



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:35 PM UTC

PDB ID : 6TOT / pdb_00006tot
Title : Crystal structure of the Orexin-1 receptor in complex with lemborexant
Authors : Rappas, M.; Ali, A.; Bennett, K.A.; Brown, J.D.; Bucknell, S.J.; Congreve, M.; Cooke, R.M.; Cseke, G.; de Graaf, C.; Dore, A.S.; Errey, J.C.; Jazayeri, A.; Marshall, F.H.; Mason, J.S.; Mould, R.; Patel, J.C.; Tehan, B.G.; Weir, M.; Christopher, J.A.
Deposited on : 2019-12-11
Resolution : 2.22 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](#) ①) 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

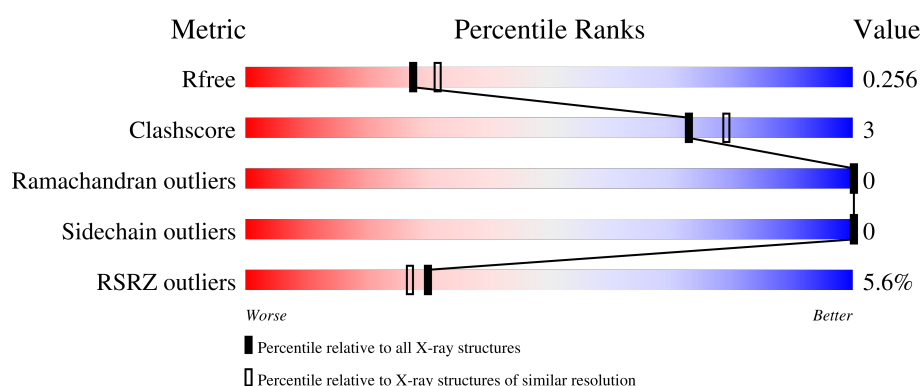
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.22 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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	336	6% 79% 10% 11%
1	B	336	4% 81% 9% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 5266 atoms, of which 40 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 Orexin receptor type 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2422	1611	400	394	17			
1	B	303	Total	C	N	O	S	0	0	0
			2404	1592	403	392	17			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	25	ALA	-	expression tag	UNP O43613
A	26	ALA	-	expression tag	UNP O43613
A	27	SER	-	expression tag	UNP O43613
A	46	ALA	GLU	engineered mutation	UNP O43613
A	85	LEU	ILE	engineered mutation	UNP O43613
A	95	ALA	VAL	engineered mutation	UNP O43613
A	162	LEU	ARG	engineered mutation	UNP O43613
A	194	ALA	ASN	engineered mutation	UNP O43613
A	198	ALA	LEU	engineered mutation	UNP O43613
A	211	ALA	TYR	engineered mutation	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	VAL	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ASN	deletion	UNP O43613
A	?	-	TRP	deletion	UNP O43613
A	?	-	LYS	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	SER	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	ASP	deletion	UNP O43613

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LEU	deletion	UNP O43613
A	?	-	GLU	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	?	-	SER	deletion	UNP O43613
A	?	-	GLY	deletion	UNP O43613
A	?	-	GLU	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	GLN	deletion	UNP O43613
A	?	-	PRO	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	ARG	deletion	UNP O43613
A	?	-	ALA	deletion	UNP O43613
A	?	-	PHE	deletion	UNP O43613
A	?	-	LEU	deletion	UNP O43613
A	304	VAL	LEU	engineered mutation	UNP O43613
A	339	ALA	CYS	engineered mutation	UNP O43613
A	375	TRP	CYS	engineered mutation	UNP O43613
A	376	TRP	CYS	engineered mutation	UNP O43613
A	381	ALA	-	expression tag	UNP O43613
A	382	ALA	-	expression tag	UNP O43613
A	383	ALA	-	expression tag	UNP O43613
A	384	HIS	-	expression tag	UNP O43613
A	385	HIS	-	expression tag	UNP O43613
A	386	HIS	-	expression tag	UNP O43613
A	387	HIS	-	expression tag	UNP O43613
A	388	HIS	-	expression tag	UNP O43613
A	389	HIS	-	expression tag	UNP O43613
A	390	HIS	-	expression tag	UNP O43613
A	391	HIS	-	expression tag	UNP O43613
A	392	HIS	-	expression tag	UNP O43613
B	25	ALA	-	expression tag	UNP O43613
B	26	ALA	-	expression tag	UNP O43613
B	27	SER	-	expression tag	UNP O43613
B	46	ALA	GLU	engineered mutation	UNP O43613
B	85	LEU	ILE	engineered mutation	UNP O43613
B	95	ALA	VAL	engineered mutation	UNP O43613
B	162	LEU	ARG	engineered mutation	UNP O43613
B	194	ALA	ASN	engineered mutation	UNP O43613
B	198	ALA	LEU	engineered mutation	UNP O43613

