B:374:PHE:O	1:B:374:PHE:CD1	2.56	0.59
1:A:408:LEU:HD13	1:A:427:ALA:HB3	1.84	0.58
2:A:601:MYR:H82	2:A:602:MYR:C2	2.34	0.57
1:B:430:LEU:CD1	1:B:456:VAL:HG11	2.34	0.57
1:A:123:MET:HB3	1:A:165:PHE:HE1	1.70	0.56
2:A:601:MYR:H82	2:A:602:MYR:H22	1.88	0.56
1:B:242:HIS:O	1:B:246:CYS:SG	2.64	0.56
1:A:5:SER:HB3	1:A:8:ALA:HB3	1.88	0.55
1:B:430:LEU:HD21	4:B:603:DAO:H61	1.89	0.55
1:B:133:THR:O	1:B:137:LYS:HB2	2.08	0.54
1:A:464:HIS:HE1	1:A:474:THR:OG1	1.91	0.54
1:B:408:LEU:HD13	1:B:427:ALA:HB2	1.90	0.54
1:A:4:LYS:CG	1:A:57:GLU:OE1	2.56	0.54
1:B:290:ILE:O	1:B:293:VAL:HG22	2.09	0.52
1:A:415:VAL:CG1	1:A:418:VAL:HG23	2.38	0.52
1:A:243:THR:O	1:A:247:HIS:CD2	2.62	0.51
1:A:511:ALA:HA	1:A:568:PHE:CE2	2.45	0.51
1:B:479:GLU:HA	1:B:479:GLU:OE1	2.11	0.51
1:A:179:LEU:N	1:A:180:PRO:CD	2.74	0.51
1:A:460:LEU:HD11	2:A:602:MYR:C13	2.41	0.50
3:B:605:RWF:O4	3:B:605:RWF:H3C1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ALA:HB3	1:A:152:PRO:HD3	1.95	0.49
1:A:408:LEU:HD13	1:A:427:ALA:HB2	1.94	0.49
1:B:305:LEU:HD13	1:B:337:ARG:HD2	1.95	0.49
1:B:374:PHE:CD1	1:B:374:PHE:C	2.87	0.48
1:A:290:ILE:O	1:A:293:VAL:HG22	2.13	0.48
1:B:231:VAL:O	1:B:235:VAL:HG23	2.13	0.48
1:A:63:ASP:OD1	1:A:63:ASP:N	2.48	0.47
1:B:446:MET:N	1:B:447:PRO:CD	2.77	0.47
1:B:380:LEU:O	1:B:384:PRO:HD2	2.14	0.47
1:B:367:HIS:HA	1:B:370:TYR:CZ	2.50	0.47
1:A:420:THR:HB	1:A:421:PRO:HD3	1.97	0.46
1:B:95:GLU:OE2	1:B:98:ARG:NE	2.41	0.46
1:B:434:GLY:O	1:B:438:CYS:HB2	2.16	0.46
1:A:446:MET:N	1:A:447:PRO:CD	2.79	0.46
1:A:458:ASN:OD1	1:A:484:ARG:NH1	2.46	0.46
1:A:463:LEU:HD23	1:A:463:LEU:HA	1.86	0.46
1:A:348:ARG:CG	1:A:482:VAL:HB	2.46	0.45
1:A:457:LEU:HD21	2:A:602:MYR:H62	1.99	0.45
1:A:275:LEU:HD23	1:A:293:VAL:HG11	2.00	0.44
1:B:34[B]:CYS:SG	1:B:38:ASP:HB2	2.58	0.44
1:A:518:GLU:OE2	1:A:521:ARG:NH1	2.50	0.44
1:B:241:VAL:HG13	1:B:257:ARG:HG3	2.00	0.44
1:B:566:THR:HG22	1:B:570:GLU:OE2	2.18	0.44
1:A:97:GLU:HA	1:A:100:GLU:OE1	2.18	0.43
1:A:344:VAL:HG23	1:A:482:VAL:HA	2.00	0.43
1:B:408:LEU:HD13	1:B:427:ALA:HB3	2.00	0.43
1:B:153:GLU:OE2	1:B:192:SER:CB	2.67	0.43
1:B:234:LEU:O	1:B:238:LEU:HB2	2.17	0.43
1:B:460:LEU:C	1:B:460:LEU:HD23	2.38	0.43
2:A:601:MYR:H82	2:A:602:MYR:H31	2.00	0.43
1:B:305:LEU:CD1	1:B:337:ARG:CZ	2.97	0.43
1:B:10:ARG:HA	1:B:10:ARG:HD2	1.75	0.43
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.65	0.43
1:A:507:PHE:HB3	2:A:603:MYR:H112	1.99	0.43
1:A:240:LYS:O	1:A:241:VAL:C	2.56	0.43
3:A:605:RWF:C7	3:A:605:RWF:O3	2.67	0.43
1:B:483:ASN:C	1:B:486:PRO:HD2	2.38	0.43
1:B:521:ARG:O	1:B:525:LYS:HG3	2.19	0.42
1:A:185:LEU:HD23	1:A:185:LEU:HA	1.91	0.42
1:A:194:ALA:HB1	1:A:455:ILE:HG23	2.01	0.42
1:A:416:PRO:HG2	1:A:497:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ALA:HA	1:A:166:THR:OG1	2.20	0.42
1:A:37:GLU:H	1:A:37:GLU:CD	2.23	0.42
1:A:25:ILE:O	1:A:29:GLN:HG3	2.20	0.41
1:A:173:ASP:OD2	1:A:176:ALA:HB2	2.20	0.41
1:A:408:LEU:HD21	1:A:526:GLN:HB3	2.01	0.41
1:A:498:VAL:O	1:A:499:PRO:C	2.59	0.41
1:B:223:PHE:N	1:B:224:PRO:CD	2.83	0.41
1:A:344:VAL:HG22	1:A:348:ARG:NH1	2.36	0.41
1:B:90:CYS:O	1:B:98:ARG:HG3	2.21	0.41
1:A:305:LEU:HD21	1:A:337:ARG:HD2	2.03	0.40
1:A:312:SER:C	1:A:313:LYS:O	2.55	0.40
1:B:408:LEU:HD21	1:B:526:GLN:HB3	2.03	0.40
1:B:263:TYR:CD1	1:B:263:TYR:C	2.94	0.40
1:B:284:LEU:HD23	1:B:284:LEU:HA	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [\(i\)](#)

