



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:45 PM UTC

PDB ID : 7YL5 / pdb_00007yl5
Title : Cell surface protein YwfG protein complexed with mannose
Authors : Tsuchiya, W.; Fujimoto, Z.; Suzuki, C.
Deposited on : 2022-07-25
Resolution : 3.00 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

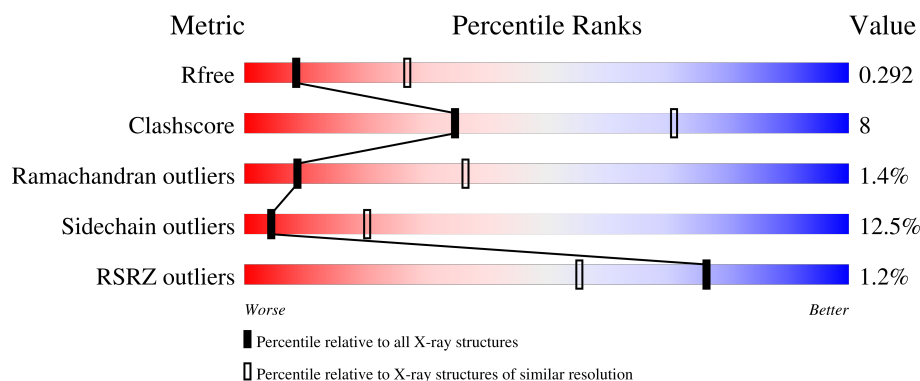
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	505	
1	B	505	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	606	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6642 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 GRAM_POS_ANCHORING domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3552	2207	590	750	5			
1	B	388	Total	C	N	O	S	0	0	0
			2894	1799	479	611	5			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP S6FKX6
A	8	GLY	-	expression tag	UNP S6FKX6
A	9	SER	-	expression tag	UNP S6FKX6
A	10	SER	-	expression tag	UNP S6FKX6
A	11	HIS	-	expression tag	UNP S6FKX6
A	12	HIS	-	expression tag	UNP S6FKX6
A	13	HIS	-	expression tag	UNP S6FKX6
A	14	HIS	-	expression tag	UNP S6FKX6
A	15	HIS	-	expression tag	UNP S6FKX6
A	16	HIS	-	expression tag	UNP S6FKX6
A	17	SER	-	expression tag	UNP S6FKX6
A	18	SER	-	expression tag	UNP S6FKX6
A	19	GLY	-	expression tag	UNP S6FKX6
A	20	LEU	-	expression tag	UNP S6FKX6
A	21	VAL	-	expression tag	UNP S6FKX6
A	22	PRO	-	expression tag	UNP S6FKX6
A	23	ARG	-	expression tag	UNP S6FKX6
A	24	GLY	-	expression tag	UNP S6FKX6
A	25	SER	-	expression tag	UNP S6FKX6
A	26	HIS	-	expression tag	UNP S6FKX6
A	27	MET	-	expression tag	UNP S6FKX6
B	7	MET	-	initiating methionine	UNP S6FKX6
B	8	GLY	-	expression tag	UNP S6FKX6
B	9	SER	-	expression tag	UNP S6FKX6
B	10	SER	-	expression tag	UNP S6FKX6

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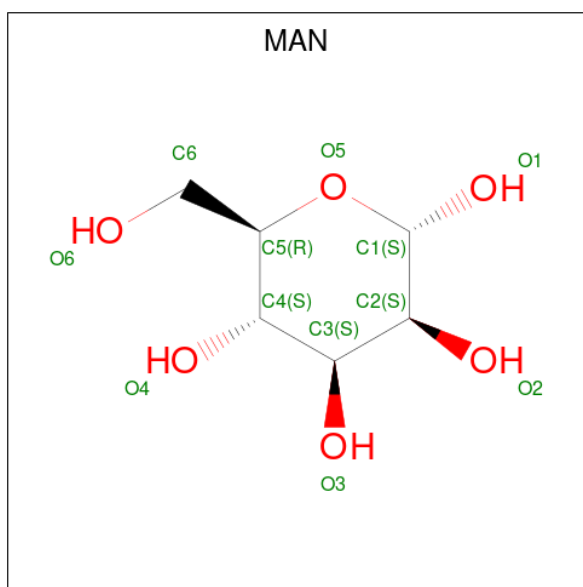
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Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP S6FKX6
B	12	HIS	-	expression tag	UNP S6FKX6
B	13	HIS	-	expression tag	UNP S6FKX6
B	14	HIS	-	expression tag	UNP S6FKX6
B	15	HIS	-	expression tag	UNP S6FKX6
B	16	HIS	-	expression tag	UNP S6FKX6
B	17	SER	-	expression tag	UNP S6FKX6
B	18	SER	-	expression tag	UNP S6FKX6
B	19	GLY	-	expression tag	UNP S6FKX6
B	20	LEU	-	expression tag	UNP S6FKX6
B	21	VAL	-	expression tag	UNP S6FKX6
B	22	PRO	-	expression tag	UNP S6FKX6
B	23	ARG	-	expression tag	UNP S6FKX6
B	24	GLY	-	expression tag	UNP S6FKX6
B	25	SER	-	expression tag	UNP S6FKX6
B	26	HIS	-	expression tag	UNP S6FKX6
B	27	MET	-	expression tag	UNP S6FKX6

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

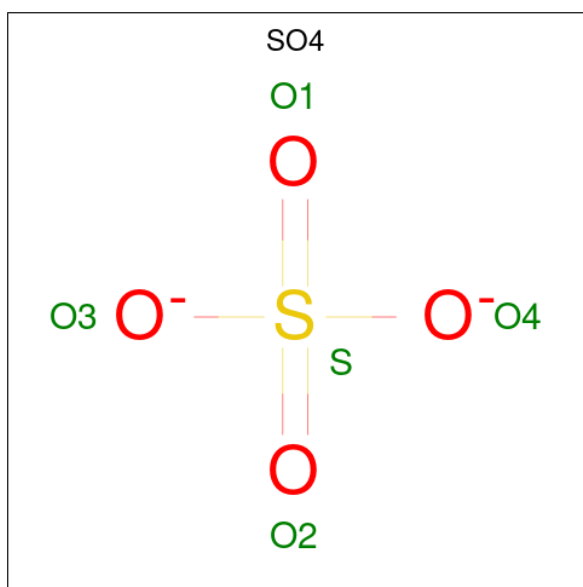
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is alpha-D-mannopyranose (CCD ID: MAN) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

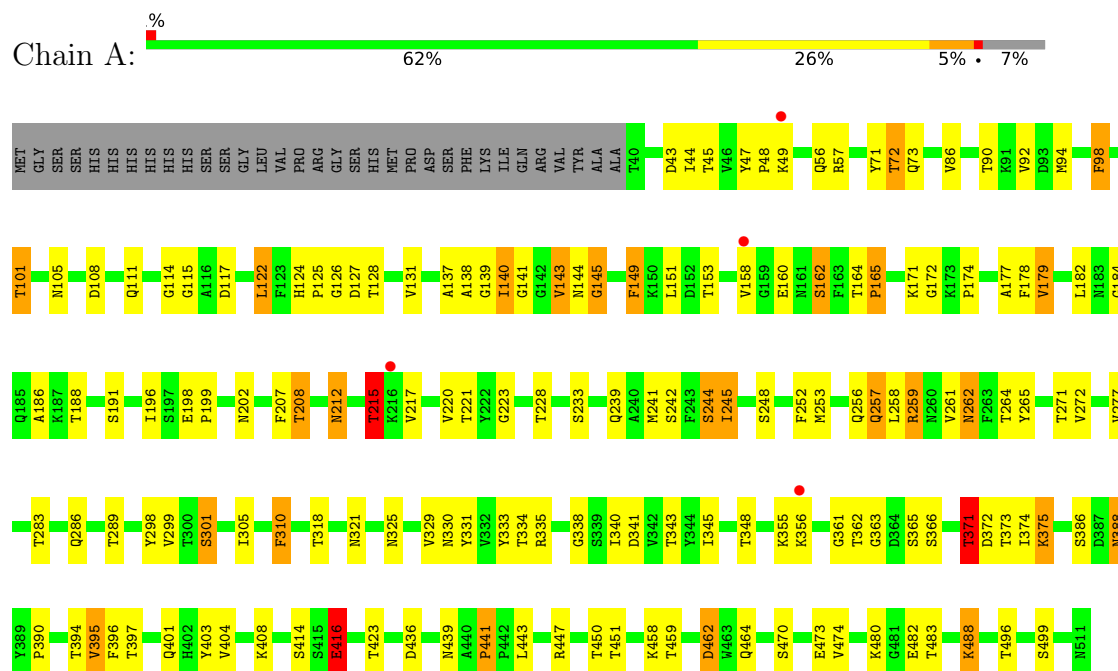
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	28	Total	O	0	0
			28	28		