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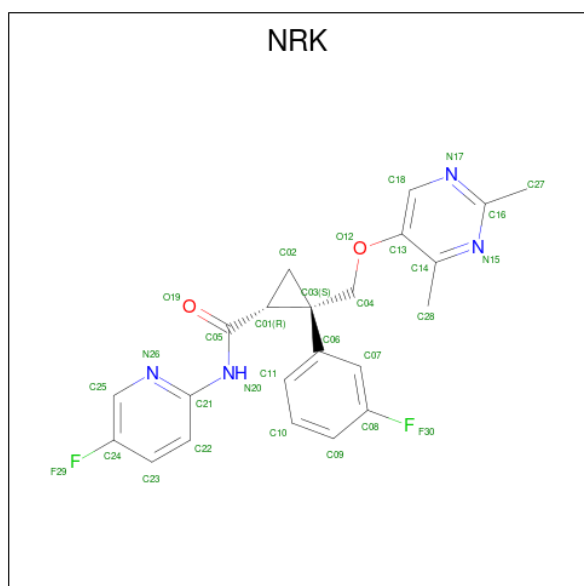
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	ASP	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	SER	deletion	UNP O43613
B	?	-	GLY	deletion	UNP O43613
B	?	-	GLU	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	GLN	deletion	UNP O43613
B	?	-	PRO	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	PHE	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	304	VAL	LEU	engineered mutation	UNP O43613
B	339	ALA	CYS	engineered mutation	UNP O43613
B	375	TRP	CYS	engineered mutation	UNP O43613
B	376	TRP	CYS	engineered mutation	UNP O43613
B	381	ALA	-	expression tag	UNP O43613
B	382	ALA	-	expression tag	UNP O43613
B	383	ALA	-	expression tag	UNP O43613
B	384	HIS	-	expression tag	UNP O43613
B	385	HIS	-	expression tag	UNP O43613

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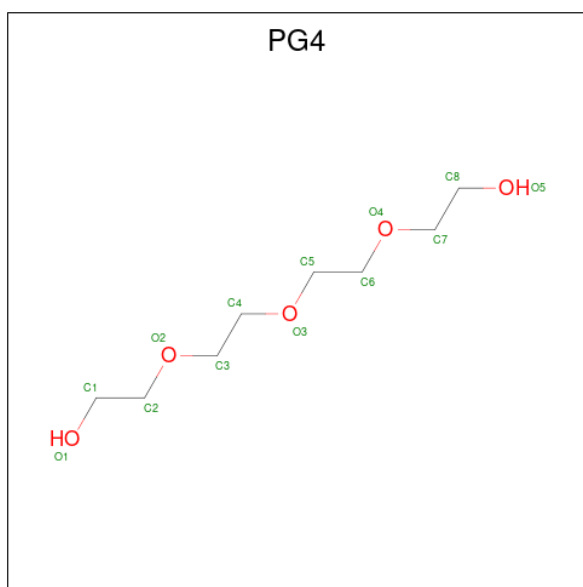
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is (1 {R},2 {S})-2-[(2,4-dimethylpyrimidin-5-yl)oxymethyl]- {N}-(5-fluoranylpyridin-2-yl)-2-(3-fluorophenyl)cyclopropane-1-carboxamide (CCD ID: NRK) (formula: C₂₂H₂₀F₂N₄O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			50	22	2	20	4	2		
2	B	1	Total	C	F	H	N	O	0	0
			50	22	2	20	4	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