5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	580/585 (99%)	553 (95%)	26 (4%)	1 (0%)	47 44
1	B	581/585 (99%)	554 (95%)	26 (4%)	1 (0%)	47 44
All	All	1161/1170 (99%)	1107 (95%)	52 (4%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ALA
1	B	479	GLU

5.3.2 Protein sidechains [\(i\)](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	457/512 (89%)	442 (97%)	15 (3%)	38 37
1	B	451/512 (88%)	438 (97%)	13 (3%)	42 43
All	All	908/1024 (89%)	880 (97%)	28 (3%)	40 40

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

Mol	Chain	Res	Type
1	A	48	GLU
1	A	63	ASP
1	A	156	TYR
1	A	219	LEU
1	A	233	LYS
1	A	238	LEU
1	A	269	ASP
1	A	281	LYS
1	A	284	LEU
1	A	292	GLU
1	A	334	TYR
1	A	371	SER
1	A	408	LEU
1	A	479	GLU
1	A	512	ASP
1	B	10	ARG
1	B	20	LYS
1	B	192	SER
1	B	232	SER
1	B	245	CYS
1	B	284	LEU
1	B	305	LEU
1	B	334	TYR
1	B	408	LEU
1	B	430	LEU
1	B	442	GLU
1	B	451	ASP

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Mol	Chain	Res	Type
1	B	479	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	247	HIS
1	A	464	HIS
1	B	196	GLN
1	B	242	HIS
1	B	397	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 monosaccharides in this entry.