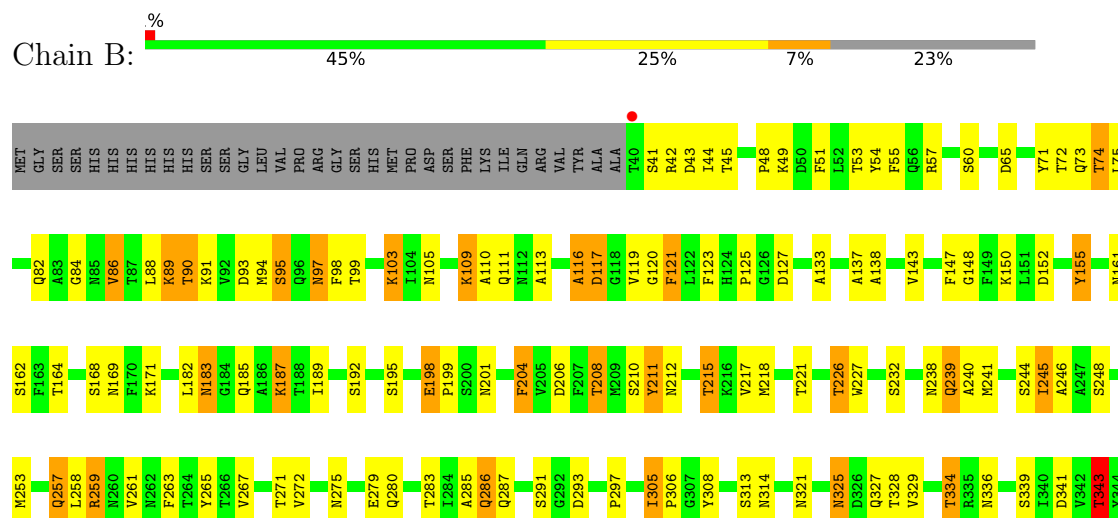
3 Residue-property plots

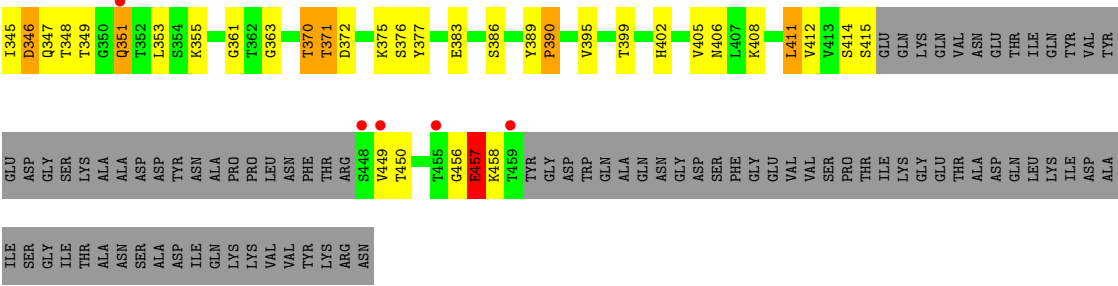
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: GRAM_POS_ANCHORING domain-containing protein



- Molecule 1: GRAM_POS_ANCHORING domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	43.31Å 273.16Å 322.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 3.00 45.57 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.57-3.00) 99.6 (45.57-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.227 , 0.295 0.231 , 0.292	Depositor DCC
R_{free} test set	1964 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6642	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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: CA, SO4, MAN

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	1.42	21/3620 (0.6%)	1.72	51/4924 (1.0%)
1	B	1.52	27/2949 (0.9%)	1.86	63/4013 (1.6%)
All	All	1.47	48/6569 (0.7%)	1.78	114/8937 (1.3%)

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	SER	CB-OG	-9.63	1.22	1.42
1	A	202	ASN	C-O	8.40	1.34	1.23
1	B	125	PRO	C-O	-8.22	1.15	1.23
1	B	119	VAL	C-O	7.94	1.32	1.23
1	A	436	ASP	C-O	7.80	1.32	1.23
1	A	144	ASN	C-O	7.21	1.32	1.24
1	B	138	ALA	C-O	-7.15	1.15	1.24
1	B	120	GLY	C-O	7.09	1.31	1.24
1	A	416	GLU	CD-OE1	7.07	1.38	1.25
1	A	416	GLU	CD-OE2	6.99	1.38	1.25
1	A	196	ILE	C-O	6.97	1.31	1.23
1	B	204	PHE	C-O	-6.86	1.15	1.24
1	A	73	GLN	C-O	6.84	1.31	1.24
1	B	73	GLN	C-O	6.72	1.31	1.24
1	B	314	ASN	C-O	6.62	1.32	1.23
1	B	82	GLN	C-O	6.60	1.32	1.24
1	B	334	THR	C-O	6.54	1.31	1.23
1	B	361	GLY	C-O	6.45	1.30	1.23
1	A	158	VAL	C-O	6.34	1.30	1.23
1	A	178	PHE	C-O	6.17	1.31	1.23
1	A	122	LEU	C-O	6.10	1.31	1.24
1	B	238	ASN	C-O	6.07	1.31	1.24
1	B	405	VAL	C-O	6.01	1.30	1.24
1	A	215	THR	C-O	6.00	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	LYS	C-O	5.95	1.31	1.23
1	B	55	PHE	C-O	5.92	1.30	1.23
1	B	84	GLY	C-O	5.87	1.31	1.24
1	B	232	SER	CA-CB	-5.87	1.44	1.53
1	B	245	ILE	C-O	5.84	1.30	1.24
1	A	259	ARG	C-O	5.79	1.30	1.23
1	B	217	VAL	C-O	-5.79	1.17	1.24
1	B	48	PRO	C-O	-5.78	1.16	1.24
1	B	339	SER	C-O	5.73	1.31	1.24
1	A	207	PHE	C-O	5.69	1.31	1.24
1	A	321	ASN	C-O	5.66	1.30	1.24
1	B	259	ARG	C-O	5.65	1.30	1.23
1	A	443	LEU	C-O	5.56	1.30	1.23
1	B	45	THR	C-O	-5.45	1.17	1.23
1	B	208	THR	C-O	-5.43	1.17	1.24
1	B	285	ALA	C-O	5.42	1.30	1.23
1	B	257	GLN	C-O	5.33	1.30	1.23
1	A	43	ASP	CG-OD2	5.23	1.35	1.25
1	A	223	GLY	C-O	5.11	1.30	1.23
1	B	345	ILE	C-O	5.11	1.29	1.24
1	B	293	ASP	C-O	-5.08	1.17	1.23
1	A	217	VAL	C-O	5.05	1.29	1.24
1	A	245	ILE	C-O	5.05	1.29	1.24
1	B	183	ASN	C-O	-5.00	1.16	1.24

