



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 08:26 AM UTC

PDB ID : 8QJ0 / pdb_00008qj0
Title : Room-temperature Serial Synchrotron Crystallography structure of Spinacia oleracea RuBisCO
Authors : Bjelcic, M.; Neutze, R.; Aurelius, O.; Nan, J.; Ursby, T.
Deposited on : 2023-09-12
Resolution : 2.30 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
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

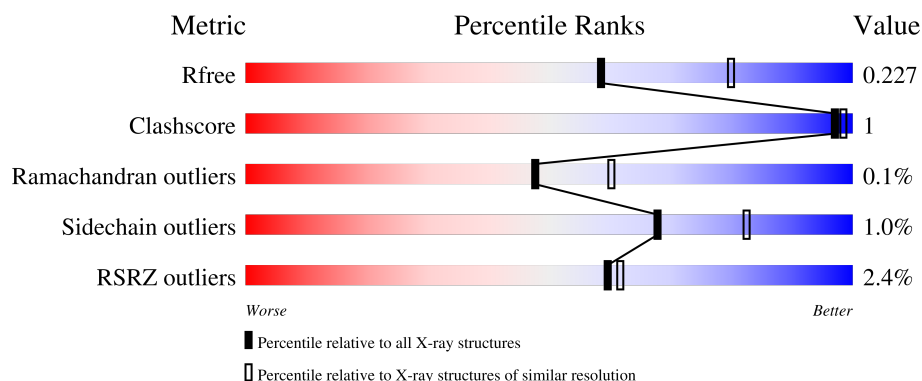
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	S	123	
1	T	123	
1	U	123	
1	V	123	
2	L	475	

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Mol	Chain	Length	Quality of chain
2	M	475	% 83% 9% 8%
2	N	475	2% 85% 7% 8%
2	O	475	3% 84% 7% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36264 atoms, of which 17380 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 Ribulose biphosphate carboxylase small subunit, chloroplastic 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	S	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	T	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	U	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			
1	V	123	Total	C	H	N	O	S	31	0	0
			2023	669	989	171	186	8			

- Molecule 2 is a protein called Ribulose biphosphate carboxylase large chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	439	Total	C	H	N	O	S	109	0	0
			6786	2175	3351	606	637	17			
2	M	439	Total	C	H	N	O	S	109	0	0
			6786	2175	3351	606	637	17			
2	N	439	Total	C	H	N	O	S	107	0	0
			6799	2178	3360	607	637	17			
2	O	439	Total	C	H	N	O	S	107	0	0
			6802	2178	3362	608	637	17			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	L	1	Total	Mg	0	0
			1	1		
3	M	1	Total	Mg	0	0
			1	1		
3	N	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	O	1	Total 1	Mg 1	0	0

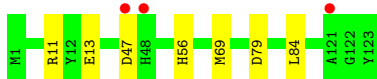
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	S	44	Total 44	O 44	0	0
4	T	50	Total 50	O 50	0	0
4	U	45	Total 45	O 45	0	0
4	V	46	Total 46	O 46	0	0
4	L	202	Total 202	O 202	0	0
4	M	198	Total 198	O 198	0	0
4	N	193	Total 193	O 193	0	0
4	O	217	Total 217	O 217	0	0

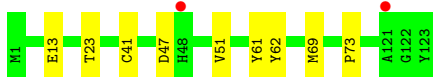
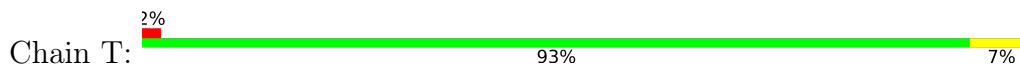
3 Residue-property plots [i](#)

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: Ribulose biphosphate carboxylase small subunit, chloroplastic 2



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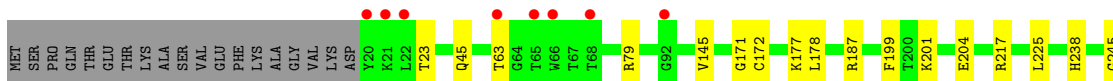
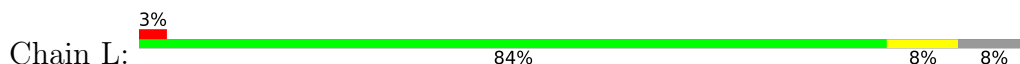
- Molecule 1: Ribulose biphosphate carboxylase small subunit, chloroplastic 2