5.6 Ligand geometry [\(i\)](#)

10 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
4	DAO	B	603	-	13,13,13	0.58	0	13,13,13	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MYR	A	601	-	15,15,15	1.14	1 (6%)	15,15,15	0.98	1 (6%)
2	MYR	A	603	-	15,15,15	1.69	2 (13%)	15,15,15	1.09	0
3	RWF	A	605	-	21,25,25	2.22	5 (23%)	26,35,35	2.54	9 (34%)
2	MYR	A	602	-	15,15,15	0.50	0	15,15,15	1.90	4 (26%)
2	MYR	B	601	-	15,15,15	0.94	0	15,15,15	0.98	0
3	RWF	B	605	-	21,25,25	1.76	4 (19%)	26,35,35	3.17	9 (34%)
2	MYR	A	604	-	15,15,15	0.87	1 (6%)	15,15,15	1.24	1 (6%)
2	MYR	B	604	-	15,15,15	1.51	2 (13%)	15,15,15	0.65	0
2	MYR	B	602	-	15,15,15	0.91	1 (6%)	15,15,15	1.06	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
4	DAO	B	603	-	-	8/11/11/11	-
2	MYR	A	601	-	-	7/13/13/13	-
2	MYR	A	603	-	-	8/13/13/13	-
3	RWF	A	605	-	-	3/12/12/12	0/3/3/3
2	MYR	A	602	-	-	8/13/13/13	-
2	MYR	B	601	-	-	5/13/13/13	-
3	RWF	B	605	-	-	3/12/12/12	0/3/3/3
2	MYR	A	604	-	-	8/13/13/13	-
2	MYR	B	604	-	-	5/13/13/13	-
2	MYR	B	602	-	-	9/13/13/13	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	RWF	O3-C4	6.49	1.46	1.21
3	B	605	RWF	O3-C4	5.40	1.42	1.21
2	A	603	MYR	C2-C1	5.35	1.63	1.50
2	B	604	MYR	C2-C1	4.24	1.60	1.50
3	A	605	RWF	O1-C19	3.96	1.43	1.36
3	A	605	RWF	C3-C4	3.95	1.57	1.51
3	A	605	RWF	C6-C2	-3.83	1.42	1.53
3	B	605	RWF	C6-C2	-3.44	1.43	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	604	MYR	C3-C2	2.53	1.61	1.52
2	A	603	MYR	C3-C2	2.29	1.60	1.52
3	A	605	RWF	C17-C18	2.28	1.41	1.36
2	A	604	MYR	C2-C1	2.26	1.55	1.50
2	B	602	MYR	C2-C1	2.25	1.55	1.50
3	B	605	RWF	O1-C19	2.18	1.40	1.36
2	A	601	MYR	C2-C1	2.15	1.55	1.50
3	B	605	RWF	C5-C4	2.12	1.57	1.49

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	RWF	O3-C4-C3	-11.65	102.96	121.72
3	B	605	RWF	C3-C2-C6	-7.10	94.27	112.31
3	A	605	RWF	C2-C3-C4	-6.08	106.34	114.47
3	A	605	RWF	O3-C4-C3	-5.48	112.90	121.72
3	A	605	RWF	O3-C4-C5	-4.85	109.08	121.40
3	A	605	RWF	C15-C1-C19	4.24	121.41	116.50
3	B	605	RWF	C5-C4-C3	-3.97	110.89	116.56
3	A	605	RWF	C5-C4-C3	-3.92	110.96	116.56
3	B	605	RWF	O3-C4-C5	-3.88	111.55	121.40
2	A	602	MYR	O2-C1-O1	3.53	132.09	123.30
2	A	602	MYR	O1-C1-C2	-3.32	112.42	123.08
2	A	602	MYR	C3-C2-C1	-3.23	106.32	114.47
3	B	605	RWF	O1-C19-C1	-2.99	118.31	121.20
3	A	605	RWF	C3-C2-C13	2.65	116.61	112.11
3	A	605	RWF	C9-C10-C12	2.48	123.97	120.19
3	A	605	RWF	C14-C13-C2	2.42	127.06	121.62
3	A	605	RWF	C10-C9-C8	-2.36	115.55	119.93
3	B	605	RWF	C15-C1-C19	2.21	119.06	116.50
2	A	601	MYR	C3-C2-C1	-2.20	108.92	114.47
3	B	605	RWF	C8-C7-C6	2.18	123.35	120.65
3	B	605	RWF	C12-C6-C7	-2.14	115.62	118.29
3	B	605	RWF	C2-C3-C4	2.13	117.31	114.47
2	A	602	MYR	C10-C9-C8	-2.04	104.05	114.42
2	A	604	MYR	O1-C1-C2	-2.03	116.55	123.08

There are no chirality outliers.