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	208	THR	CA-CB-OG1	-11.34	92.60	109.60
1	B	117	ASP	CA-CB-CG	10.37	122.97	112.60
1	B	305	ILE	CA-C-O	8.77	124.03	119.12
1	A	208	THR	CA-CB-OG1	-8.18	97.32	109.60
1	B	287	GLN	CA-C-O	-8.14	112.24	121.19
1	B	325	ASN	CA-CB-CG	-8.03	104.57	112.60
1	B	95	SER	N-CA-C	-7.88	103.80	113.50
1	A	397	THR	CA-CB-OG1	-7.87	97.80	109.60
1	A	371	THR	CA-CB-OG1	-7.79	97.91	109.60
1	B	261	VAL	CA-C-O	-7.71	112.00	120.71
1	A	117	ASP	CA-CB-CG	7.10	119.70	112.60
1	A	271	THR	CB-CA-C	7.03	122.24	109.37
1	A	128	THR	CA-CB-OG1	7.00	120.09	109.60
1	B	182	LEU	O-C-N	6.97	129.51	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	53	THR	CA-CB-OG1	-6.96	99.17	109.60
1	B	210	SER	CA-C-O	-6.96	113.19	120.70
1	A	325	ASN	CA-CB-CG	-6.96	105.64	112.60
1	B	271	THR	CA-CB-OG1	-6.83	99.36	109.60
1	B	98	PHE	CA-CB-CG	6.81	120.61	113.80
1	B	121	PHE	CA-C-O	-6.81	113.18	120.46
1	A	184	GLY	CA-C-N	6.80	131.03	121.24
1	A	184	GLY	C-N-CA	6.80	131.03	121.24
1	A	153	THR	CA-CB-OG1	6.79	119.79	109.60
1	B	91	LYS	N-CA-C	-6.72	100.01	109.69
1	B	240	ALA	CA-C-O	-6.64	111.02	120.51
1	B	49	LYS	O-C-N	6.60	128.87	122.07
1	B	155	TYR	CB-CA-C	-6.58	99.25	110.16
1	B	275	ASN	CA-CB-CG	-6.55	106.05	112.60
1	B	261	VAL	O-C-N	6.50	130.37	122.95
1	A	388	ASN	CB-CA-C	-6.48	96.01	110.21
1	A	86	VAL	CA-C-O	-6.41	113.17	120.67
1	B	297	PRO	CA-C-O	-6.36	114.11	121.86
1	A	423	THR	CA-CB-OG1	-6.33	100.10	109.60
1	B	51	PHE	O-C-N	6.31	128.59	122.03
1	B	399	THR	CA-CB-OG1	-6.30	100.14	109.60
1	B	390	PRO	CB-CA-C	6.29	119.62	111.64
1	B	286	GLN	CA-C-O	-6.24	113.63	120.81
1	A	355	LYS	CA-C-O	-6.19	112.45	120.25
1	A	143	VAL	O-C-N	6.17	129.40	122.98
1	A	47	TYR	CB-CA-C	6.16	117.72	108.86
1	A	101	THR	CA-CB-OG1	-6.05	100.53	109.60
1	A	348	THR	CA-C-O	-6.00	114.15	120.63
1	B	370	THR	CA-CB-OG1	-6.00	100.61	109.60
1	A	86	VAL	N-CA-C	-5.97	99.88	108.48
1	A	127	ASP	CA-CB-CG	5.97	118.57	112.60
1	B	343	THR	CA-CB-OG1	-5.94	100.68	109.60
1	B	116	ALA	CA-C-O	-5.94	115.08	121.38
1	A	127	ASP	CB-CA-C	5.90	119.52	109.72
1	B	263	PHE	CA-C-O	-5.90	113.96	120.33
1	B	155	TYR	O-C-N	5.89	130.10	123.27
1	A	145	GLY	O-C-N	5.88	128.54	122.54
1	A	356	LYS	CA-C-O	-5.88	114.81	120.92
1	A	482	GLU	CB-CG-CD	5.85	122.55	112.60
1	B	346	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	366	SER	N-CA-C	-5.83	106.29	113.41
1	B	457	GLU	CB-CA-C	5.83	117.81	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	TYR	CA-C-O	-5.80	112.81	119.60
1	A	151	LEU	CA-C-O	-5.80	113.98	121.11
1	B	103	LYS	CA-C-O	-5.74	114.39	121.11
1	A	386	SER	CA-C-O	-5.74	115.13	121.33
1	B	386	SER	CA-C-N	5.74	130.56	121.72
1	B	386	SER	C-N-CA	5.74	130.56	121.72
1	A	188	THR	CB-CA-C	-5.72	100.91	110.29
1	B	123	PHE	CA-C-O	-5.70	114.16	120.38
1	A	341	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	143	VAL	CA-C-O	-5.61	114.59	120.76
1	A	436	ASP	CA-CB-CG	5.58	118.18	112.60
1	B	226	THR	CA-CB-OG1	-5.58	101.24	109.60
1	B	363	GLY	N-CA-C	-5.57	107.85	114.48
1	B	43	ASP	CA-C-N	-5.57	115.83	123.46
1	B	43	ASP	C-N-CA	-5.57	115.83	123.46
1	B	375	LYS	CA-C-O	-5.52	113.86	120.10
1	A	310	PHE	CA-C-O	-5.45	115.02	120.96
1	B	283	THR	CA-C-O	-5.44	114.49	120.69
1	B	336	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	182	LEU	CA-C-O	-5.39	114.84	120.55
1	B	211	TYR	CA-C-O	-5.37	114.55	120.24
1	A	199	PRO	CB-CA-C	-5.36	104.84	111.64
1	A	330	ASN	CB-CA-C	5.36	118.59	109.75
1	B	120	GLY	O-C-N	5.36	127.57	123.23
1	B	280	GLN	N-CA-C	-5.34	106.60	113.23
1	B	74	THR	CA-CB-OG1	-5.32	101.63	109.60
1	A	143	VAL	CA-C-N	5.30	129.67	122.19
1	A	143	VAL	C-N-CA	5.30	129.67	122.19
1	B	347	GLN	CA-C-O	-5.29	115.45	120.90
1	B	201	ASN	CB-CA-C	-5.29	104.02	111.95
1	A	470	SER	CA-C-N	5.29	128.98	121.42
1	A	470	SER	C-N-CA	5.29	128.98	121.42
1	B	371	THR	CA-CB-OG1	-5.28	101.68	109.60
1	B	363	GLY	O-C-N	5.24	128.09	122.22
1	B	328	THR	CA-CB-OG1	-5.24	101.74	109.60
1	A	335	ARG	CA-C-O	-5.23	114.69	120.60
1	A	149	PHE	CA-C-O	-5.22	114.69	120.38
1	A	462	ASP	CA-CB-CG	5.22	117.82	112.60
1	A	261	VAL	O-C-N	5.21	128.67	122.83
1	B	105	ASN	CA-C-O	-5.20	115.02	120.58
1	B	283	THR	CA-CB-OG1	-5.19	101.81	109.60
1	B	246	ALA	O-C-N	5.18	129.61	123.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	395	VAL	CA-C-O	-5.17	115.37	120.90
1	B	321	ASN	CB-CA-C	5.17	119.17	109.71
1	B	99	THR	CA-CB-OG1	-5.14	101.89	109.60
1	B	215	THR	N-CA-C	-5.13	107.19	113.50
1	B	91	LYS	CA-C-O	-5.13	115.40	121.60
1	A	365	SER	CA-C-O	-5.12	115.93	121.87
1	A	212	ASN	CA-C-N	5.08	125.73	119.99
1	A	212	ASN	C-N-CA	5.08	125.73	119.99
1	A	473	GLU	CA-C-O	-5.08	115.47	121.16
1	A	72	THR	CA-CB-OG1	5.07	117.20	109.60
1	B	206	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	108	ASP	CA-CB-CG	-5.06	107.54	112.60
1	A	462	ASP	CA-C-O	-5.05	115.83	121.23
1	A	139	GLY	O-C-N	5.03	128.37	122.38
1	B	164	THR	N-CA-CB	5.03	116.82	110.04
1	A	153	THR	N-CA-CB	5.02	118.18	110.70

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	3552	0	3355	44	0
1	B	2894	0	2729	52	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	12	0	0
3	B	24	0	24	0	0
4	A	45	0	0	1	0
4	B	80	0	0	4	0
5	A	5	0	0	0	0
5	B	28	0	0	2	0
All	All	6642	0	6120	96	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 8.