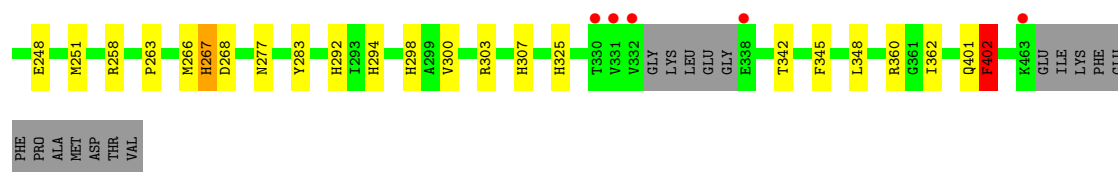


- Molecule 1: Ribulose biphosphate carboxylase small subunit, chloroplastic 2

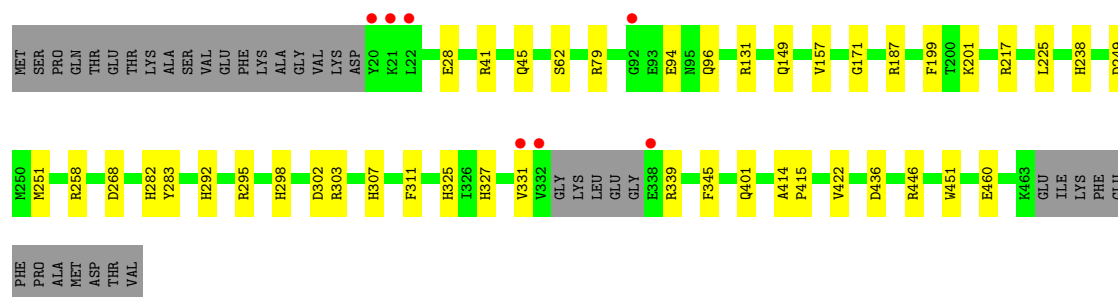
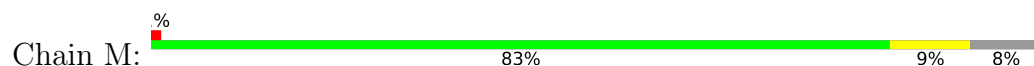


- Molecule 2: Ribulose biphosphate carboxylase large chain

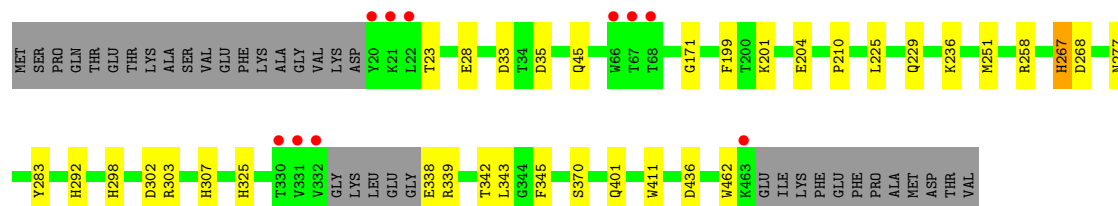
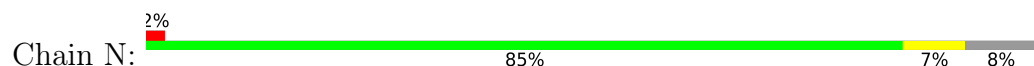




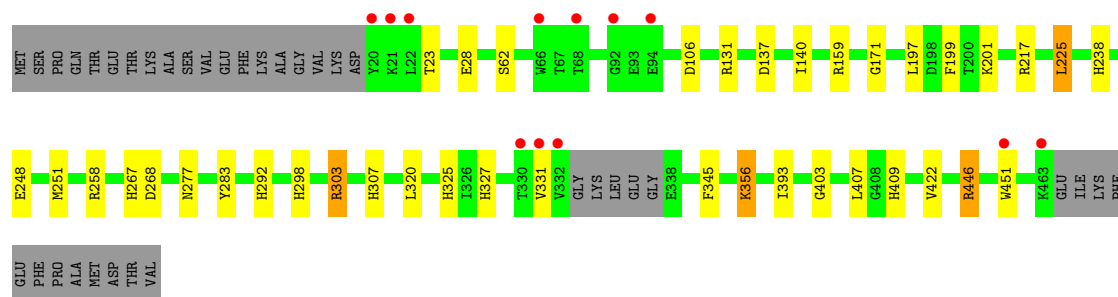
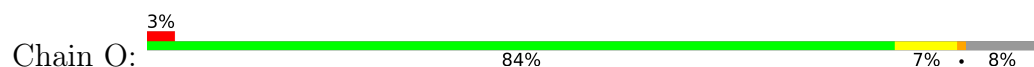
- Molecule 2: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase large chain



- Molecule 2: Ribulose biphosphate carboxylase large chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	158.60Å 157.12Å 202.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	97.78 – 2.30 97.78 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (97.78-2.30) 99.9 (97.78-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.74 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0419	Depositor
R, R_{free}	0.181 , 0.227 0.181 , 0.227	Depositor DCC
R_{free} test set	5452 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	36264	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7999e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, MG

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	S	0.80	0/1069	1.32	4/1453 (0.3%)
1	T	0.82	0/1069	1.36	4/1453 (0.3%)
1	U	0.81	0/1069	1.37	5/1453 (0.3%)
1	V	0.82	0/1069	1.34	3/1453 (0.2%)
2	L	0.92	2/3507 (0.1%)	1.46	28/4763 (0.6%)
2	M	0.90	2/3507 (0.1%)	1.43	20/4763 (0.4%)
2	N	0.93	1/3511 (0.0%)	1.45	21/4767 (0.4%)
2	O	0.94	1/3512 (0.0%)	1.46	21/4767 (0.4%)
All	All	0.90	6/18313 (0.0%)	1.43	106/24872 (0.4%)

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	S	0	1
2	L	0	6
2	M	0	7
2	N	0	3
2	O	0	5
All	All	0	22

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	267	HIS	CG-CD2	-5.75	1.29	1.35
2	O	409	HIS	CG-CD2	-5.56	1.29	1.35
2	M	238	HIS	CE1-NE2	-5.53	1.27	1.32
2	L	294	HIS	CE1-NE2	5.46	1.38	1.32
2	M	249	ASP	CG-OD1	-5.34	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	267	HIS	CG-CD2	-5.02	1.30	1.35

