



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:01 AM UTC

PDB ID : 8A9Q / pdb_00008a9q
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 ⓘ 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

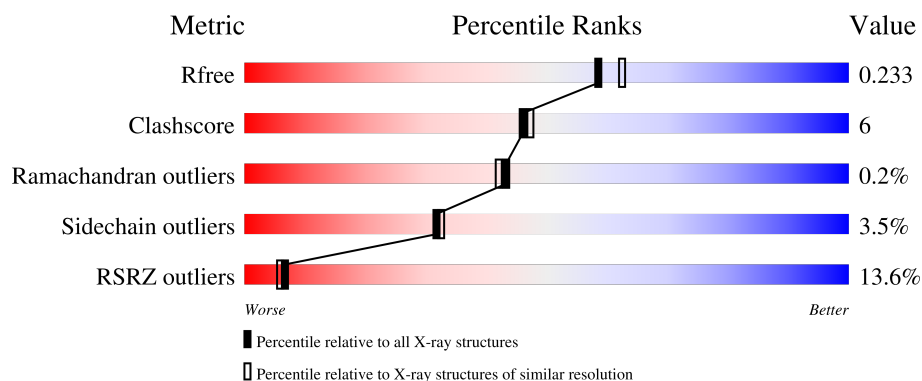
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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.

Mol	Chain	Length	Quality of chain
1	A	585	11% 81% 17% ..
1	B	585	16% 82% 15% ..

2 Entry composition

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:

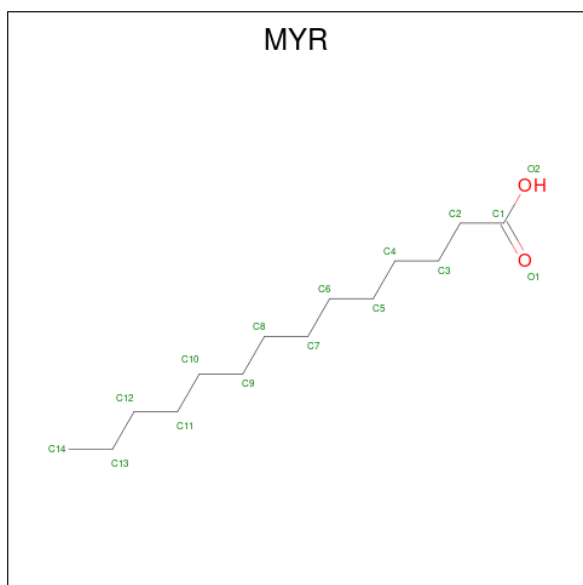
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	LEU	HIS	engineered mutation	UNP P02768
A	42	MET	LEU	engineered mutation	UNP P02768
A	120	PRO	VAL	engineered mutation	UNP P02768
A	156	TYR	PHE	engineered mutation	UNP P02768
A	187	GLU	ASP	engineered mutation	UNP P02768
A	198	HIS	LEU	engineered mutation	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

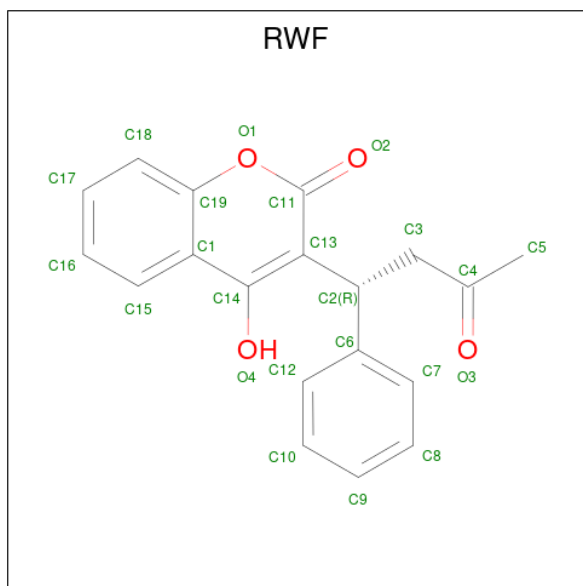
- Molecule 2 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



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

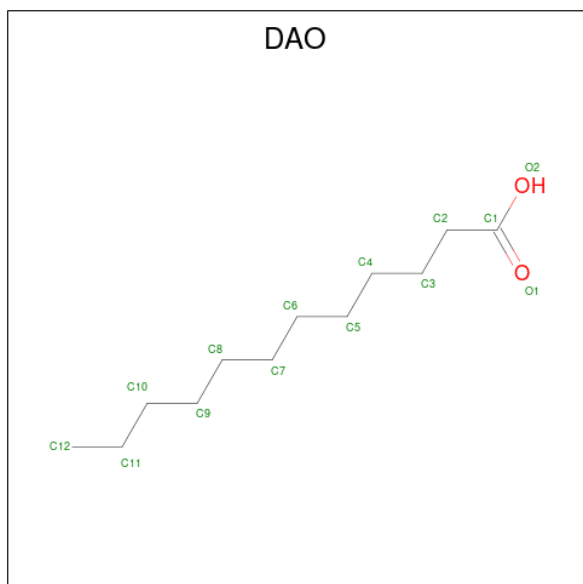
- Molecule 3 is R-WARFARIN (CCD ID: RWF) (formula: $C_{19}H_{16}O_4$) (labeled as "Ligand of

Interest" by depositor).



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

- Molecule 4 is LAURIC ACID (CCD ID: DAO) (formula: $C_{12}H_{24}O_2$).