All (64) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MYR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
2	A	603	MYR	C1-C2-C3-C4
4	B	603	DAO	C5-C6-C7-C8
3	B	605	RWF	C2-C3-C4-O3
4	B	603	DAO	C11-C10-C9-C8
2	B	601	MYR	C2-C3-C4-C5
2	A	601	MYR	C11-C10-C9-C8
2	B	604	MYR	C5-C6-C7-C8
2	B	602	MYR	C6-C7-C8-C9
2	B	601	MYR	C11-C10-C9-C8
2	A	604	MYR	C9-C10-C11-C12
4	B	603	DAO	C2-C3-C4-C5
2	A	604	MYR	C1-C2-C3-C4
2	A	602	MYR	C10-C11-C12-C13
2	A	601	MYR	C5-C6-C7-C8
2	B	602	MYR	C7-C8-C9-C10
2	A	604	MYR	C3-C4-C5-C6
2	A	602	MYR	C6-C7-C8-C9
2	B	601	MYR	C6-C7-C8-C9
2	A	601	MYR	C10-C11-C12-C13
2	A	604	MYR	C5-C6-C7-C8
2	A	603	MYR	C3-C4-C5-C6
2	B	604	MYR	C2-C3-C4-C5
2	A	604	MYR	C4-C5-C6-C7
4	B	603	DAO	C1-C2-C3-C4
2	B	602	MYR	C5-C6-C7-C8
2	A	603	MYR	C4-C5-C6-C7
2	A	603	MYR	C11-C10-C9-C8
2	A	601	MYR	C11-C12-C13-C14
4	B	603	DAO	C3-C4-C5-C6
2	A	602	MYR	C11-C12-C13-C14
2	B	602	MYR	C11-C12-C13-C14
2	B	602	MYR	C9-C10-C11-C12
2	A	602	MYR	C11-C10-C9-C8
4	B	603	DAO	C7-C8-C9-C10
2	A	603	MYR	C6-C7-C8-C9
2	B	604	MYR	C7-C8-C9-C10
3	A	605	RWF	C6-C2-C3-C4
3	A	605	RWF	C13-C2-C3-C4
2	A	604	MYR	C7-C8-C9-C10
2	A	603	MYR	C10-C11-C12-C13
3	B	605	RWF	C13-C2-C6-C7
2	B	602	MYR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	B	605	RWF	C13-C2-C6-C12
3	A	605	RWF	C2-C3-C4-C5
2	B	604	MYR	O1-C1-C2-C3
2	B	602	MYR	O2-C1-C2-C3
2	B	604	MYR	O2-C1-C2-C3
2	B	602	MYR	O1-C1-C2-C3
2	B	601	MYR	O1-C1-C2-C3
2	A	603	MYR	O1-C1-C2-C3
2	A	603	MYR	O2-C1-C2-C3
2	A	601	MYR	O2-C1-C2-C3
2	A	602	MYR	O1-C1-C2-C3
2	A	602	MYR	O2-C1-C2-C3
2	B	601	MYR	O2-C1-C2-C3
2	A	602	MYR	C2-C3-C4-C5
2	A	604	MYR	O2-C1-C2-C3
2	A	602	MYR	C9-C10-C11-C12
4	B	603	DAO	O1-C1-C2-C3
2	A	604	MYR	O1-C1-C2-C3
4	B	603	DAO	O2-C1-C2-C3
2	A	601	MYR	O1-C1-C2-C3
2	B	602	MYR	C2-C3-C4-C5