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	307	HIS	CB-CG-CD2	8.71	142.52	131.20
2	L	307	HIS	CB-CG-CD2	8.45	142.18	131.20
2	O	307	HIS	CB-CG-CD2	8.39	142.11	131.20
2	N	307	HIS	CB-CG-CD2	8.23	141.90	131.20
2	M	292	HIS	CB-CG-CD2	8.16	141.81	131.20
2	O	298	HIS	CB-CG-CD2	7.89	141.45	131.20
2	L	402	PHE	CB-CA-C	7.83	122.73	109.50
2	L	268	ASP	CA-CB-CG	7.67	120.27	112.60
2	O	292	HIS	CB-CG-CD2	7.64	141.13	131.20
2	L	307	HIS	CB-CG-ND1	-7.61	111.29	122.70
2	M	268	ASP	CA-CB-CG	7.45	120.05	112.60
2	M	307	HIS	CB-CG-ND1	-7.42	111.58	122.70
2	N	268	ASP	CA-CB-CG	7.28	119.88	112.60
2	M	298	HIS	CB-CG-CD2	7.25	140.63	131.20
2	O	268	ASP	CA-CB-CG	7.25	119.85	112.60
2	N	292	HIS	CB-CG-CD2	7.24	140.61	131.20
2	M	238	HIS	CB-CG-CD2	7.03	140.34	131.20
2	O	307	HIS	CB-CG-ND1	-7.00	112.20	122.70
2	L	238	HIS	CB-CG-CD2	6.92	140.19	131.20
2	N	307	HIS	CB-CG-ND1	-6.91	112.34	122.70
1	U	24	ASP	CA-CB-CG	6.88	119.48	112.60
1	S	47	ASP	CB-CA-C	6.85	124.05	110.42
2	N	298	HIS	CB-CG-CD2	6.75	139.97	131.20
2	L	266	MET	CG-SD-CE	6.70	115.63	100.90
2	M	292	HIS	CB-CG-ND1	-6.67	112.70	122.70
2	M	325	HIS	CA-CB-CG	6.59	120.39	113.80
2	O	238	HIS	CB-CG-CD2	6.47	139.60	131.20
2	O	345	PHE	CA-CB-CG	6.44	120.24	113.80
2	L	298	HIS	CB-CG-CD2	6.42	139.55	131.20
2	O	325	HIS	CA-CB-CG	6.41	120.21	113.80
1	U	23	THR	CA-CB-OG1	-6.35	100.08	109.60
2	O	292	HIS	CB-CG-ND1	-6.35	113.17	122.70
2	N	33	ASP	CA-CB-CG	6.34	118.94	112.60
2	N	345	PHE	CA-CB-CG	6.33	120.14	113.80
2	M	345	PHE	CA-CB-CG	6.33	120.13	113.80
2	N	292	HIS	CB-CG-ND1	-6.25	113.32	122.70
1	V	47	ASP	CB-CA-C	6.23	122.82	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	13	GLU	CB-CA-C	6.14	122.63	110.42
1	T	47	ASP	CB-CA-C	6.13	122.62	110.42
2	N	325	HIS	CA-CB-CG	6.13	119.93	113.80
2	O	356	LYS	CB-CA-C	6.07	118.95	109.84
2	L	325	HIS	CA-CB-CG	6.07	119.87	113.80
2	L	292	HIS	CB-CG-ND1	-5.92	113.83	122.70
2	L	360	ARG	NE-CZ-NH2	-5.92	113.88	119.20
2	M	298	HIS	CB-CG-ND1	-5.89	113.86	122.70
2	L	345	PHE	CA-CB-CG	5.89	119.69	113.80
1	U	57	ASN	CB-CA-C	-5.83	100.64	110.44
2	O	298	HIS	CB-CG-ND1	-5.78	114.03	122.70
1	V	13	GLU	CB-CA-C	5.76	121.89	110.42
2	O	225	LEU	CA-C-O	-5.73	114.48	120.55
1	S	13	GLU	CB-CA-C	5.71	121.78	110.42
2	N	436	ASP	CA-CB-CG	5.70	118.30	112.60
1	S	56	HIS	CB-CG-CD2	-5.70	123.79	131.20
2	O	131	ARG	NE-CZ-NH2	5.65	124.28	119.20
2	L	238	HIS	CB-CG-ND1	-5.63	114.25	122.70
2	M	28	GLU	CB-CG-CD	5.62	122.15	112.60
2	M	249	ASP	CA-CB-CG	5.61	118.21	112.60
1	U	79	ASP	CA-CB-CG	5.59	118.19	112.60
2	N	45	GLN	CB-CA-C	5.55	118.21	109.27
2	L	292	HIS	CB-CG-CD2	5.54	138.40	131.20
2	N	401	GLN	N-CA-CB	-5.48	101.94	110.55
2	N	204	GLU	CB-CG-CD	5.47	121.90	112.60
2	O	356	LYS	CA-CB-CG	5.46	125.03	114.10
2	O	238	HIS	CB-CG-ND1	-5.43	114.56	122.70
2	M	327	HIS	CB-CG-CD2	-5.39	124.20	131.20
2	M	131	ARG	CA-CB-CG	5.39	124.88	114.10
1	V	48	HIS	CA-CB-CG	5.38	119.18	113.80
2	N	28	GLU	CB-CG-CD	5.38	121.75	112.60
2	N	302	ASP	CA-CB-CG	5.38	117.98	112.60
2	L	45	GLN	CB-CA-C	5.34	118.22	109.46
2	L	263	PRO	N-CA-C	5.33	121.59	114.18
1	T	23	THR	CA-CB-OG1	-5.32	101.62	109.60
2	N	267	HIS	CB-CG-ND1	5.32	130.69	122.70
2	L	267	HIS	CB-CG-CD2	-5.29	124.32	131.20
2	L	145	VAL	N-CA-CB	5.29	116.38	110.51
2	M	436	ASP	CA-CB-CG	5.27	117.87	112.60
2	L	300	VAL	CA-C-N	5.26	128.56	122.35
2	L	300	VAL	C-N-CA	5.26	128.56	122.35
2	L	245	GLY	CA-C-O	-5.25	115.10	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	GLN	N-CA-CB	-5.25	102.31	110.55
2	O	327	HIS	CB-CG-CD2	-5.24	124.39	131.20
2	M	460	GLU	CB-CG-CD	-5.23	103.71	112.60
1	U	47	ASP	CB-CA-C	5.20	120.76	110.42
2	N	35	ASP	CA-CB-CG	5.19	117.79	112.60
2	N	267	HIS	CB-CG-CD2	-5.18	124.46	131.20
2	N	401	GLN	CB-CA-C	5.16	118.65	110.19
2	N	342	THR	CA-CB-OG1	-5.16	101.87	109.60
2	L	63	THR	CA-CB-OG1	-5.15	101.87	109.60
2	L	401	GLN	CB-CA-C	5.15	118.63	110.19
2	L	402	PHE	N-CA-C	-5.13	101.91	110.17
2	O	225	LEU	N-CA-CB	5.12	117.65	110.12
2	O	137	ASP	CA-CB-CG	5.10	117.70	112.60
2	M	311	PHE	CA-CB-CG	-5.08	108.72	113.80
1	T	61	TYR	N-CA-CB	5.08	118.70	110.42
2	M	45	GLN	CB-CA-C	5.08	117.78	109.46
2	O	303	ARG	CD-NE-CZ	5.07	131.50	124.40
2	L	248	GLU	CB-CG-CD	5.05	121.19	112.60
2	O	248	GLU	CB-CG-CD	5.05	121.19	112.60
2	O	28	GLU	CB-CG-CD	5.05	121.18	112.60
2	L	402	PHE	O-C-N	-5.03	117.31	123.10
2	L	342	THR	CA-CB-OG1	-5.02	102.07	109.60
2	N	298	HIS	CB-CG-ND1	-5.02	115.17	122.70
2	L	204	GLU	CB-CG-CD	5.02	121.13	112.60
1	S	79	ASP	CA-CB-CG	5.01	117.61	112.60
2	M	302	ASP	CA-CB-CG	5.01	117.61	112.60
2	M	94	GLU	CB-CA-C	5.01	118.01	109.84