All (96) 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:117:ASP:HB2	1:B:248:SER:O	1.87	0.75
1:B:189:ILE:HG23	4:B:609:SO4:O2	1.87	0.75
1:B:341:ASP:OD1	1:B:402:HIS:HA	1.93	0.67
1:A:56:GLN:HA	4:A:603:SO4:O4	1.94	0.67
1:B:97:ASN:HA	1:B:211:TYR:O	1.99	0.63
1:B:54:TYR:O	1:B:88:LEU:HD12	2.01	0.61
1:B:208:THR:HB	1:B:221:THR:OG1	2.02	0.60
1:A:114:GLY:HA2	1:A:252:PHE:CD2	2.41	0.56
1:A:137:ALA:HB2	1:A:162:SER:HB2	1.88	0.55
1:A:208:THR:O	1:A:220:VAL:HA	2.06	0.55
1:A:318:THR:HB	1:A:331:TYR:OH	2.07	0.55
1:A:174:PRO:HG3	1:A:198:GLU:HG2	1.89	0.55
1:B:42:ARG:O	1:B:44:ILE:HG23	2.07	0.55
1:A:122:LEU:HD13	1:A:140:ILE:HA	1.90	0.53
1:B:221:THR:HG22	1:B:226:THR:HG23	1.90	0.53
1:A:212:ASN:HB3	1:A:215:THR:OG1	2.08	0.53
1:B:192:SER:O	1:B:227:TRP:CD1	2.62	0.53
1:B:110:ALA:HB2	1:B:198:GLU:HG2	1.91	0.53
1:B:57:ARG:NH2	4:B:604:SO4:O2	2.41	0.53
1:B:110:ALA:CB	1:B:198:GLU:HG2	2.38	0.52
1:A:496:THR:O	1:A:499:SER:HB2	2.09	0.51
1:A:71:TYR:O	1:A:259:ARG:HA	2.10	0.51
1:A:416:GLU:HG2	1:A:447:ARG:HH21	1.76	0.51
1:A:371:THR:OG1	1:A:372:ASP:N	2.45	0.50
1:A:390:PRO:HD3	1:A:403:TYR:CE1	2.48	0.49
1:B:90:THR:OG1	1:B:267:VAL:HG13	2.12	0.49
1:B:346:ASP:HB2	1:B:353:LEU:HD21	1.94	0.49
1:B:183:ASN:OD1	1:B:187:LYS:HE3	2.13	0.49
1:B:155:TYR:OH	1:B:168:SER:HA	2.12	0.49
1:A:401:GLN:HB3	1:A:403:TYR:CE2	2.48	0.48
1:B:121:PHE:O	1:B:148:GLY:HA3	2.13	0.48
1:A:92:VAL:HG13	1:A:265:TYR:HD2	1.79	0.48
1:A:141:GLY:CA	1:A:186:ALA:HB2	2.43	0.48
1:A:340:ILE:HG12	1:A:401:GLN:HB2	1.96	0.48
1:A:451:THR:HG23	1:A:458:LYS:HG2	1.95	0.47
1:B:71:TYR:O	1:B:259:ARG:HA	2.14	0.47
1:B:109:LYS:O	1:B:199:PRO:HB2	2.13	0.47
1:B:308:TYR:HE2	5:B:706:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:PHE:HE2	1:B:218:MET:HE1	1.80	0.47
1:B:95:SER:HB3	1:B:239:GLN:HG3	1.97	0.47
1:B:93:ASP:CG	1:B:95:SER:HG	2.23	0.47
1:A:124:HIS:ND1	1:A:143:VAL:HG11	2.29	0.46
1:A:164:THR:O	1:A:165:PRO:C	2.58	0.46
1:B:116:ALA:HB1	1:B:117:ASP:HA	1.98	0.46
1:A:44:ILE:HD11	1:A:265:TYR:CE1	2.51	0.46
1:A:98:PHE:CD1	1:A:98:PHE:C	2.94	0.45
1:B:74:THR:HA	1:B:257:GLN:HG2	1.99	0.45
1:B:94:MET:HG3	1:B:241:MET:HG3	1.99	0.45
1:A:122:LEU:HB3	1:A:244:SER:OG	2.17	0.45
1:B:325:ASN:HB2	4:B:605:SO4:O4	2.16	0.45
1:B:133:ALA:O	1:B:137:ALA:HB3	2.17	0.45
1:A:361:GLY:O	1:A:363:GLY:N	2.50	0.44
1:B:349:THR:CG2	1:B:351:GLN:HB2	2.48	0.44
1:B:133:ALA:HB3	1:B:137:ALA:CB	2.47	0.44
1:A:125:PRO:HD3	1:A:145:GLY:O	2.17	0.44
1:A:212:ASN:CG	1:A:215:THR:OG1	2.60	0.44
1:B:103:LYS:HB3	1:B:204:PHE:HB3	1.99	0.44
1:A:212:ASN:CB	1:A:215:THR:OG1	2.66	0.44
1:A:310:PHE:HA	1:A:333:TYR:CD1	2.53	0.44
1:A:388:ASN:HB2	1:A:404:VAL:H	1.83	0.44
1:B:89:LYS:HA	1:B:89:LYS:HD2	1.62	0.43
1:A:272:VAL:HG21	1:A:298:TYR:CG	2.53	0.43
1:A:105:ASN:HD22	1:A:257:GLN:HG3	1.82	0.43
1:A:115:GLY:HA2	1:A:253:MET:O	2.19	0.43
1:B:411:LEU:HB2	1:B:450:THR:HG22	1.99	0.43
1:B:272:VAL:HG22	1:B:327:GLN:HB2	2.00	0.42
1:A:48:PRO:HD3	1:A:262:ASN:HD22	1.85	0.42
1:A:140:ILE:HG21	1:A:179:VAL:HB	2.01	0.42
1:A:277:VAL:HG12	1:A:283:THR:HA	2.00	0.42
1:B:86:VAL:O	1:B:244:SER:HA	2.19	0.42
1:B:212:ASN:HB3	1:B:215:THR:OG1	2.19	0.42
1:B:370:THR:O	1:B:372:ASP:N	2.52	0.42
1:B:75:LEU:HD23	1:B:75:LEU:HA	1.88	0.42
1:B:279:GLU:OE1	1:B:334:THR:HA	2.18	0.42
1:B:341:ASP:OD2	1:B:402:HIS:ND1	2.52	0.42
1:B:110:ALA:O	1:B:111:GLN:C	2.63	0.42
1:A:94:MET:HG3	1:A:241:MET:HG3	2.02	0.42
1:B:72:THR:HA	1:B:258:LEU:O	2.19	0.42
1:B:89:LYS:HE3	5:B:708:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:TYR:CE2	1:B:267:VAL:HG22	2.55	0.42
1:A:44:ILE:HD11	1:A:265:TYR:HE1	1.85	0.42
1:A:374:ILE:O	1:A:375:LYS:C	2.62	0.42
1:B:198:GLU:O	1:B:199:PRO:C	2.62	0.41
1:B:389:TYR:O	1:B:390:PRO:C	2.63	0.41
1:A:145:GLY:HA2	1:A:182:LEU:HD23	2.01	0.41
1:B:390:PRO:HA	4:B:611:SO4:O1	2.19	0.41
1:A:45:THR:HA	1:A:264:THR:HA	2.02	0.41
1:B:305:ILE:O	1:B:306:PRO:C	2.61	0.41
1:A:149:PHE:CD1	1:A:177:ALA:O	2.74	0.41
1:B:161:ASN:O	1:B:185:GLN:HG3	2.20	0.41
1:A:72:THR:HA	1:A:258:LEU:O	2.19	0.41
1:A:124:HIS:HB2	1:A:125:PRO:HD2	2.03	0.41
1:A:338:GLY:HA3	1:A:396:PHE:HB3	2.03	0.41
1:B:343:THR:HG23	1:B:355:LYS:HG3	2.03	0.41
1:B:456:GLY:O	1:B:457:GLU:C	2.64	0.40
1:B:389:TYR:HA	1:B:390:PRO:HD3	1.93	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	470/505 (93%)	431 (92%)	31 (7%)	8 (2%)	7	32
1	B	384/505 (76%)	357 (93%)	23 (6%)	4 (1%)	12	45
All	All	854/1010 (85%)	788 (92%)	54 (6%)	12 (1%)	9	36

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	371	THR

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Mol	Chain	Res	Type
1	B	371	THR
1	A	126	GLY
1	A	172	GLY
1	A	362	THR
1	B	348	THR
1	B	41	SER
1	B	113	ALA
1	A	138	ALA
1	A	375	LYS
1	A	441	PRO
1	A	165	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	383/411 (93%)	333 (87%)	50 (13%)	4	19
1	B	313/411 (76%)	276 (88%)	37 (12%)	5	22
All	All	696/822 (85%)	609 (88%)	87 (12%)	4	20

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	57	ARG
1	A	90	THR
1	A	98	PHE
1	A	101	THR
1	A	111	GLN
1	A	131	VAL
1	A	140	ILE
1	A	160	GLU
1	A	162	SER
1	A	171	LYS
1	A	179	VAL

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Mol	Chain	Res	Type
1	A	191	SER
1	A	215	THR
1	A	221	THR
1	A	228	THR
1	A	233	SER
1	A	239	GLN
1	A	242	SER
1	A	244	SER
1	A	245	ILE
1	A	248	SER
1	A	256	GLN
1	A	257	GLN
1	A	262	ASN
1	A	286	GLN
1	A	289	THR
1	A	299	VAL
1	A	301	SER
1	A	305	ILE
1	A	329	VAL
1	A	334	THR
1	A	343	THR
1	A	345	ILE
1	A	373	THR
1	A	394	THR
1	A	395	VAL
1	A	408	LYS
1	A	414	SER
1	A	416	GLU
1	A	439	ASN
1	A	441	PRO
1	A	450	THR
1	A	459	THR
1	A	462	ASP
1	A	464	GLN
1	A	474	VAL
1	A	480	LYS
1	A	483	THR
1	A	488	LYS
1	B	60	SER
1	B	65	ASP
1	B	86	VAL
1	B	89	LYS

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Mol	Chain	Res	Type
1	B	90	THR
1	B	97	ASN
1	B	109	LYS
1	B	127	ASP
1	B	150	LYS
1	B	152	ASP
1	B	162	SER
1	B	169	ASN
1	B	171	LYS
1	B	187	LYS
1	B	195	SER
1	B	198	GLU
1	B	239	GLN
1	B	245	ILE
1	B	253	MET
1	B	286	GLN
1	B	291	SER
1	B	313	SER
1	B	329	VAL
1	B	343	THR
1	B	351	GLN
1	B	376	SER
1	B	383	GLU
1	B	395	VAL
1	B	406	ASN
1	B	408	LYS
1	B	411	LEU
1	B	412	VAL
1	B	414	SER
1	B	415	SER
1	B	449	VAL
1	B	457	GLU
1	B	458	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	82	GLN
1	A	194	GLN
1	A	262	ASN
1	A	388	ASN