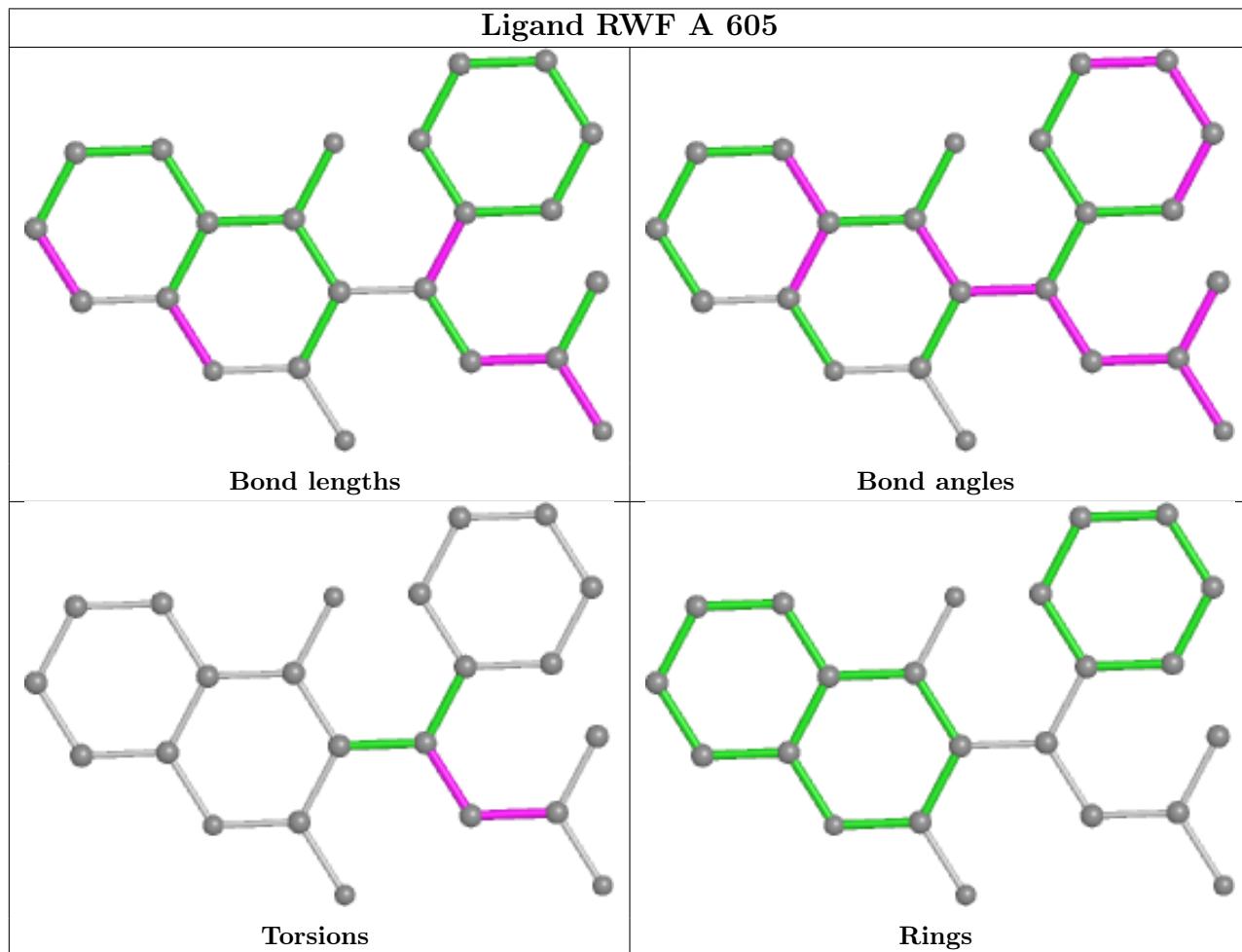
There are no ring outliers.