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

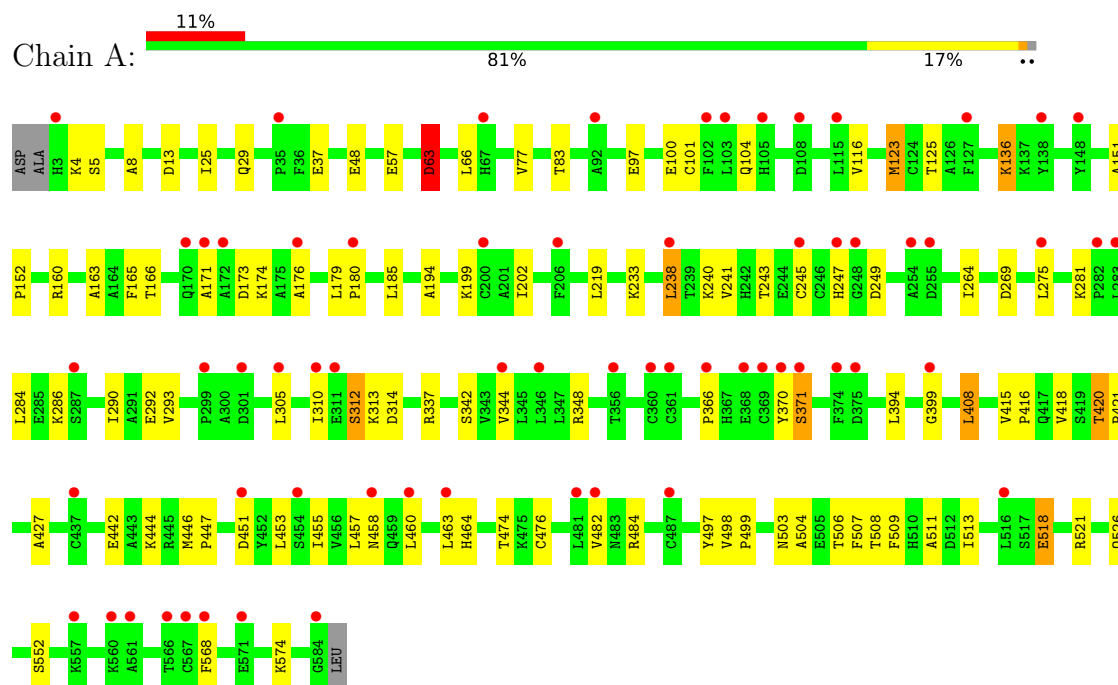
- Molecule 5 is water.

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

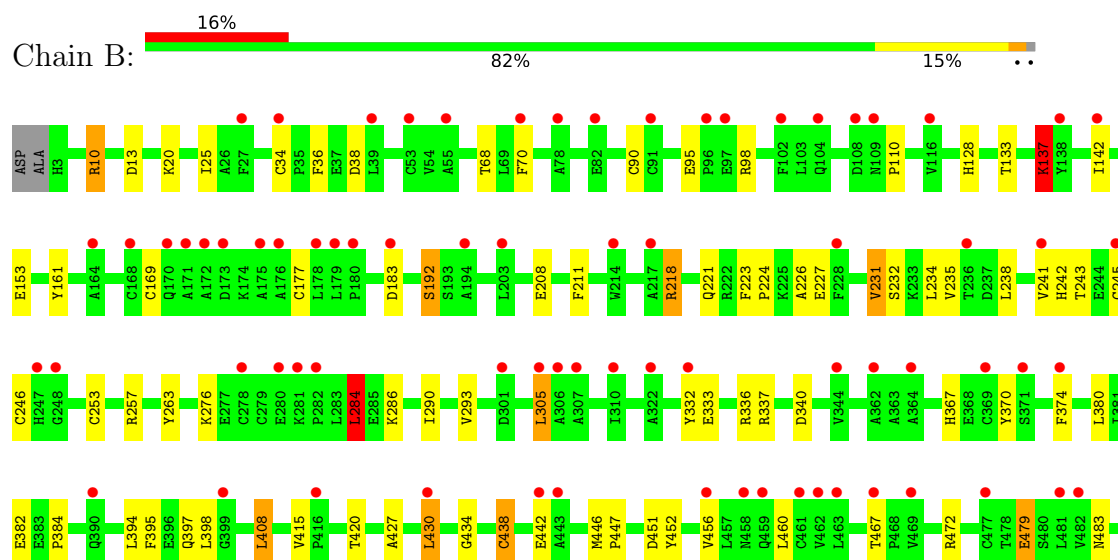
3 Residue-property plots [i](#)

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

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 46.02 – 2.00	Depositor EDS
% Data completeness (in resolution range)	89.0 (46.02-2.00) 89.0 (46.02-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.15.2	Depositor
R, R_{free}	0.220 , 0.271 0.236 , 0.233	Depositor DCC
R_{free} test set	3603 reflections (4.31%)	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)	0.33 , 25.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.23	7/4548 (0.2%)	1.63	25/6165 (0.4%)
1	B	1.23	6/4535 (0.1%)	1.69	44/6152 (0.7%)
All	All	1.23	13/9083 (0.1%)	1.66	69/12317 (0.6%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	444	LYS	C-O	7.00	1.33	1.24
1	A	66	LEU	C-O	5.90	1.31	1.24
1	A	342	SER	C-O	5.82	1.31	1.23
1	A	123	MET	C-O	5.51	1.30	1.24
1	B	438	CYS	C-O	-5.47	1.17	1.24
1	B	208	GLU	C-O	-5.21	1.18	1.24
1	A	451	ASP	C-O	5.16	1.30	1.24
1	B	218	ARG	C-O	5.11	1.30	1.24
1	A	394	LEU	C-O	5.09	1.30	1.24
1	B	394	LEU	C-O	5.04	1.30	1.24
1	B	227	GLU	C-O	5.04	1.30	1.23
1	A	476	CYS	C-O	-5.03	1.17	1.24
1	B	36	PHE	C-O	5.03	1.29	1.24