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



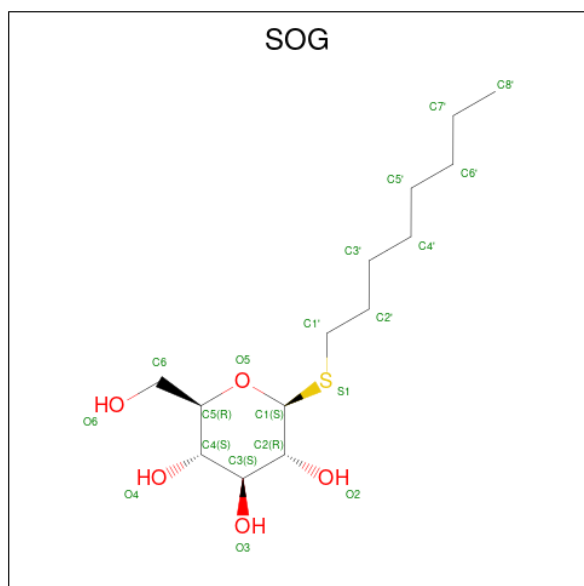
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

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

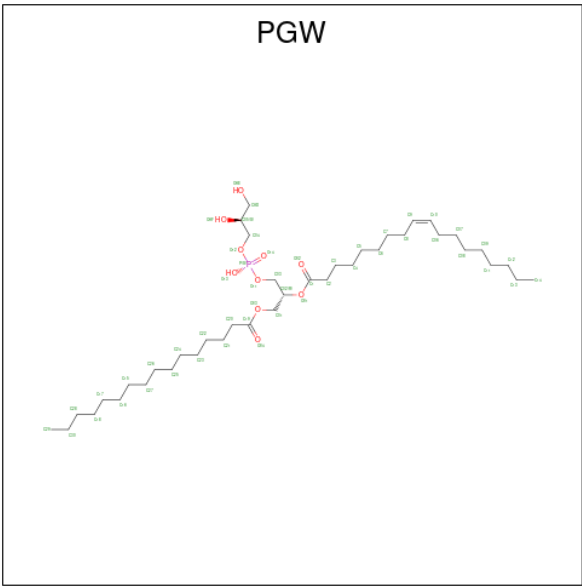
- Molecule 5 is octyl 1-thio-beta-D-glucopyranoside (CCD ID: SOG) (formula: C₁₄H₂₈O₅S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			20	14	5	1		
5	A	1	Total	C	O	S	0	0
			20	14	5	1		
5	A	1	Total	C	O	S	0	0
			13	7	5	1		
5	A	1	Total	C	O	S	0	0
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			13	7	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		
5	B	1	Total	C	O	S	0	0
			16	10	5	1		
5	B	1	Total	C	O	S	0	0
			20	14	5	1		

- Molecule 6 is (1R)-2-{[(S)-{[(2S)-2,3-dihydroxypropyl]oxy}(hydroxy)phosphoryl]oxy}-1-[(hexadecanoyloxy)methyl]ethyl (9Z)-octadec-9-enoate (CCD ID: PGW) (formula:

C₄₀H₇₇O₁₀P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	P	0	0
			51	40	10	1		
6	A	1	Total	C	O	P	0	0
			51	40	10	1		

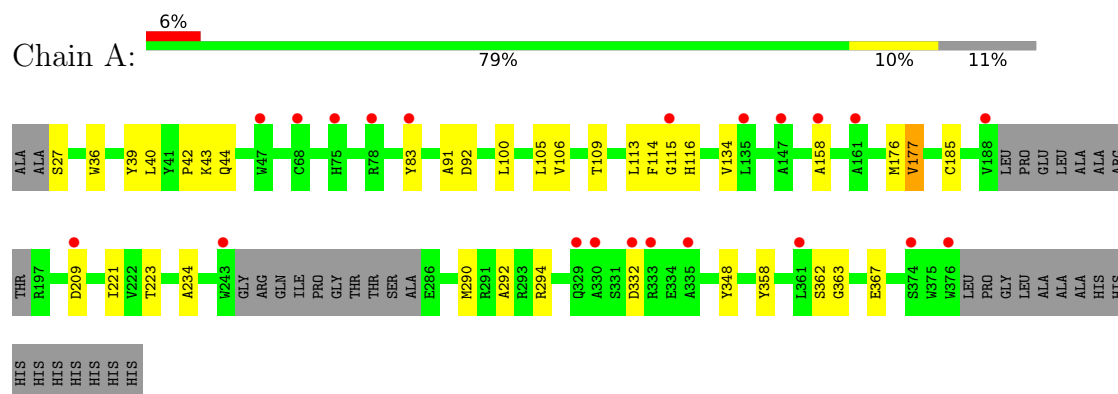
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total	O	0	0
			18	18		
7	B	25	Total	O	0	0
			25	25		