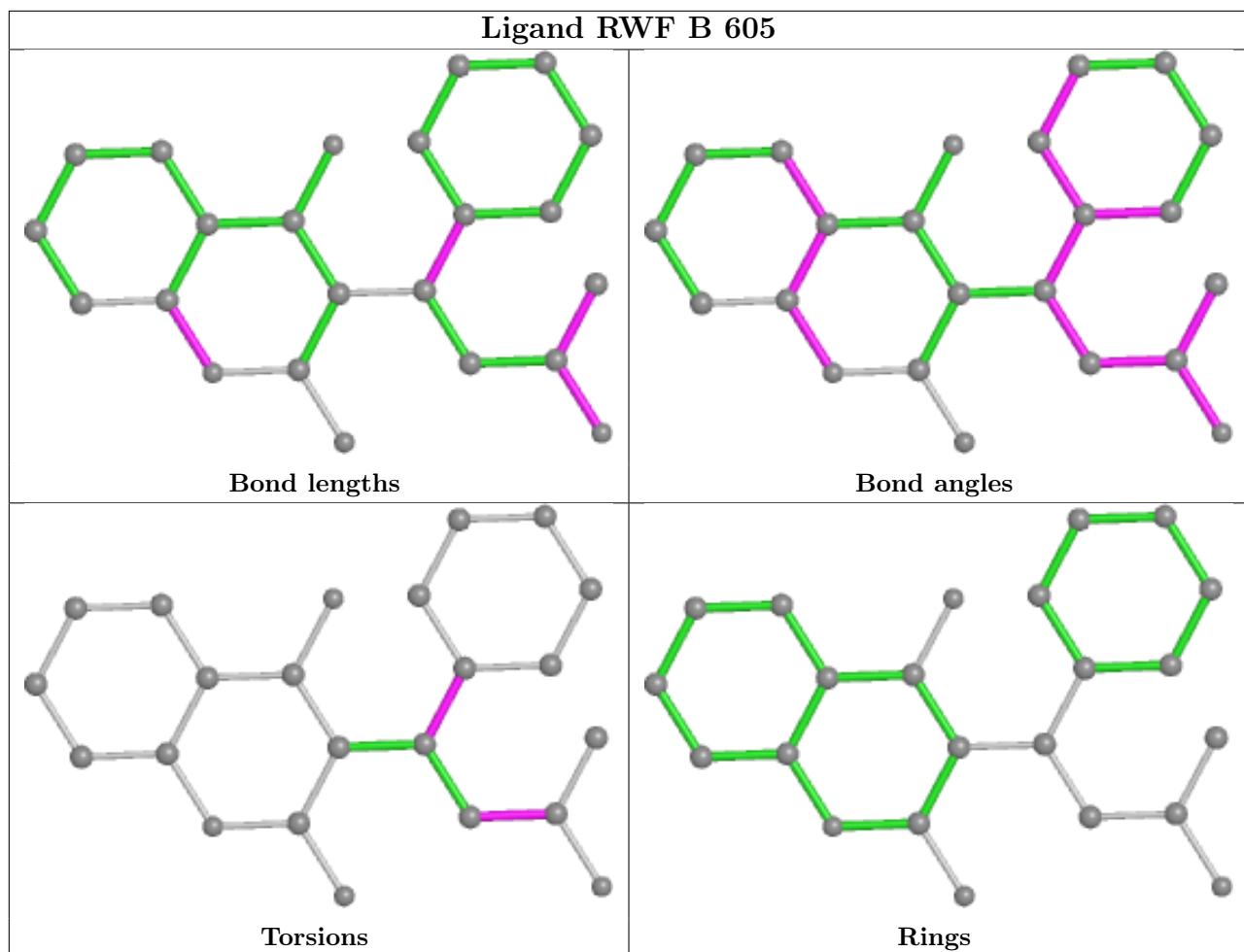
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	DAO	2	0
2	A	601	MYR	4	0
2	A	603	MYR	2	0
3	A	605	RWF	1	0
2	A	602	MYR	8	0
3	B	605	RWF	2	0
2	B	602	MYR	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	582/585 (99%)	0.15	12 (2%) 63 62	27, 41, 59, 88	0
1	B	582/585 (99%)	0.19	27 (4%) 32 31	25, 42, 59, 85	0
All	All	1164/1170 (99%)	0.17	39 (3%) 45 44	25, 41, 60, 88	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	11.8
1	B	514	CYS	6.7
1	B	168	CYS	6.6
1	A	171	ALA	6.3
1	B	568	PHE	6.2
1	B	179	LEU	4.7
1	B	172	ALA	4.6
1	B	584	GLY	4.3
1	B	559	CYS	3.9
1	B	562	ASP	3.7
1	B	175	ALA	3.6
1	B	178	LEU	3.6
1	B	138	TYR	3.5
1	A	559	CYS	3.4
1	A	92	ALA	3.4
1	B	171	ALA	3.1
1	B	173	ASP	3.0
1	B	103	LEU	3.0
1	B	247	HIS	2.9
1	A	103	LEU	2.9
1	A	370	TYR	2.8
1	A	138	TYR	2.8
1	B	305	LEU	2.6
1	B	515	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	287	SER	2.5
1	B	564	LYS	2.5
1	B	509	PHE	2.5
1	B	166	THR	2.5
1	A	374	PHE	2.3
1	A	301	ASP	2.3
1	A	568	PHE	2.2
1	A	584	GLY	2.2
1	B	104	GLN	2.2
1	B	170	GLN	2.2
1	B	443	ALA	2.2
1	B	567	CYS	2.2
1	B	569	ALA	2.1
1	B	228	PHE	2.1
1	B	558	CYS	2.1