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	110	PRO	CA-C-N	-7.03	112.37	122.77
1	B	110	PRO	C-N-CA	-7.03	112.37	122.77
1	B	13	ASP	CA-CB-CG	7.03	119.62	112.60
1	A	420	THR	CA-CB-OG1	-7.02	99.08	109.60
1	B	398	LEU	CA-C-N	-7.00	111.95	122.04
1	B	398	LEU	C-N-CA	-7.00	111.95	122.04
1	A	125	THR	CA-CB-OG1	-6.73	99.51	109.60
1	B	286	LYS	CA-C-N	6.51	130.59	120.82
1	B	286	LYS	C-N-CA	6.51	130.59	120.82
1	B	336	ARG	NE-CZ-NH2	-6.50	113.35	119.20
1	B	494	ASP	CA-C-N	6.42	130.45	120.82
1	B	494	ASP	C-N-CA	6.42	130.45	120.82
1	B	169	CYS	CA-C-N	6.29	128.95	120.65
1	B	169	CYS	C-N-CA	6.29	128.95	120.65
1	B	276	LYS	CA-C-N	6.27	128.59	120.44
1	B	276	LYS	C-N-CA	6.27	128.59	120.44
1	A	264	ILE	N-CA-C	-6.21	104.45	110.72
1	A	238	LEU	CA-C-N	6.16	128.82	120.38
1	A	238	LEU	C-N-CA	6.16	128.82	120.38
1	B	183	ASP	CA-CB-CG	6.05	118.65	112.60
1	B	509	PHE	CA-C-O	-6.05	114.33	121.16
1	A	77	VAL	CA-C-N	6.02	128.35	120.28
1	A	77	VAL	C-N-CA	6.02	128.35	120.28
1	B	572	GLY	CA-C-N	5.97	128.20	120.44
1	B	572	GLY	C-N-CA	5.97	128.20	120.44
1	B	420	THR	CA-CB-OG1	-5.95	100.67	109.60
1	B	542	GLU	CA-C-N	5.93	128.71	120.29
1	B	542	GLU	C-N-CA	5.93	128.71	120.29
1	A	63	ASP	CB-CA-C	5.82	120.90	109.72
1	A	310	ILE	CA-C-O	-5.77	113.56	120.78
1	A	199	LYS	CB-CA-C	5.67	120.48	110.85
1	B	573	LYS	CA-C-N	5.66	128.13	120.44
1	B	573	LYS	C-N-CA	5.66	128.13	120.44
1	B	137	LYS	N-CA-C	-5.63	105.05	111.07
1	B	397	GLN	CB-CA-C	-5.56	102.12	110.90
1	A	286	LYS	CA-C-N	5.49	127.95	120.54
1	A	286	LYS	C-N-CA	5.49	127.95	120.54
1	B	70	PHE	CA-C-N	5.47	126.17	119.99
1	B	70	PHE	C-N-CA	5.47	126.17	119.99
1	B	488	PHE	CA-C-N	5.46	127.86	120.38
1	B	488	PHE	C-N-CA	5.46	127.86	120.38
1	A	202	ILE	N-CA-C	-5.40	105.06	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	382	GLU	CA-C-N	5.38	127.44	120.44
1	B	382	GLU	C-N-CA	5.38	127.44	120.44
1	A	370	TYR	CA-C-N	5.36	127.74	120.44
1	A	370	TYR	C-N-CA	5.36	127.74	120.44
1	A	442	GLU	CB-CG-CD	5.35	121.69	112.60
1	B	253	CYS	N-CA-C	-5.33	105.36	111.07
1	B	243	THR	CA-CB-OG1	-5.33	101.60	109.60
1	B	161	TYR	N-CA-C	-5.24	105.65	111.36
1	B	25	ILE	N-CA-C	-5.21	105.42	110.42
1	A	249	ASP	CA-C-N	5.20	127.20	120.44
1	A	249	ASP	C-N-CA	5.20	127.20	120.44
1	A	371	SER	O-C-N	5.15	127.65	122.09
1	B	177	CYS	CA-C-N	5.13	127.42	120.44
1	B	177	CYS	C-N-CA	5.13	127.42	120.44
1	A	160	ARG	CA-C-O	-5.12	114.99	120.42
1	B	452	TYR	CB-CA-C	5.12	119.56	110.85
1	B	231	VAL	CA-C-N	5.12	127.40	120.38
1	B	231	VAL	C-N-CA	5.12	127.40	120.38
1	A	83	THR	CA-CB-OG1	-5.11	101.93	109.60
1	B	221	GLN	CB-CG-CD	-5.09	103.95	112.60
1	A	366	PRO	CA-C-N	5.07	127.07	120.28
1	A	366	PRO	C-N-CA	5.07	127.07	120.28
1	B	284	LEU	O-C-N	5.05	127.34	122.09
1	B	549	ASP	O-C-N	5.05	127.47	122.12
1	B	340	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	509	PHE	CB-CA-C	5.00	118.72	109.71

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 ⓘ

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	44	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	102	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 (102) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:374:PHE:CD1	1:B:374:PHE:C	2.87	0.53
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
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:460:LEU:C	1:B:460:LEU:HD23	2.38	0.48
1:B:226:ALA:O	1:B:332:TYR:OH	2.28	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:B:483:ASN:C	1:B:486:PRO:HD2	2.38	0.47
1:A:63:ASP:OD1	1:A:63:ASP:N	2.48	0.47
1:A:240:LYS:O	1:A:241:VAL:C	2.56	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:37:GLU:H	1:A:37:GLU:CD	2.23	0.46
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:498:VAL:O	1:A:499:PRO:C	2.59	0.46
1:B:153:GLU:OE2	1:B:192:SER:OG	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:C	1:A:313:LYS:O	2.55	0.45
1:B:263:TYR:C	1:B:263:TYR:CD1	2.94	0.45
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:B:395:PHE:CD1	1:B:395:PHE:C	2.95	0.44
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
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
3:A:605:RWF:C7	3:A:605:RWF:O3	2.67	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
1:A:163:ALA:HA	1:A:166:THR:OG1	2.20	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: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:B:408:LEU:HD21	1:B:526:GLN:HB3	2.03	0.40
1:B:211:PHE:CD1	1:B:211:PHE:C	2.99	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