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Mol	Chain	Res	Type
1	A	425	GLN
1	A	503	GLN
1	B	78	ASN
1	B	229	GLN
1	B	238	ASN
1	B	256	GLN
1	B	321	ASN
1	B	406	ASN
1	B	453	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 2 are monoatomic - leaving 28 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	$\# Z > 2$
4	SO4	B	611	-	4,4,4	0.26	0	6,6,6	0.33	0
4	SO4	A	603	-	4,4,4	0.39	0	6,6,6	0.28	0
4	SO4	B	615	-	4,4,4	0.35	0	6,6,6	0.25	0
4	SO4	B	610	-	4,4,4	0.32	0	6,6,6	0.23	0
4	SO4	A	609	-	4,4,4	0.32	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	B	614	-	4,4,4	0.32	0	6,6,6	0.09	0
4	SO4	B	608	-	4,4,4	0.27	0	6,6,6	0.43	0
4	SO4	B	617	-	4,4,4	2.80	3 (75%)	6,6,6	0.70	0
4	SO4	A	610	-	4,4,4	2.94	2 (50%)	6,6,6	0.29	0
4	SO4	B	612	-	4,4,4	0.36	0	6,6,6	0.15	0
4	SO4	A	607	-	4,4,4	0.31	0	6,6,6	0.46	0
4	SO4	A	606	-	4,4,4	2.61	4 (100%)	6,6,6	0.74	0
4	SO4	B	618	-	4,4,4	0.32	0	6,6,6	0.15	0
4	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.43	0
4	SO4	B	606	-	4,4,4	2.57	3 (75%)	6,6,6	0.68	0
3	MAN	B	603	-	12,12,12	3.66	11 (91%)	17,17,17	1.89	5 (29%)
4	SO4	A	605	-	4,4,4	0.29	0	6,6,6	0.28	0
4	SO4	B	619	-	4,4,4	3.03	3 (75%)	6,6,6	0.48	0
4	SO4	B	605	-	4,4,4	0.26	0	6,6,6	0.24	0
4	SO4	A	611	-	4,4,4	3.02	3 (75%)	6,6,6	0.24	0
4	SO4	B	616	-	4,4,4	0.29	0	6,6,6	0.28	0
4	SO4	B	609	-	4,4,4	0.41	0	6,6,6	0.54	0
3	MAN	A	602	-	12,12,12	1.55	2 (16%)	17,17,17	1.84	4 (23%)
4	SO4	B	607	-	4,4,4	0.37	0	6,6,6	0.20	0
4	SO4	A	608	-	4,4,4	0.39	0	6,6,6	0.70	0
3	MAN	B	602	-	12,12,12	1.51	3 (25%)	17,17,17	2.30	6 (35%)
4	SO4	B	604	-	4,4,4	0.48	0	6,6,6	0.87	0
4	SO4	B	613	-	4,4,4	0.22	0	6,6,6	0.21	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
3	MAN	A	602	-	-	0/2/22/22	0/1/1/1
3	MAN	B	603	-	-	1/2/22/22	0/1/1/1
3	MAN	B	602	-	-	0/2/22/22	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	MAN	O5-C1	5.36	1.56	1.42
3	B	603	MAN	O3-C3	4.62	1.54	1.43
3	B	603	MAN	C1-C2	4.54	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	MAN	O2-C2	4.05	1.53	1.43
3	B	603	MAN	C3-C2	4.03	1.62	1.52
4	A	610	SO4	O2-S	3.92	1.68	1.44
4	B	619	SO4	O2-S	3.90	1.68	1.44
4	B	619	SO4	O1-S	3.80	1.67	1.44
3	B	603	MAN	O5-C5	3.80	1.53	1.44
4	A	611	SO4	O2-S	3.75	1.67	1.44
4	A	611	SO4	O1-S	3.74	1.67	1.44
4	B	617	SO4	O1-S	3.51	1.65	1.44
4	B	617	SO4	O2-S	3.43	1.65	1.44
4	A	610	SO4	O1-S	3.39	1.65	1.44
3	B	603	MAN	C4-C3	3.39	1.61	1.52
4	A	606	SO4	O1-S	3.37	1.64	1.44
3	B	603	MAN	O1-C1	3.15	1.49	1.39
4	B	606	SO4	O1-S	2.98	1.62	1.44
4	B	606	SO4	O2-S	2.97	1.62	1.44
3	B	603	MAN	O6-C6	2.83	1.54	1.42
3	B	602	MAN	C4-C5	2.83	1.59	1.53
3	B	603	MAN	C6-C5	2.77	1.61	1.51
3	A	602	MAN	C3-C2	2.50	1.58	1.52
4	A	606	SO4	O3-S	2.46	1.68	1.48
3	B	602	MAN	C4-C3	2.33	1.58	1.52
4	A	606	SO4	O2-S	2.30	1.58	1.44
3	A	602	MAN	O1-C1	2.28	1.46	1.39
3	B	603	MAN	C4-C5	2.26	1.57	1.53
4	B	619	SO4	O3-S	2.25	1.66	1.48
4	B	606	SO4	O4-S	2.25	1.66	1.48
3	B	602	MAN	C3-C2	2.21	1.58	1.52
4	A	611	SO4	O3-S	2.18	1.66	1.48
4	A	606	SO4	O4-S	2.14	1.65	1.48
4	B	617	SO4	O3-S	2.07	1.65	1.48

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	MAN	O2-C2-C3	4.71	121.47	110.38
3	B	602	MAN	O5-C1-C2	4.61	118.40	110.30
3	B	602	MAN	O2-C2-C3	4.26	120.41	110.38
3	B	603	MAN	C4-C3-C2	-4.22	103.43	110.83
3	A	602	MAN	O3-C3-C2	4.20	120.27	110.38
3	B	602	MAN	O1-C1-O5	-3.35	100.46	110.41
3	B	603	MAN	O5-C1-C2	3.24	116.00	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	MAN	C1-O5-C5	-3.02	107.82	113.65
3	B	602	MAN	C4-C3-C2	2.91	115.94	110.83
3	B	603	MAN	C3-C4-C5	2.87	115.43	110.23
3	B	602	MAN	C3-C4-C5	2.59	114.92	110.23
3	B	603	MAN	O6-C6-C5	-2.51	102.79	111.33
3	B	603	MAN	O3-C3-C2	2.29	115.78	110.38
3	A	602	MAN	O4-C4-C5	2.27	114.92	109.32
3	A	602	MAN	O5-C5-C4	2.17	113.61	109.70

There are no chirality outliers.

All (1) torsion outliers are listed below:

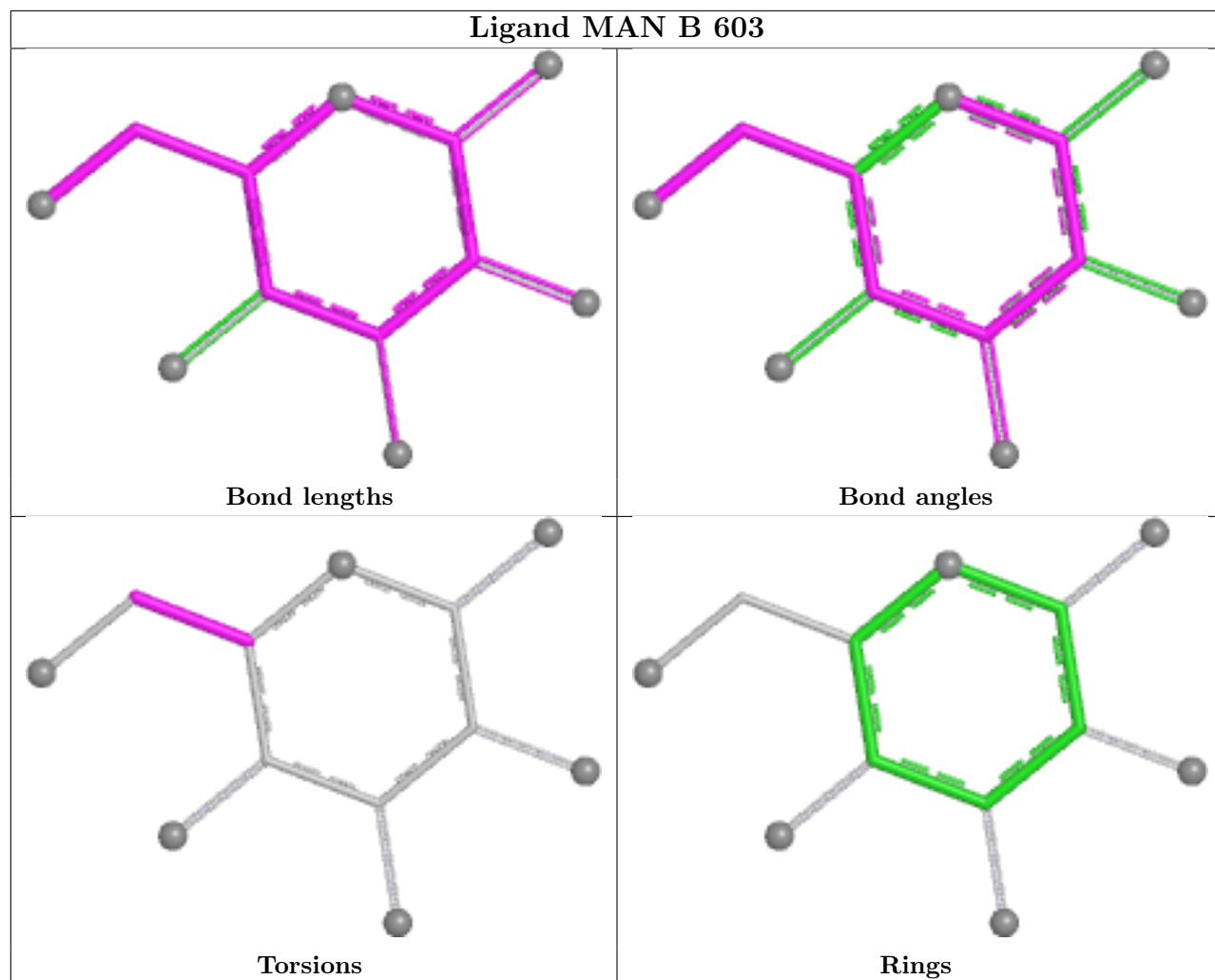
Mol	Chain	Res	Type	Atoms
3	B	603	MAN	O5-C5-C6-O6