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

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

6.3 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

6.4 Ligands [\(i\)](#)

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

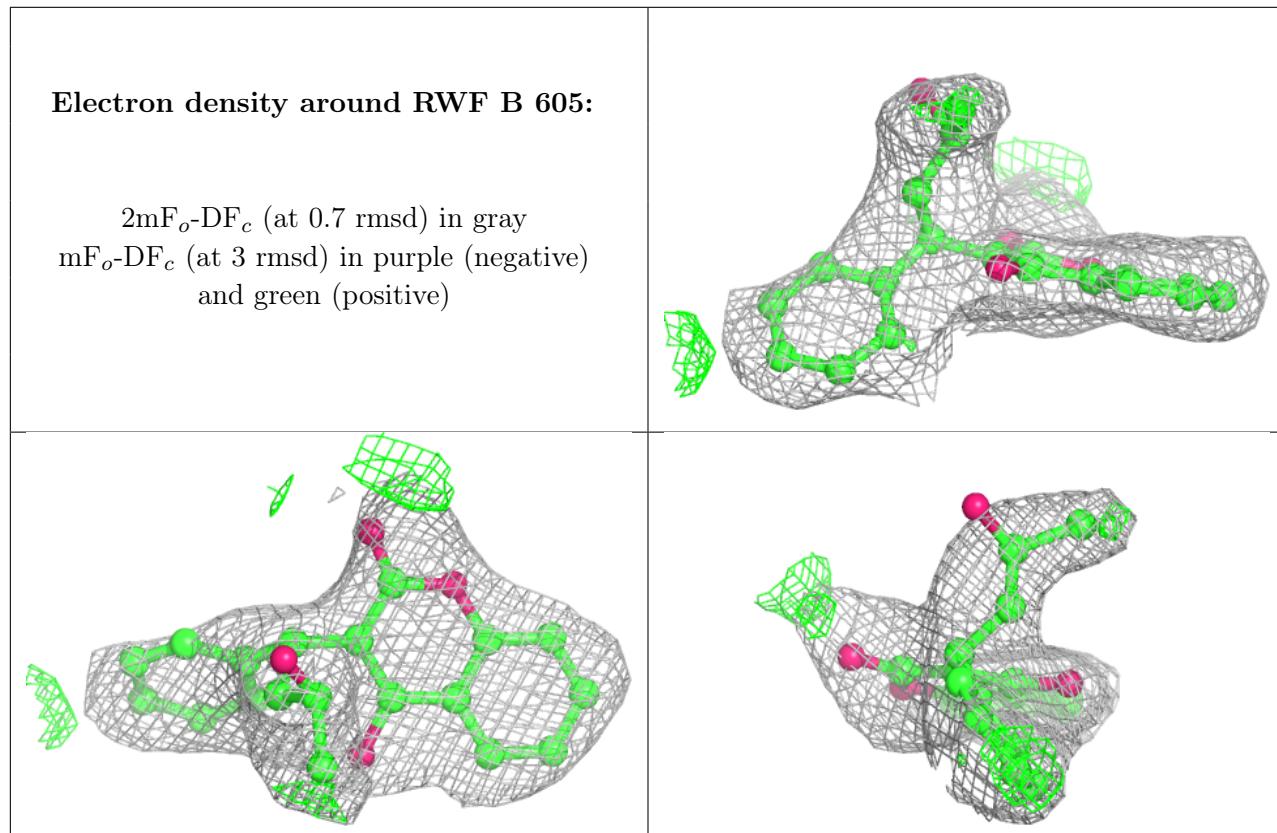
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MYR	A	603	16/16	0.72	0.18	33,39,51,57	0
3	RWF	B	605	23/23	0.74	0.18	55,66,72,76	0
3	RWF	A	605	23/23	0.77	0.23	57,66,77,82	0
2	MYR	A	602	16/16	0.82	0.23	52,64,68,68	0
2	MYR	A	604	16/16	0.82	0.21	44,54,66,72	0
4	DAO	B	603	14/14	0.83	0.17	50,56,72,74	0
2	MYR	B	602	16/16	0.84	0.17	39,47,57,57	0
2	MYR	B	604	16/16	0.87	0.14	35,43,56,57	0