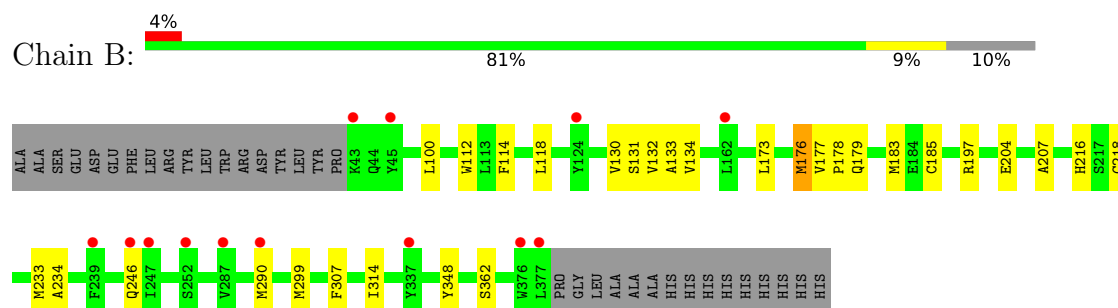
3 Residue-property plots

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: Orexin receptor type 1



• Molecule 1: Orexin receptor type 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.73Å 145.72Å 71.70Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	24.02 – 2.22 24.02 – 2.22	Depositor EDS
% Data completeness (in resolution range)	63.9 (24.02-2.22) 83.1 (24.02-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.36 (at 2.22Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.206 , 0.239 0.231 , 0.256	Depositor DCC
R_{free} test set	2831 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5266	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NRK, SO4, SOG, PG4, PGW

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.84	1/2491 (0.0%)	1.43	16/3393 (0.5%)
1	B	0.86	2/2470 (0.1%)	1.44	9/3368 (0.3%)
All	All	0.85	3/4961 (0.1%)	1.43	25/6761 (0.4%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	177	VAL	CA-C	6.07	1.57	1.52
1	B	177	VAL	CA-C	5.76	1.57	1.52
1	B	177	VAL	CA-CB	5.55	1.57	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	VAL	N-CA-C	-7.46	103.19	110.72
1	A	91	ALA	N-CA-C	-6.04	104.77	111.36
1	A	176	MET	CA-C-N	5.94	123.98	120.24
1	A	176	MET	C-N-CA	5.94	123.98	120.24
1	A	42	PRO	N-CA-C	5.63	121.97	113.81
1	B	176	MET	CA-C-N	5.62	123.78	120.24
1	B	176	MET	C-N-CA	5.62	123.78	120.24
1	A	115	GLY	CA-C-N	5.58	127.76	120.28
1	A	115	GLY	C-N-CA	5.58	127.76	120.28
1	B	133	ALA	CA-C-N	5.46	127.44	120.56
1	B	133	ALA	C-N-CA	5.46	127.44	120.56
1	A	44	GLN	N-CA-C	-5.46	105.33	111.28
1	A	292	ALA	CA-C-N	5.27	127.34	120.28
1	A	292	ALA	C-N-CA	5.27	127.34	120.28
1	A	92	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	132	VAL	CA-C-N	5.23	127.24	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	132	VAL	C-N-CA	5.23	127.24	120.44
1	B	314	ILE	CA-C-N	5.12	127.09	120.44
1	B	314	ILE	C-N-CA	5.12	127.09	120.44
1	A	332	ASP	CA-C-N	5.09	127.10	120.28
1	A	332	ASP	C-N-CA	5.09	127.10	120.28
1	B	197	ARG	N-CA-C	-5.08	106.49	113.30
1	A	27	SER	CA-C-N	5.08	127.34	120.38
1	A	27	SER	C-N-CA	5.08	127.34	120.38
1	A	209	ASP	CA-CB-CG	5.02	117.62	112.60

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	2422	0	2464	19	0
1	B	2404	0	2474	16	0
2	A	30	20	0	0	0
2	B	30	20	0	0	0
3	A	13	0	18	1	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
5	A	73	0	95	0	0
5	B	89	0	112	1	0
6	A	102	0	152	6	0
7	A	18	0	0	0	0
7	B	25	0	0	0	0
All	All	5226	40	5315	34	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 3.