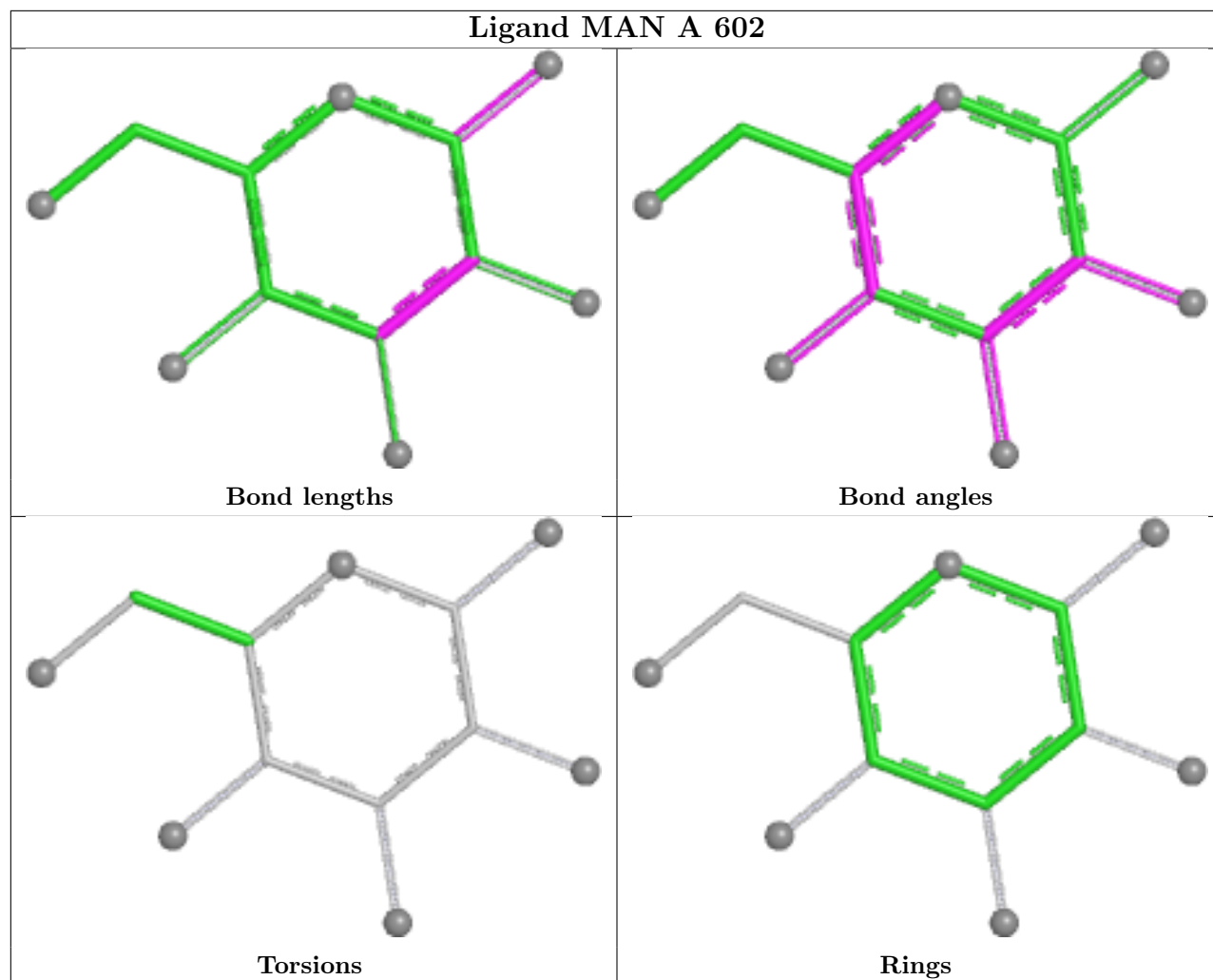
There are no ring outliers.

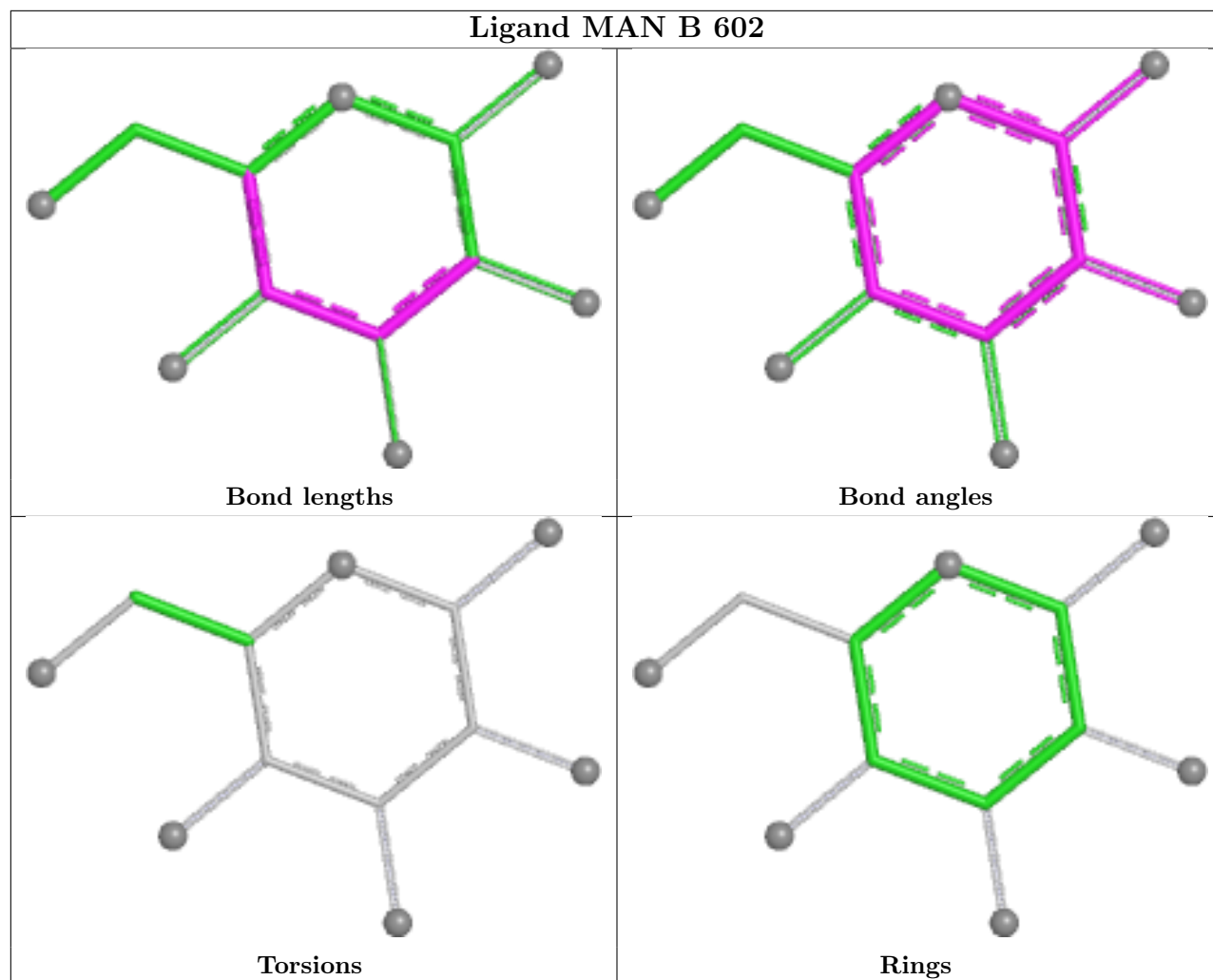
5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	611	SO4	1	0
4	A	603	SO4	1	0
4	B	605	SO4	1	0
4	B	609	SO4	1	0
4	B	604	SO4	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	472/505 (93%)	0.17	4 (0%) 82 64	62, 93, 120, 150	0
1	B	388/505 (76%)	-0.07	6 (1%) 72 49	42, 71, 119, 169	0
All	All	860/1010 (85%)	0.06	10 (1%) 76 55	42, 85, 121, 169	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	40	THR	2.9
1	B	449	VAL	2.5
1	A	49	LYS	2.3
1	B	455	THR	2.3
1	A	216	LYS	2.3
1	B	459	THR	2.3
1	A	356	LYS	2.2
1	B	448	SER	2.1
1	B	351	GLN	2.1
1	A	158	VAL	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 ⓘ