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	580/585 (99%)	553 (95%)	26 (4%)	1 (0%)	43	42
1	B	581/585 (99%)	554 (95%)	26 (4%)	1 (0%)	43	42
All	All	1161/1170 (99%)	1107 (95%)	52 (4%)	2 (0%)	43	42

All (2) Ramachandran outliers are listed below:

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

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	457/512 (89%)	441 (96%)	16 (4%)	32	32
1	B	451/512 (88%)	435 (96%)	16 (4%)	32	32
All	All	908/1024 (89%)	876 (96%)	32 (4%)	32	32

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	63	ASP
1	A	136	LYS
1	A	174	LYS

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Mol	Chain	Res	Type
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	371	SER
1	A	408	LEU
1	A	513	ILE
1	A	518	GLU
1	A	574	LYS
1	B	10	ARG
1	B	20	LYS
1	B	68	THR
1	B	137	LYS
1	B	142	ILE
1	B	192	SER
1	B	232	SER
1	B	245	CYS
1	B	284	LEU
1	B	305	LEU
1	B	408	LEU
1	B	415	VAL
1	B	430	LEU
1	B	442	GLU
1	B	451	ASP
1	B	467	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	196	GLN
1	A	247	HIS
1	A	288	HIS
1	A	464	HIS
1	A	510	HIS
1	B	104	GLN
1	B	242	HIS
1	B	288	HIS
1	B	397	GLN

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Mol	Chain	Res	Type
1	B	483	ASN

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](#)

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$
2	MYR	A	601	-	15,15,15	1.19	1 (6%)	15,15,15	0.98	1 (6%)
2	MYR	A	604	-	15,15,15	0.90	1 (6%)	15,15,15	1.24	1 (6%)
2	MYR	B	604	-	15,15,15	1.54	2 (13%)	15,15,15	0.65	0
2	MYR	A	602	-	15,15,15	0.54	0	15,15,15	1.88	4 (26%)
2	MYR	B	602	-	15,15,15	0.94	1 (6%)	15,15,15	1.06	0
3	RWF	A	605	-	25,25,25	2.92	7 (28%)	34,35,35	2.61	14 (41%)
3	RWF	B	605	-	25,25,25	2.23	7 (28%)	34,35,35	3.19	14 (41%)
4	DAO	B	603	-	13,13,13	0.60	0	13,13,13	0.63	0
2	MYR	A	603	-	15,15,15	1.72	2 (13%)	15,15,15	1.10	0
2	MYR	B	601	-	15,15,15	0.98	0	15,15,15	0.98	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MYR	A	601	-	-	7/13/13/13	-
2	MYR	A	604	-	-	8/13/13/13	-
2	MYR	B	604	-	-	5/13/13/13	-
2	MYR	A	602	-	-	8/13/13/13	-
2	MYR	B	602	-	-	8/13/13/13	-
3	RWF	A	605	-	-	3/12/12/12	0/3/3/3
3	RWF	B	605	-	-	3/12/12/12	0/3/3/3
4	DAO	B	603	-	-	8/11/11/11	-
2	MYR	A	603	-	-	8/13/13/13	-
2	MYR	B	601	-	-	5/13/13/13	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	RWF	C2-C13	-7.73	1.42	1.52
3	A	605	RWF	O3-C4	6.77	1.46	1.21
3	A	605	RWF	C6-C2	-6.27	1.42	1.52
3	B	605	RWF	O3-C4	5.63	1.42	1.21
3	B	605	RWF	C6-C2	-5.59	1.43	1.52
2	A	603	MYR	C2-C1	5.38	1.63	1.50
3	B	605	RWF	C14-C13	4.69	1.44	1.36
2	B	604	MYR	C2-C1	4.26	1.60	1.50
3	A	605	RWF	C14-C13	3.92	1.43	1.36
3	A	605	RWF	C3-C4	3.74	1.57	1.51
3	A	605	RWF	C1-C14	-3.51	1.40	1.45
3	A	605	RWF	O1-C19	3.16	1.43	1.38
3	B	605	RWF	C2-C13	-3.08	1.48	1.52
3	B	605	RWF	O4-C14	2.60	1.40	1.33
2	B	604	MYR	C3-C2	2.55	1.61	1.52
2	A	603	MYR	C3-C2	2.30	1.60	1.52
2	A	604	MYR	C2-C1	2.27	1.55	1.50
2	B	602	MYR	C2-C1	2.26	1.55	1.50
3	B	605	RWF	C1-C14	-2.24	1.42	1.45
3	B	605	RWF	C5-C4	2.17	1.57	1.49
2	A	601	MYR	C2-C1	2.16	1.55	1.50