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	187	ARG	Sidechain
2	L	217	ARG	Sidechain
2	L	258	ARG	Sidechain
2	L	303	ARG	Sidechain
2	L	402	PHE	Mainchain
2	L	79	ARG	Sidechain
2	M	217	ARG	Sidechain
2	M	258	ARG	Sidechain
2	M	295	ARG	Sidechain
2	M	303	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	M	339	ARG	Sidechain
2	M	446	ARG	Sidechain
2	M	79	ARG	Sidechain
2	N	258	ARG	Sidechain
2	N	303	ARG	Sidechain
2	N	462	TRP	Peptide
2	O	159	ARG	Sidechain
2	O	217	ARG	Sidechain
2	O	258	ARG	Sidechain
2	O	303	ARG	Sidechain
2	O	446	ARG	Sidechain
1	S	11	ARG	Sidechain

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	S	1034	989	986	1	0
1	T	1034	989	986	3	0
1	U	1034	989	986	1	0
1	V	1034	989	986	1	0
2	L	3435	3351	3330	5	0
2	M	3435	3351	3330	8	0
2	N	3439	3360	3341	5	1
2	O	3440	3362	3343	8	1
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
4	L	202	0	0	0	0
4	M	198	0	0	0	0
4	N	193	0	0	1	0
4	O	217	0	0	2	0
4	S	44	0	0	0	0
4	T	50	0	0	0	0
4	U	45	0	0	0	0
4	V	46	0	0	0	0
All	All	18884	17380	17288	30	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (30) 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:T:69:MET:HE1	1:T:73:PRO:HD3	1.81	0.61
1:S:69:MET:HE2	2:M:187:ARG:HD3	1.86	0.57
2:O:407:LEU:HD22	4:O:774:HOH:O	2.07	0.54
2:N:229:GLN:HE21	2:N:236:LYS:H	1.55	0.54
2:L:251:MET:HE1	2:L:283:TYR:CD1	2.43	0.54
2:N:251:MET:HE1	2:N:283:TYR:CD1	2.43	0.53
2:O:197:LEU:HD23	4:O:709:HOH:O	2.09	0.52
2:O:331:VAL:HG11	2:O:393:ILE:HD13	1.92	0.51
2:M:251:MET:HE1	2:M:283:TYR:CD1	2.46	0.50
2:O:140:ILE:HD13	2:O:320:LEU:HD11	1.95	0.49
2:M:41:ARG:HH11	2:M:96:GLN:NE2	2.11	0.48
2:O:251:MET:HE1	2:O:283:TYR:CD1	2.49	0.48
2:L:348:LEU:HD11	2:L:362:ILE:HD12	1.96	0.47
2:M:149:GLN:HE22	2:M:282:HIS:HA	1.79	0.47
2:L:172:CYS:HA	2:L:402:PHE:O	2.15	0.46
2:L:171:GLY:HA2	2:L:199:PHE:O	2.16	0.46
2:M:157:VAL:HG13	4:N:773:HOH:O	2.16	0.45
2:M:171:GLY:HA2	2:M:199:PHE:O	2.17	0.44
2:N:171:GLY:HA2	2:N:199:PHE:O	2.17	0.44
1:V:51:VAL:HG13	1:V:62:TYR:HB3	1.99	0.44
1:T:51:VAL:HG13	1:T:62:TYR:HB3	1.98	0.44
1:U:1:MET:HE3	2:N:411:TRP:HA	2.00	0.43
2:L:267:HIS:HD2	2:L:277:ASN:OD1	2.02	0.42
2:O:171:GLY:HA2	2:O:199:PHE:O	2.19	0.41
1:T:41:CYS:SG	1:T:69:MET:HE3	2.61	0.41
2:N:267:HIS:HD2	2:N:277:ASN:OD1	2.04	0.41
2:M:414:ALA:HB3	2:M:415:PRO:HD3	2.03	0.40
2:M:422:VAL:HG13	2:M:451:TRP:CH2	2.56	0.40
2:O:267:HIS:HD2	2:O:277:ASN:OD1	2.04	0.40
2:O:422:VAL:HG13	2:O:451:TRP:CH2	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:370:SER:HG	2:O:106:ASP:OD2[4_555]	1.55	0.05