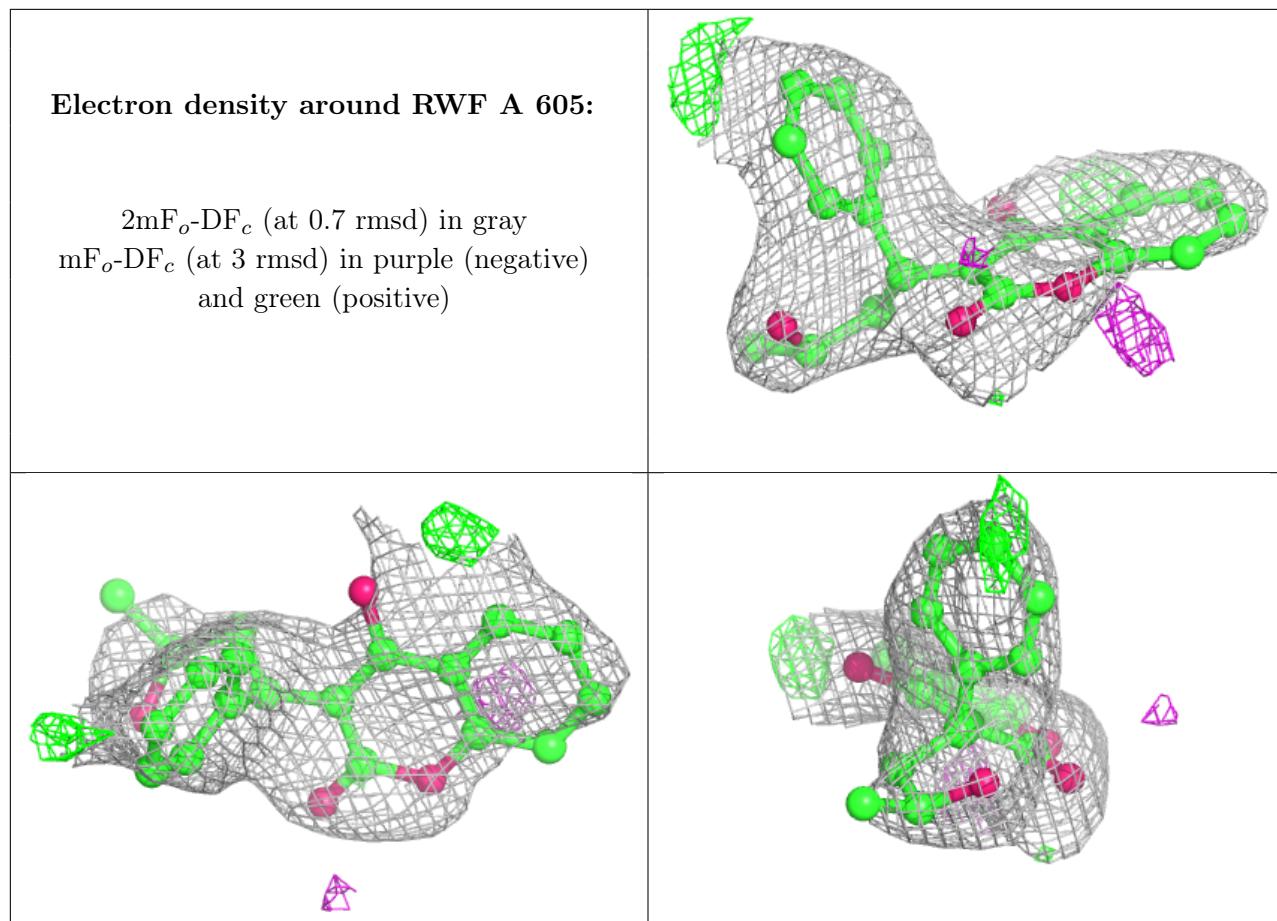
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MYR	A	601	16/16	0.87	0.17	36,47,52,53	0
2	MYR	B	601	16/16	0.90	0.20	48,57,63,64	0

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.





6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.