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	605	RWF	O3-C4-C3	-11.98	102.96	121.74
3	B	605	RWF	C3-C2-C6	-6.82	94.27	111.75
3	A	605	RWF	C2-C3-C4	-5.96	106.34	114.57
3	B	605	RWF	C6-C2-C13	5.71	122.34	111.94
3	A	605	RWF	O3-C4-C3	-5.64	112.90	121.74
3	A	605	RWF	O2-C11-C13	-5.09	118.68	125.56
3	A	605	RWF	O3-C4-C5	-4.95	109.08	121.48
3	A	605	RWF	O1-C19-C18	4.66	122.46	116.25
3	B	605	RWF	C5-C4-C3	-4.05	110.89	116.53
3	A	605	RWF	C5-C4-C3	-4.00	110.96	116.53
3	B	605	RWF	O3-C4-C5	-3.96	111.55	121.48
3	B	605	RWF	O1-C19-C18	3.65	121.11	116.25
3	B	605	RWF	O1-C19-C1	-3.58	118.31	121.57
3	A	605	RWF	O1-C11-O2	3.42	120.73	116.22
2	A	602	MYR	O2-C1-O1	3.40	132.09	123.33
2	A	602	MYR	O1-C1-C2	-3.37	112.42	123.09
3	A	605	RWF	C10-C9-C8	-3.15	115.55	119.87
2	A	602	MYR	C3-C2-C1	-3.14	106.32	114.51
3	B	605	RWF	C2-C13-C11	3.08	121.95	117.76
3	A	605	RWF	C9-C10-C12	3.02	123.97	120.24
3	A	605	RWF	C2-C13-C11	-2.95	113.75	117.76
3	B	605	RWF	C12-C6-C2	2.79	125.99	120.90
3	B	605	RWF	C14-C13-C11	-2.50	116.86	119.11
3	A	605	RWF	C15-C1-C19	2.43	121.41	118.21
3	B	605	RWF	C19-O1-C11	2.29	124.44	122.26
3	B	605	RWF	C8-C7-C6	2.26	123.35	120.65
3	A	605	RWF	O1-C19-C1	-2.20	119.57	121.57
3	B	605	RWF	C12-C6-C7	-2.17	115.62	118.30
2	A	601	MYR	C3-C2-C1	-2.14	108.92	114.51
3	B	605	RWF	C9-C10-C12	2.09	122.82	120.24
2	A	604	MYR	O1-C1-C2	-2.06	116.55	123.09
2	A	602	MYR	C10-C9-C8	-2.04	104.05	114.37
3	A	605	RWF	C3-C2-C13	2.03	116.61	113.25
3	A	605	RWF	C12-C6-C2	2.02	124.59	120.90

There are no chirality outliers.

All (63) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	MYR	C9-C10-C11-C12
2	A	603	MYR	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	B	605	RWF	C2-C3-C4-O3
4	B	603	DAO	C5-C6-C7-C8
4	B	603	DAO	C11-C10-C9-C8
2	B	601	MYR	C2-C3-C4-C5
2	B	602	MYR	C6-C7-C8-C9
2	A	601	MYR	C11-C10-C9-C8
2	B	604	MYR	C5-C6-C7-C8
2	A	602	MYR	C10-C11-C12-C13
2	A	604	MYR	C1-C2-C3-C4
2	B	601	MYR	C11-C10-C9-C8
2	B	602	MYR	C7-C8-C9-C10
4	B	603	DAO	C2-C3-C4-C5
2	A	604	MYR	C9-C10-C11-C12
2	A	602	MYR	C6-C7-C8-C9
2	A	601	MYR	C5-C6-C7-C8
2	B	601	MYR	C6-C7-C8-C9
2	A	604	MYR	C3-C4-C5-C6
2	A	601	MYR	C10-C11-C12-C13
2	A	604	MYR	C4-C5-C6-C7
2	A	604	MYR	C5-C6-C7-C8
2	A	603	MYR	C3-C4-C5-C6
2	B	604	MYR	C2-C3-C4-C5
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	602	MYR	C11-C12-C13-C14
2	B	602	MYR	C11-C12-C13-C14
2	A	601	MYR	C11-C12-C13-C14
4	B	603	DAO	C3-C4-C5-C6
2	B	602	MYR	C9-C10-C11-C12
2	A	602	MYR	C11-C10-C9-C8
4	B	603	DAO	C7-C8-C9-C10
3	A	605	RWF	C13-C2-C3-C4
2	A	603	MYR	C6-C7-C8-C9
2	B	604	MYR	C7-C8-C9-C10
2	A	604	MYR	C7-C8-C9-C10
2	A	603	MYR	C10-C11-C12-C13
2	B	602	MYR	C10-C11-C12-C13
2	B	604	MYR	O1-C1-C2-C3
2	B	601	MYR	O1-C1-C2-C3
3	B	605	RWF	C13-C2-C6-C7