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	S	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	T	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
1	U	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
1	V	121/123 (98%)	115 (95%)	6 (5%)	0	100	100
2	L	434/475 (91%)	423 (98%)	11 (2%)	0	100	100
2	M	434/475 (91%)	424 (98%)	9 (2%)	1 (0%)	43	55
2	N	434/475 (91%)	423 (98%)	11 (2%)	0	100	100
2	O	434/475 (91%)	424 (98%)	8 (2%)	2 (0%)	24	31
All	All	2220/2392 (93%)	2152 (97%)	65 (3%)	3 (0%)	48	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	62	SER
2	O	62	SER
2	O	403	GLY

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	S	112/112 (100%)	111 (99%)	1 (1%)	70	84
1	T	112/112 (100%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	112/112 (100%)	111 (99%)	1 (1%)	70	84
1	V	112/112 (100%)	112 (100%)	0	100	100
2	L	354/386 (92%)	350 (99%)	4 (1%)	65	81
2	M	354/386 (92%)	351 (99%)	3 (1%)	73	86
2	N	355/386 (92%)	349 (98%)	6 (2%)	53	72
2	O	355/386 (92%)	351 (99%)	4 (1%)	65	81
All	All	1866/1992 (94%)	1847 (99%)	19 (1%)	68	82

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	84	LEU
1	U	48	HIS
2	L	23	THR
2	L	177	LYS
2	L	178	LEU
2	L	225	LEU
2	M	225	LEU
2	M	331	VAL
2	M	401	GLN
2	N	23	THR
2	N	210	PRO
2	N	225	LEU
2	N	338	GLU
2	N	339	ARG
2	N	343	LEU
2	O	23	THR
2	O	225	LEU
2	O	356	LYS
2	O	446	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	S	55	HIS
1	S	109	GLN
1	T	82	GLN
1	T	109	GLN
1	U	8	ASN

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Mol	Chain	Res	Type
1	U	55	HIS
1	U	109	GLN
1	V	36	ASN
1	V	57	ASN
1	V	107	ASN
2	L	115	ASN
2	L	238	HIS
2	L	267	HIS
2	L	292	HIS
2	L	298	HIS
2	L	327	HIS
2	L	383	HIS
2	L	386	HIS
2	L	420	ASN
2	M	45	GLN
2	M	96	GLN
2	M	115	ASN
2	M	123	ASN
2	M	149	GLN
2	M	163	ASN
2	M	238	HIS
2	M	267	HIS
2	M	292	HIS
2	M	298	HIS
2	M	327	HIS
2	M	383	HIS
2	M	386	HIS
2	M	401	GLN
2	N	76	ASN
2	N	115	ASN
2	N	163	ASN
2	N	229	GLN
2	N	267	HIS
2	N	292	HIS
2	N	298	HIS
2	N	327	HIS
2	N	383	HIS
2	N	386	HIS
2	N	420	ASN
2	O	115	ASN
2	O	238	HIS
2	O	267	HIS

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Mol	Chain	Res	Type
2	O	292	HIS
2	O	298	HIS
2	O	304	GLN
2	O	327	HIS
2	O	383	HIS
2	O	420	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	KCX	L	201	2,3	10,11,12	1.44	1 (10%)	6,12,14	4.01	3 (50%)
2	KCX	O	201	2,3	10,11,12	1.53	1 (10%)	6,12,14	2.00	3 (50%)
2	KCX	M	201	2,3	10,11,12	1.62	1 (10%)	6,12,14	2.52	2 (33%)
2	KCX	N	201	2,3	10,11,12	1.64	1 (10%)	6,12,14	4.09	3 (50%)

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	KCX	L	201	2,3	-	1/9/10/12	-
2	KCX	O	201	2,3	-	1/9/10/12	-
2	KCX	M	201	2,3	-	1/9/10/12	-
2	KCX	N	201	2,3	-	0/9/10/12	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	201	KCX	CX-NZ	4.79	1.43	1.35
2	M	201	KCX	CX-NZ	4.51	1.43	1.35
2	O	201	KCX	CX-NZ	4.23	1.42	1.35
2	L	201	KCX	CX-NZ	3.92	1.42	1.35