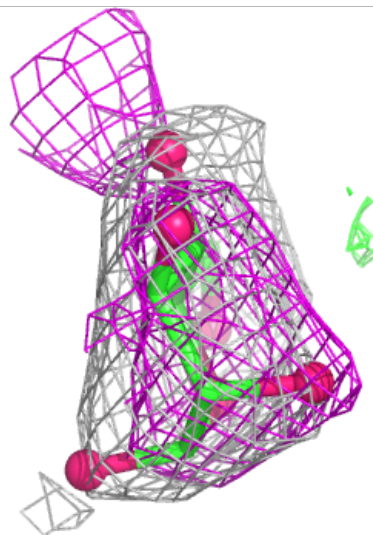
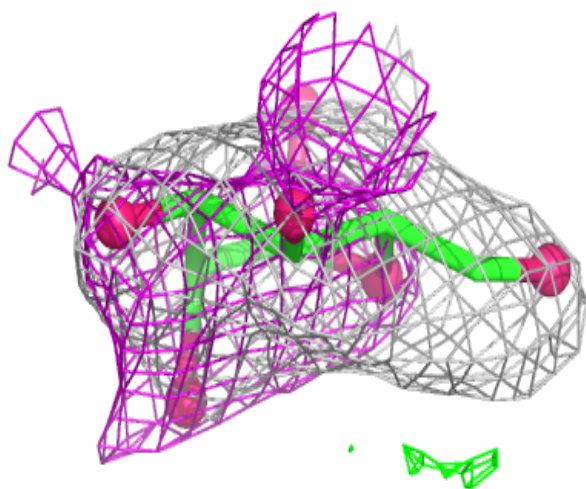
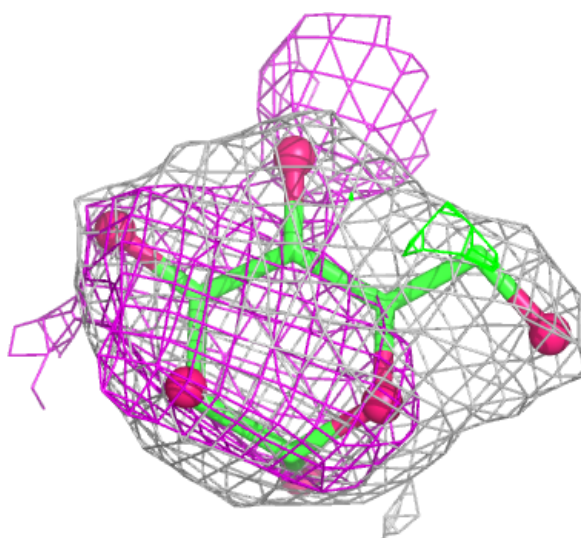
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	B	616	5/5	0.52	0.11	107,131,158,178	0
4	SO4	B	614	5/5	0.74	0.10	137,140,163,179	0
4	SO4	A	609	5/5	0.75	0.17	121,147,199,208	0
4	SO4	B	618	5/5	0.75	0.09	120,136,159,162	0
4	SO4	B	606	5/5	0.76	0.31	75,75,76,89	0
4	SO4	B	615	5/5	0.78	0.29	77,86,155,181	0
3	MAN	B	603	12/12	0.79	0.12	58,62,68,73	0
4	SO4	A	605	5/5	0.80	0.12	114,116,171,191	0
4	SO4	B	612	5/5	0.80	0.09	117,138,169,170	0
4	SO4	B	611	5/5	0.81	0.12	90,115,138,149	0
4	SO4	B	619	5/5	0.83	0.33	63,71,84,87	0
4	SO4	A	606	5/5	0.85	0.26	65,70,82,88	0
4	SO4	B	610	5/5	0.87	0.10	107,109,122,131	0
4	SO4	A	611	5/5	0.87	0.23	69,70,83,89	0
4	SO4	B	617	5/5	0.87	0.21	64,71,80,86	0
4	SO4	B	605	5/5	0.87	0.22	76,99,115,154	0
4	SO4	A	610	5/5	0.87	0.27	70,76,86,88	0
4	SO4	B	607	5/5	0.88	0.18	105,108,127,129	0
4	SO4	A	608	5/5	0.88	0.13	75,79,111,117	0
4	SO4	B	613	5/5	0.88	0.17	94,108,150,162	0
4	SO4	B	608	5/5	0.89	0.10	74,81,134,146	0
3	MAN	A	602	12/12	0.91	0.12	79,108,125,136	0
4	SO4	A	607	5/5	0.92	0.07	75,97,103,105	0
3	MAN	B	602	12/12	0.94	0.08	65,86,93,105	0
4	SO4	B	609	5/5	0.94	0.11	64,66,139,149	0
4	SO4	A	603	5/5	0.95	0.08	77,79,113,113	0
4	SO4	B	604	5/5	0.96	0.08	56,59,64,78	0
4	SO4	A	604	5/5	0.96	0.07	70,70,128,152	0
2	CA	B	601	1/1	0.98	0.04	75,75,75,75	0
2	CA	A	601	1/1	0.99	0.03	96,96,96,96	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.

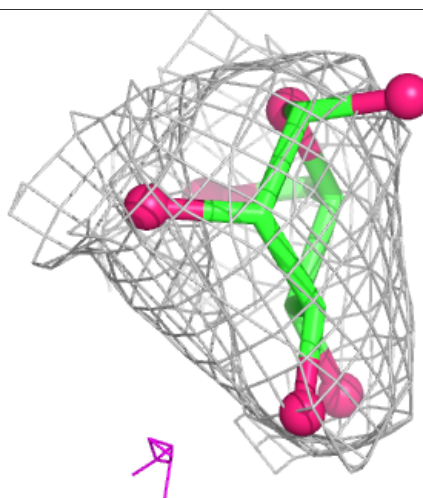
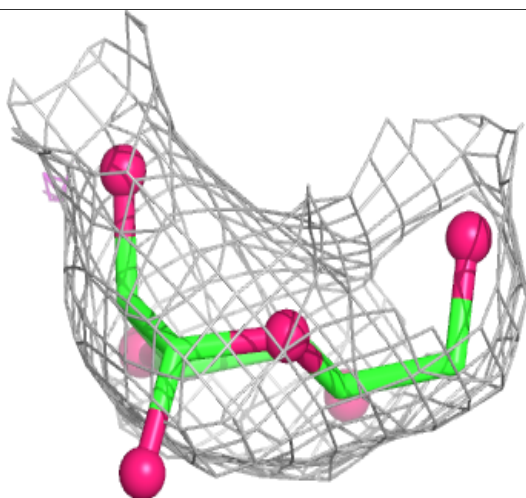
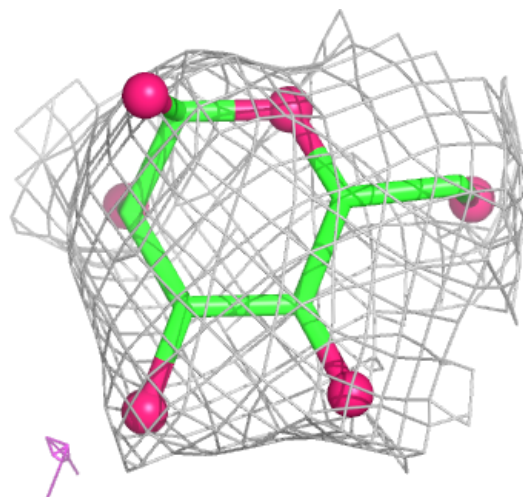
Electron density around MAN B 603:

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



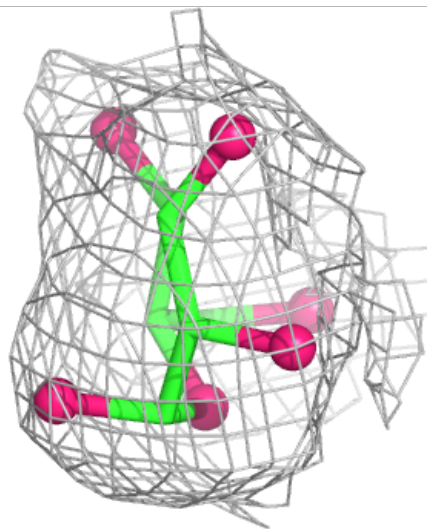
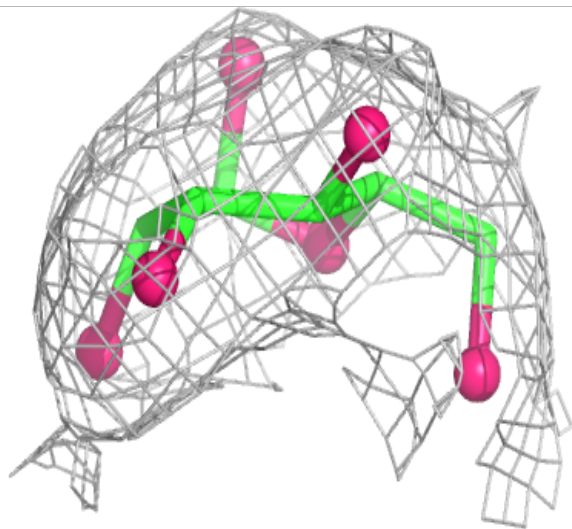
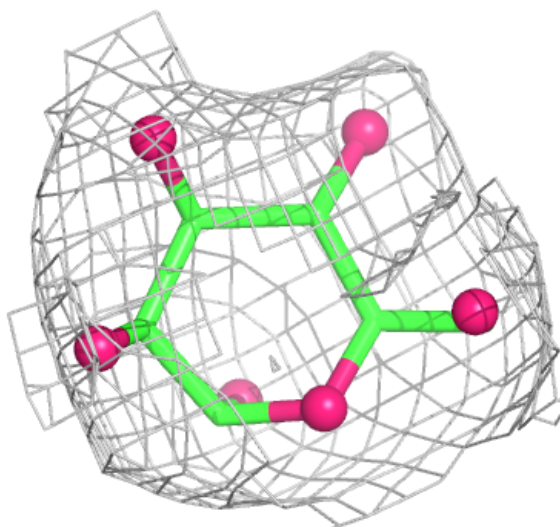
Electron density around MAN A 602:

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



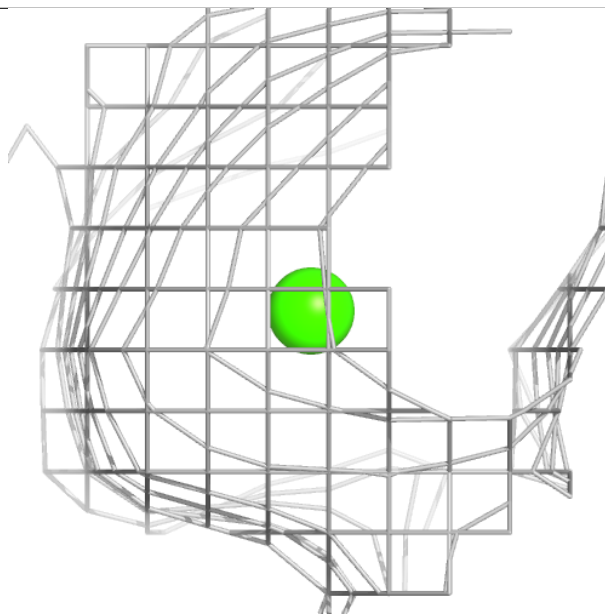
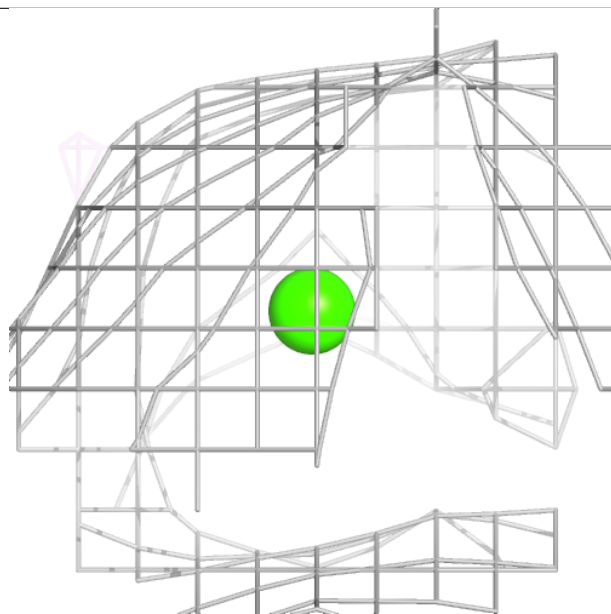
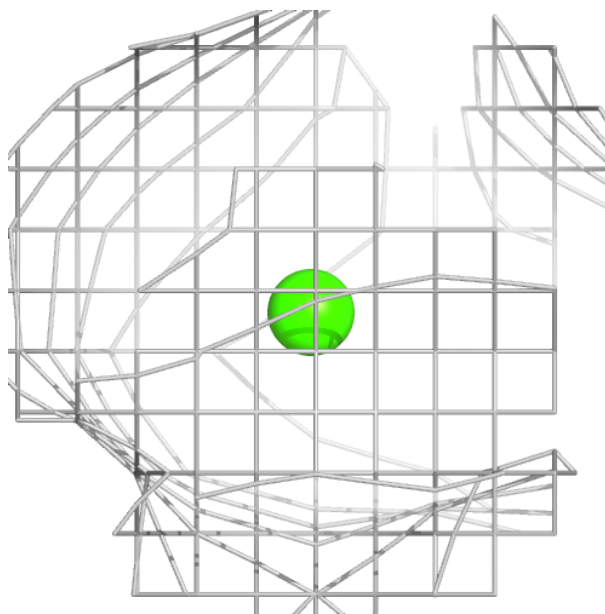
Electron density around MAN B 602:

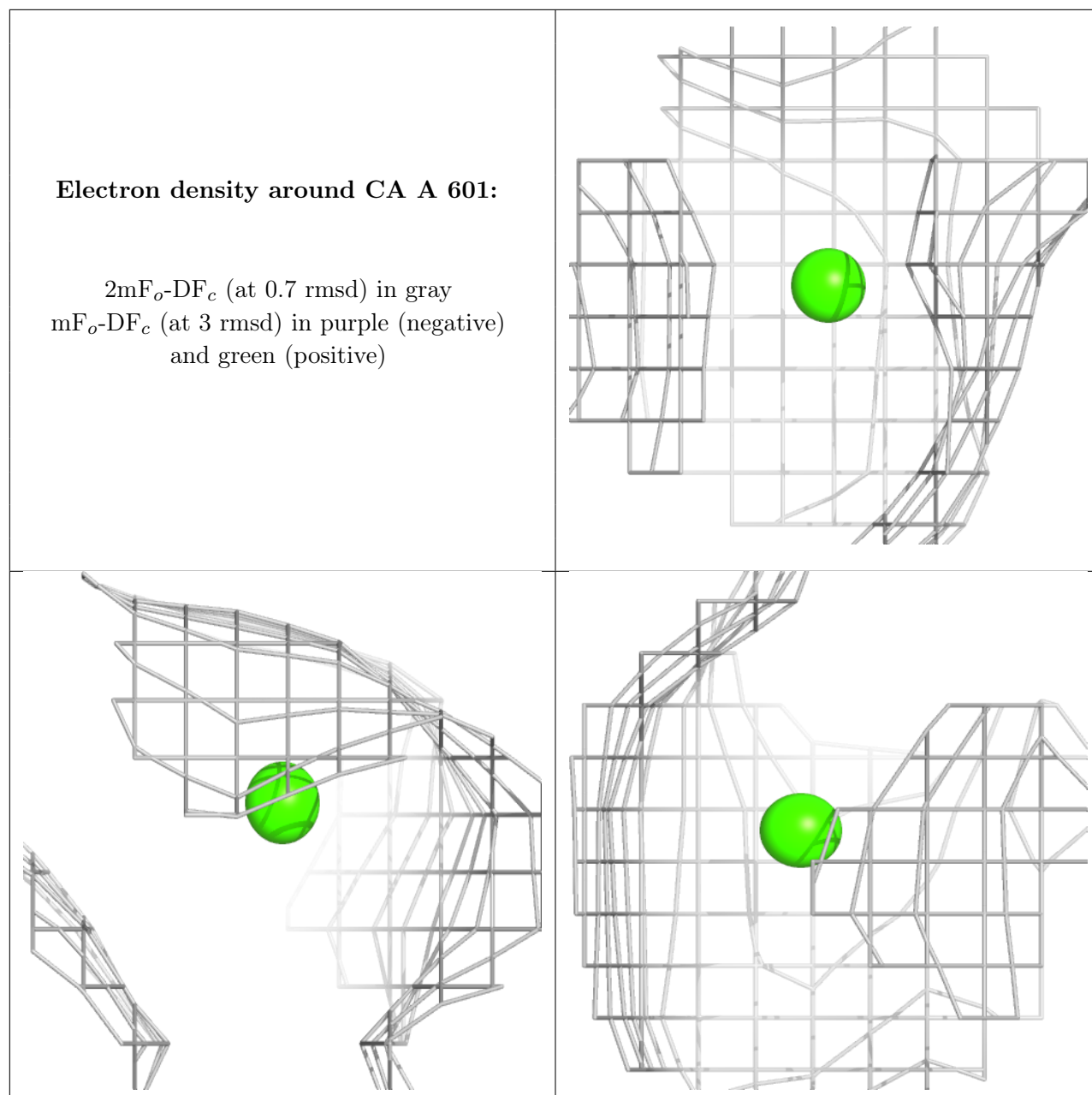
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CA B 601:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.