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

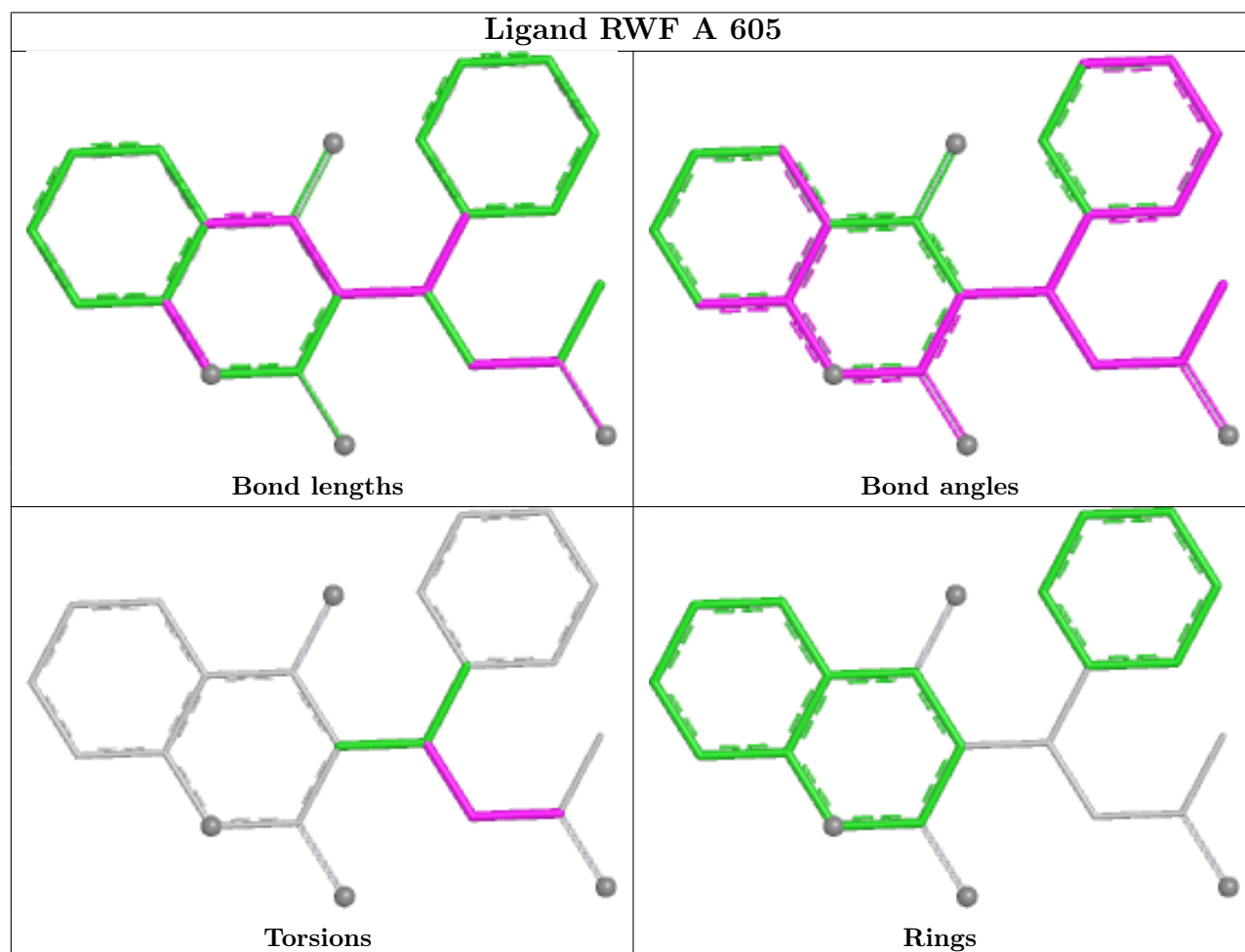
There are no ring outliers.

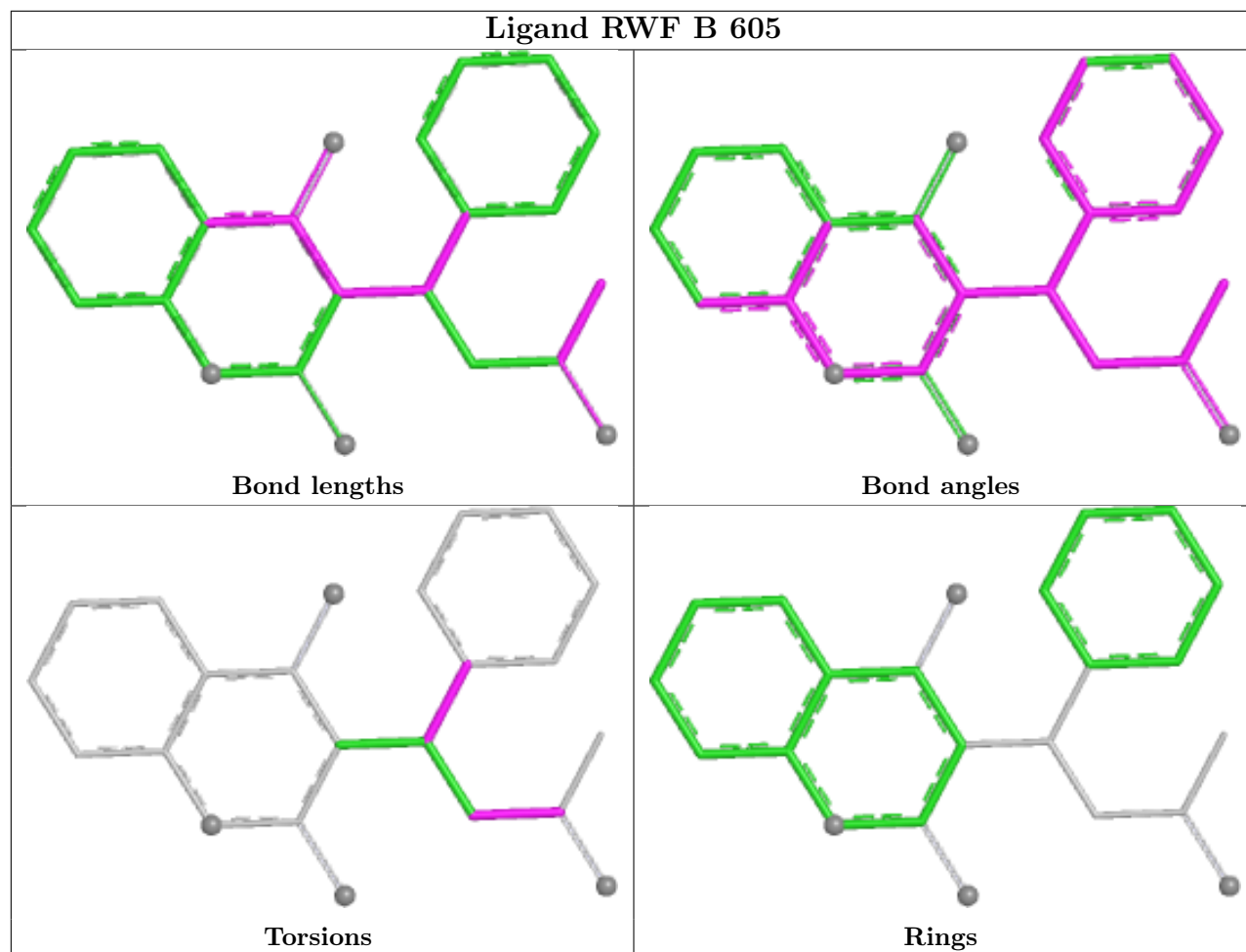
7 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	MYR	4	0
2	A	602	MYR	8	0
2	B	602	MYR	1	0
3	A	605	RWF	1	0
3	B	605	RWF	2	0
4	B	603	DAO	2	0
2	A	603	MYR	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	582/585 (99%)	0.91	65 (11%) 10 9	27, 41, 59, 88	0
1	B	582/585 (99%)	1.02	93 (15%) 5 4	20, 42, 59, 85	1 (0%)
All	All	1164/1170 (99%)	0.96	158 (13%) 7 6	20, 41, 60, 88	1 (0%)