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	201	KCX	OQ1-CX-NZ	8.36	137.63	124.92
2	L	201	KCX	OQ1-CX-NZ	8.13	137.27	124.92
2	M	201	KCX	OQ1-CX-NZ	4.94	132.43	124.92
2	N	201	KCX	CE-NZ-CX	-4.88	113.70	121.98
2	L	201	KCX	CE-NZ-CX	-4.79	113.85	121.98
2	O	201	KCX	CE-NZ-CX	-3.62	115.84	121.98
2	M	201	KCX	CE-NZ-CX	-2.94	116.99	121.98
2	L	201	KCX	CG-CD-CE	-2.38	102.58	113.56
2	O	201	KCX	OQ1-CX-NZ	2.20	128.26	124.92
2	N	201	KCX	CG-CD-CE	-2.14	103.69	113.56
2	O	201	KCX	CG-CD-CE	-2.10	103.86	113.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	201	KCX	C-CA-CB-CG
2	L	201	KCX	C-CA-CB-CG
2	M	201	KCX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	S	123/123 (100%)	-0.11	3 (2%) 59 62	12, 28, 55, 73	0
1	T	123/123 (100%)	-0.17	2 (1%) 70 72	15, 27, 58, 77	0
1	U	123/123 (100%)	0.11	4 (3%) 49 51	13, 29, 55, 71	0
1	V	123/123 (100%)	0.03	2 (1%) 70 72	12, 29, 62, 77	0
2	L	438/475 (92%)	-0.33	13 (2%) 52 54	8, 18, 52, 109	0
2	M	438/475 (92%)	-0.41	7 (1%) 70 72	9, 18, 49, 108	0
2	N	438/475 (92%)	-0.30	10 (2%) 61 63	9, 18, 51, 96	0
2	O	438/475 (92%)	-0.21	12 (2%) 56 58	9, 19, 50, 94	0
All	All	2244/2392 (93%)	-0.25	53 (2%) 59 62	8, 20, 54, 109	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	332	VAL	6.2
2	M	20	TYR	6.2
2	N	332	VAL	6.1
2	N	22	LEU	5.8
2	M	332	VAL	5.7
2	O	332	VAL	5.6
2	M	22	LEU	5.4
2	N	20	TYR	5.0
2	L	22	LEU	4.9
2	O	22	LEU	4.5
2	L	331	VAL	4.3
2	O	20	TYR	4.3
2	L	65	THR	4.1
2	N	66	TRP	4.0
2	N	68	THR	3.9
1	U	48	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	68	THR	3.7
2	O	331	VAL	3.6
2	L	330	THR	3.6
1	S	48	HIS	3.5
2	L	20	TYR	3.4
1	V	121	ALA	3.3
2	N	331	VAL	3.2
1	V	48	HIS	3.2
1	U	121	ALA	3.1
2	L	21	LYS	3.1
2	N	330	THR	2.9
2	L	92	GLY	2.8
1	S	121	ALA	2.7
2	O	66	TRP	2.7
2	N	463	LYS	2.7
2	L	66	TRP	2.7
2	M	21	LYS	2.7
2	O	94	GLU	2.7
1	T	121	ALA	2.6
2	O	21	LYS	2.6
2	M	331	VAL	2.6
2	M	92	GLY	2.5
2	O	330	THR	2.5
2	L	338	GLU	2.4
1	U	76	GLY	2.4
2	L	463	LYS	2.4
2	L	63	THR	2.4
2	N	21	LYS	2.4
2	O	92	GLY	2.2
1	T	48	HIS	2.2
2	N	67	THR	2.2
1	S	47	ASP	2.2
1	U	47	ASP	2.2
2	O	451	TRP	2.1
2	M	338	GLU	2.1
2	O	68	THR	2.0
2	O	463	LYS	2.0

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

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	KCX	O	201	12/13	0.94	0.07	12,16,20,21	0
2	KCX	L	201	12/13	0.95	0.07	11,19,19,23	0
2	KCX	N	201	12/13	0.96	0.07	12,18,20,21	0
2	KCX	M	201	12/13	0.96	0.06	12,16,19,19	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

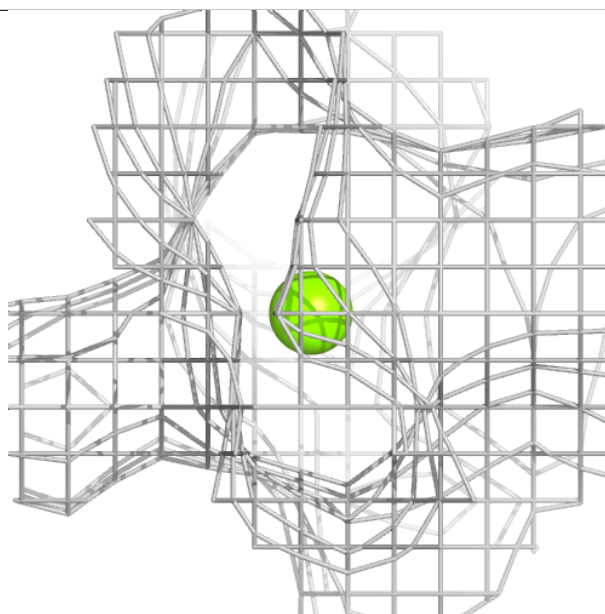
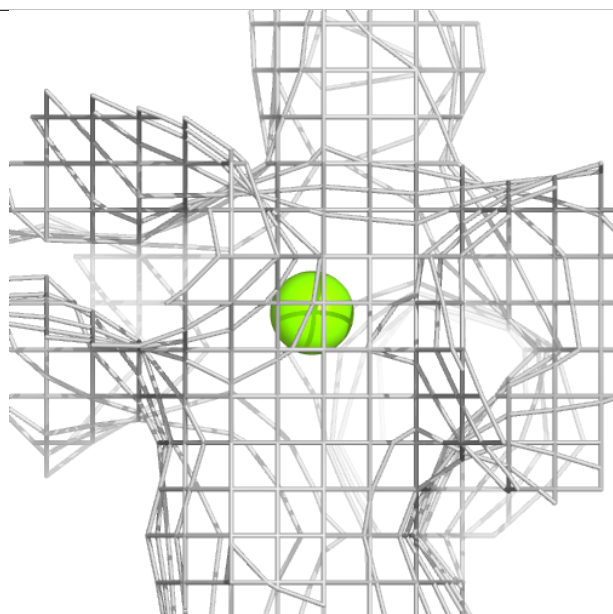
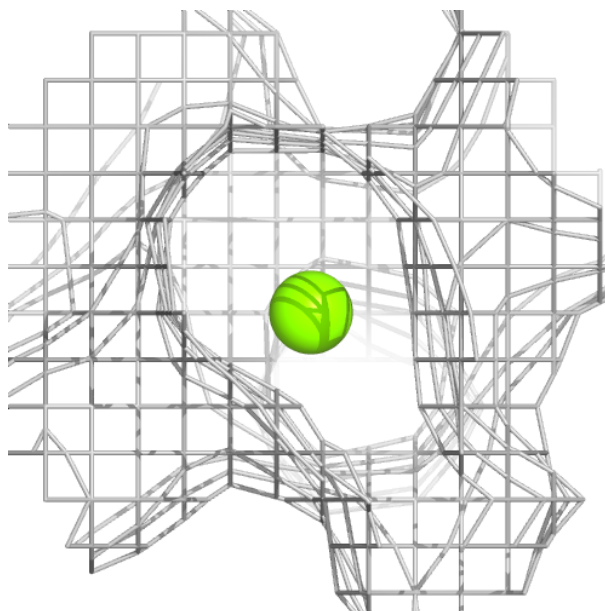
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	L	501	1/1	0.98	0.03	17,17,17,17	0
3	MG	N	501	1/1	0.98	0.04	16,16,16,16	0
3	MG	M	501	1/1	0.99	0.06	18,18,18,18	0
3	MG	O	501	1/1	0.99	0.03	20,20,20,20	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.

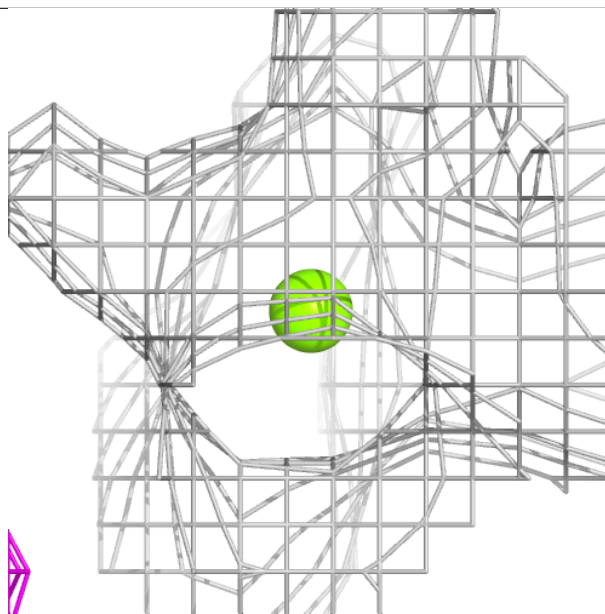
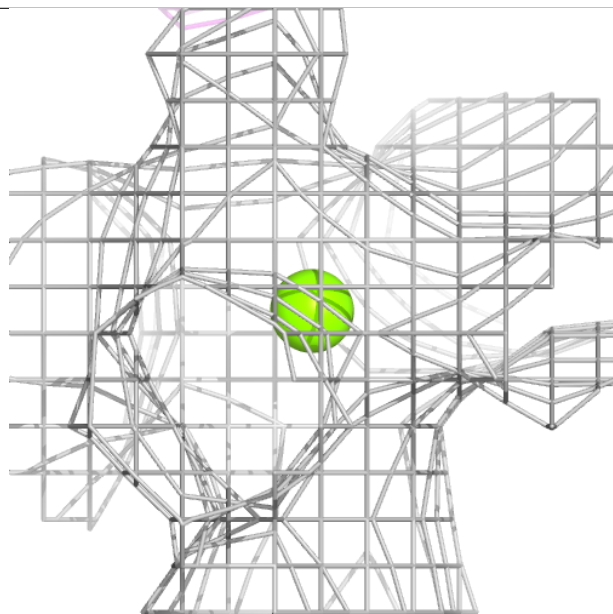
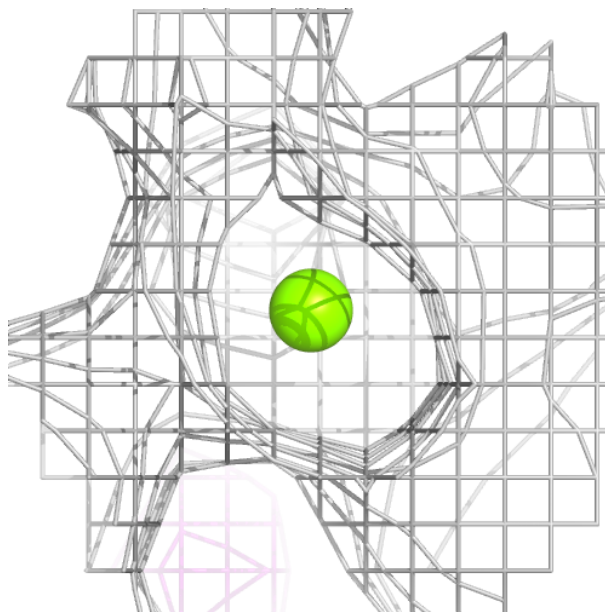
Electron density around MG L 501:

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



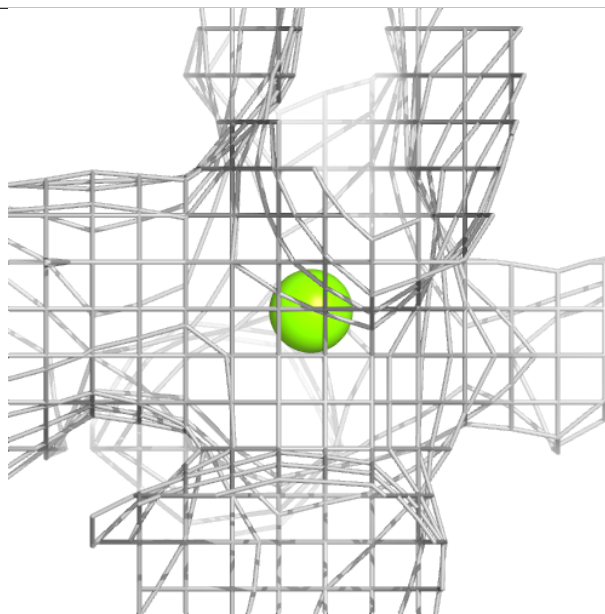
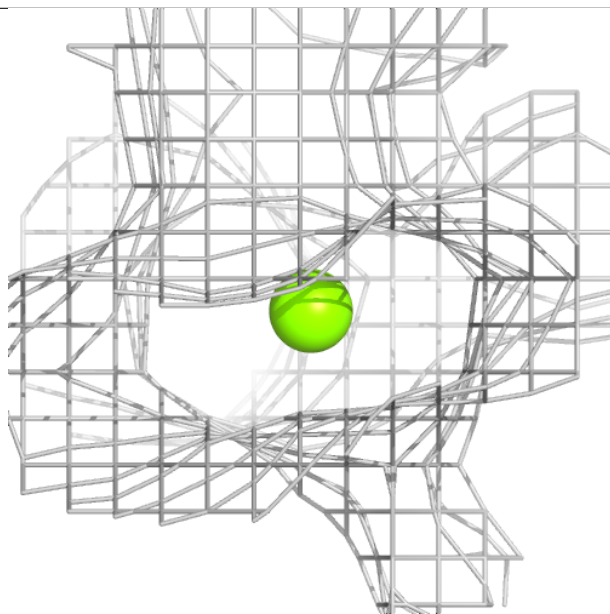
Electron density around MG N 501:

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



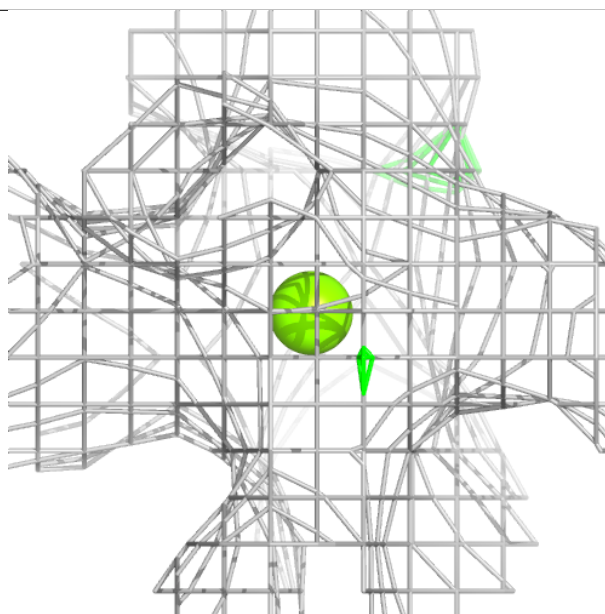
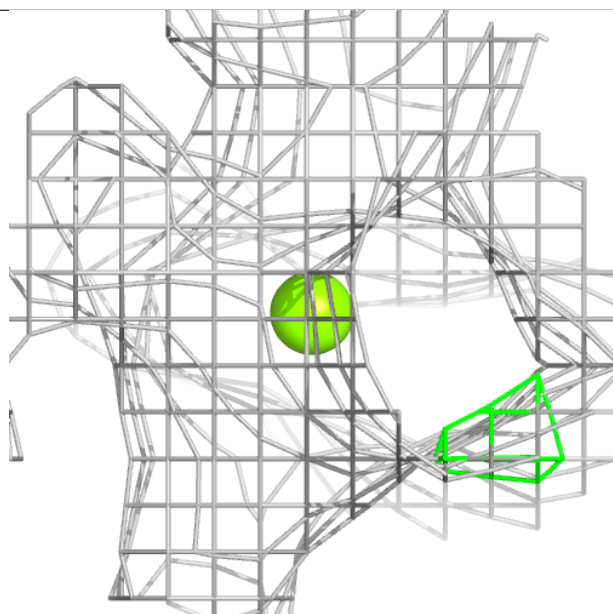
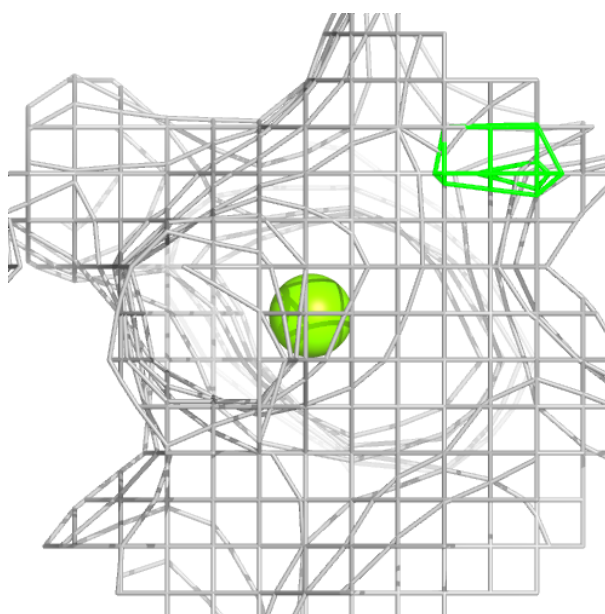
Electron density around MG M 501:

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



Electron density around MG O 501:

$2mF_o-DF_c$ (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.