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	168	CYS	6.7
1	B	568	PHE	5.5
1	B	248	GLY	5.3
1	B	514	CYS	5.3
1	A	172	ALA	5.1
1	B	567	CYS	5.1
1	B	247	HIS	5.1
1	B	179	LEU	5.0
1	A	360	CYS	4.7
1	A	92	ALA	4.4
1	B	305	LEU	4.3
1	A	370	TYR	4.2
1	B	104	GLN	4.1
1	A	310	ILE	3.8
1	B	310	ILE	3.7
1	B	172	ALA	3.7
1	B	481	LEU	3.6
1	A	375	ASP	3.6
1	B	175	ALA	3.6
1	A	171	ALA	3.5
1	A	275	LEU	3.5
1	B	458	ASN	3.5
1	B	173	ASP	3.4
1	B	558	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	515	THR	3.3
1	A	287	SER	3.3
1	A	305	LEU	3.3
1	A	361	CYS	3.3
1	B	282	PRO	3.3
1	A	481	LEU	3.2
1	B	178	LEU	3.2
1	B	564	LYS	3.2
1	B	278	CYS	3.2
1	A	369	CYS	3.2
1	B	482	VAL	3.2
1	B	462	VAL	3.1
1	A	371	SER	3.1
1	A	571	GLU	3.1
1	B	108	ASP	3.1
1	A	3	HIS	3.1
1	B	241	VAL	3.1
1	B	39	LEU	3.0
1	B	461	CYS	3.0
1	A	482	VAL	3.0
1	A	108	ASP	3.0
1	A	344	VAL	3.0
1	B	138	TYR	3.0
1	A	255	ASP	2.9
1	B	569	ALA	2.9
1	B	183	ASP	2.8
1	B	559	CYS	2.8
1	A	437	CYS	2.8
1	A	366	PRO	2.8
1	A	374	PHE	2.8
1	A	451	ASP	2.8
1	B	519	GLU	2.8
1	A	463	LEU	2.8
1	B	513	ILE	2.8
1	B	554	PHE	2.7
1	A	557	LYS	2.7
1	B	116	VAL	2.7
1	B	562	ASP	2.7
1	A	568	PHE	2.7
1	B	170	GLN	2.7
1	A	567	CYS	2.7
1	B	53	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	463	LEU	2.6
1	B	561	ALA	2.6
1	A	103	LEU	2.6
1	A	299	PRO	2.6
1	B	459	GLN	2.6
1	A	356	THR	2.6
1	B	228	PHE	2.6
1	B	280	GLU	2.6
1	A	105	HIS	2.6
1	A	247	HIS	2.6
1	A	176	ALA	2.6
1	B	374	PHE	2.5
1	B	390	GLN	2.5
1	A	584	GLY	2.5
1	B	91	CYS	2.5
1	B	301	ASP	2.5
1	A	138	TYR	2.5
1	B	34[A]	CYS	2.5
1	A	283	LEU	2.5
1	A	127	PHE	2.5
1	A	301	ASP	2.5
1	B	194	ALA	2.5
1	B	364	ALA	2.5
1	A	516	LEU	2.5
1	A	248	GLY	2.5
1	A	311	GLU	2.4
1	B	245	CYS	2.4
1	B	477	CYS	2.4
1	A	346	LEU	2.4
1	A	460	LEU	2.4
1	B	430	LEU	2.4
1	B	27	PHE	2.4
1	A	35	PRO	2.4
1	A	254	ALA	2.4
1	B	516	LEU	2.4
1	B	70	PHE	2.4
1	B	180	PRO	2.4
1	B	55	ALA	2.3
1	B	164	ALA	2.3
1	B	176	ALA	2.3
1	A	566	THR	2.3
1	B	214	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	148	TYR	2.3
1	B	322	ALA	2.3
1	A	454	SER	2.3
1	A	170	GLN	2.3
1	A	458	ASN	2.3
1	B	399	GLY	2.3
1	B	332	TYR	2.3
1	A	282	PRO	2.2
1	A	200	CYS	2.2
1	B	577	ALA	2.2
1	B	584	GLY	2.2
1	B	82	GLU	2.2
1	B	362	ALA	2.2
1	A	487	CYS	2.2
1	A	206	PHE	2.2
1	B	469	VAL	2.2
1	B	555	VAL	2.2
1	A	368	GLU	2.2
1	B	306	ALA	2.2
1	B	443	ALA	2.2
1	B	203	LEU	2.2
1	B	416	PRO	2.1
1	A	102	PHE	2.1
1	B	217	ALA	2.1
1	B	109	ASN	2.1
1	B	96	PRO	2.1
1	B	467	THR	2.1
1	A	399	GLY	2.1
1	B	307	ALA	2.1
1	A	245	CYS	2.1
1	B	369	CYS	2.1
1	A	180	PRO	2.1
1	B	281	LYS	2.1
1	B	78	ALA	2.1
1	B	553	ALA	2.1
1	B	236	THR	2.1
1	A	560	LYS	2.1
1	B	142	ILE	2.1
1	B	344	VAL	2.1
1	B	509	PHE	2.1
1	B	442	GLU	2.0
1	B	97	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	102	PHE	2.0
1	B	456	VAL	2.0
1	B	371	SER	2.0
1	A	561	ALA	2.0
1	B	171	ALA	2.0
1	A	115	LEU	2.0
1	A	238	LEU	2.0
1	A	67	HIS	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](#)

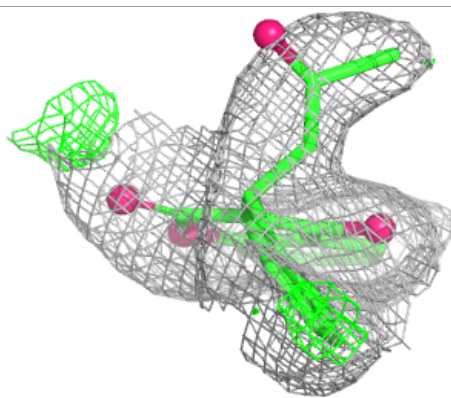
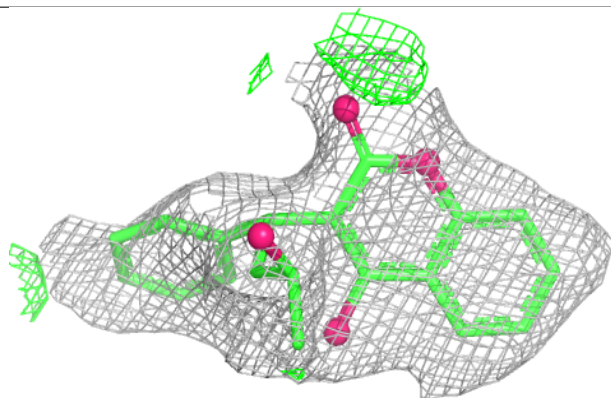
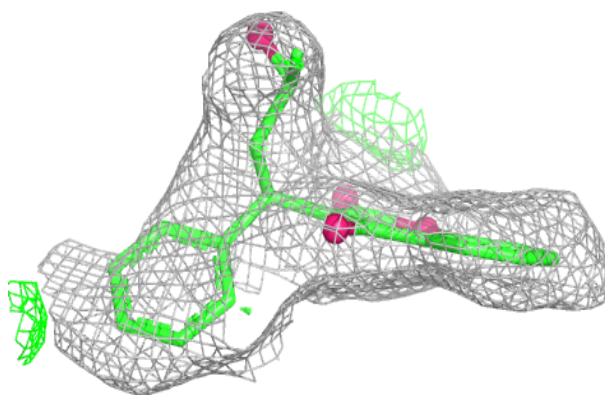
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	RWF	B	605	23/23	0.76	0.18	55,66,72,76	0
3	RWF	A	605	23/23	0.82	0.21	57,66,77,82	0
2	MYR	A	603	16/16	0.82	0.15	33,39,51,57	0
2	MYR	A	604	16/16	0.85	0.17	44,54,66,72	0
2	MYR	B	602	16/16	0.85	0.18	39,47,57,57	0
4	DAO	B	603	14/14	0.85	0.19	50,56,72,74	0
2	MYR	B	601	16/16	0.87	0.19	48,57,63,64	0
2	MYR	B	604	16/16	0.88	0.10	35,43,56,57	0
2	MYR	A	602	16/16	0.88	0.18	52,64,68,68	0
2	MYR	A	601	16/16	0.91	0.15	36,47,52,53	0

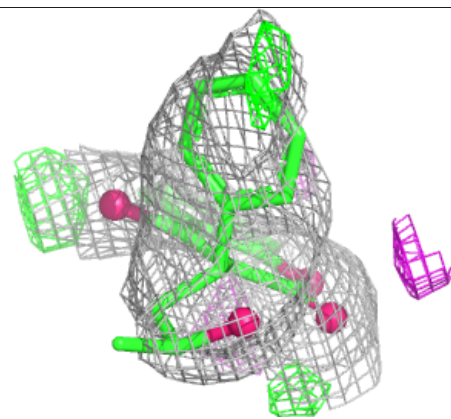
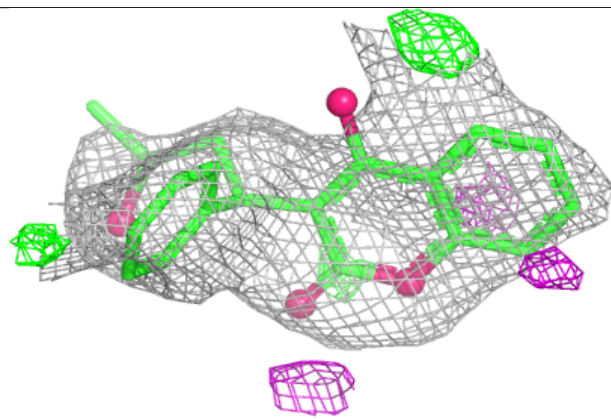
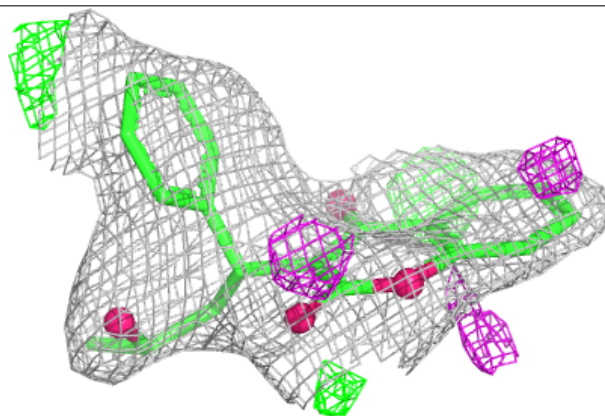
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around RWF B 605:

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

**Electron density around RWF A 605:**

$2mF_o-DF_c$ (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.