All (34) 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:290:MET:HE2	1:A:294:ARG:HH21	1.11	1.08
1:A:39:TYR:CE1	1:A:43:LYS:HD2	2.13	0.83
6:A:410:PGW:HADA	1:B:207:ALA:H	1.52	0.74
1:A:290:MET:HE2	1:A:294:ARG:NH2	1.97	0.71
1:A:105:LEU:HD12	1:A:114:PHE:HZ	1.56	0.69
6:A:409:PGW:H7A	1:B:234:ALA:HB2	1.77	0.66
1:A:105:LEU:HD12	1:A:114:PHE:CZ	2.31	0.65
1:A:234:ALA:HB2	6:A:410:PGW:H9	1.80	0.63
1:A:100:LEU:HD12	1:A:348:TYR:HB3	1.84	0.57
1:A:363:GLY:O	1:A:367:GLU:HG2	2.09	0.53
1:B:246:GLN:CD	1:B:290:MET:SD	2.93	0.52
1:B:204:GLU:OE1	1:B:216:HIS:HE1	1.95	0.50
1:A:39:TYR:CE1	1:A:43:LYS:CD	2.89	0.49
1:B:134:VAL:HG22	1:B:307:PHE:CZ	2.49	0.46
1:B:131:SER:HB2	1:B:176:MET:HE2	1.97	0.46
1:B:112:TRP:CD1	1:B:185:CYS:HG	2.33	0.46
1:B:179:GLN:O	1:B:183:MET:HG2	2.16	0.46
6:A:410:PGW:H20A	1:B:178:PRO:HB3	1.97	0.45
1:A:358:TYR:O	1:A:362:SER:HB3	2.17	0.45
1:A:36:TRP:HA	1:A:40:LEU:HB2	2.00	0.44
1:A:221:ILE:HG21	1:B:218:CYS:HA	2.00	0.43
1:A:134:VAL:HG21	1:A:223:THR:O	2.17	0.43
1:A:177:VAL:HG22	3:A:402:PG4:H62	2.01	0.43
1:A:109:THR:HG21	1:A:113:LEU:HD11	2.01	0.43
1:A:116:HIS:CD2	1:A:185:CYS:HB3	2.53	0.43
1:B:173:LEU:HB3	5:B:406:SOG:H8'2	2.00	0.42
1:A:83:TYR:CE1	1:A:158:ALA:HB1	2.55	0.41
1:A:234:ALA:CB	6:A:410:PGW:H9	2.47	0.41
1:B:114:PHE:HB3	1:B:118:LEU:HD12	2.02	0.41
6:A:409:PGW:H2A	1:B:233:MET:HB3	2.02	0.41
1:A:83:TYR:HE1	1:A:158:ALA:HB1	1.86	0.41
1:B:100:LEU:HD12	1:B:348:TYR:HB3	2.03	0.40
1:B:299:MET:SD	1:B:362:SER:HB2	2.61	0.40
1:B:130:VAL:O	1:B:134:VAL:HG23	2.21	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	294/336 (88%)	289 (98%)	5 (2%)	0	100	100
1	B	301/336 (90%)	296 (98%)	5 (2%)	0	100	100
All	All	595/672 (88%)	585 (98%)	10 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	254/279 (91%)	254 (100%)	0	100	100
1	B	252/279 (90%)	252 (100%)	0	100	100
All	All	506/558 (91%)	506 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	116	HIS
1	A	368	GLN
1	B	126	GLN
1	B	150	HIS
1	B	216	HIS

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Mol	Chain	Res	Type
1	B	350	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](#)

18 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$
5	SOG	A	406	-	20,20,20	0.94	1 (5%)	24,25,25	1.05	1 (4%)
5	SOG	B	404	-	20,20,20	0.92	2 (10%)	24,25,25	0.70	0
5	SOG	B	406	-	20,20,20	1.07	1 (5%)	24,25,25	1.19	2 (8%)
2	NRK	A	401	-	31,33,33	1.34	4 (12%)	38,48,48	2.20	11 (28%)
4	SO4	B	402	-	4,4,4	0.24	0	6,6,6	0.25	0
6	PGW	A	409	-	50,50,50	1.00	2 (4%)	53,56,56	1.06	3 (5%)
4	SO4	A	404	-	4,4,4	0.27	0	6,6,6	0.06	0
4	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.16	0
5	SOG	B	408	-	20,20,20	1.10	2 (10%)	24,25,25	0.94	2 (8%)
5	SOG	A	407	-	12,13,20	0.64	0	17,18,25	1.32	2 (11%)
6	PGW	A	410	-	50,50,50	0.98	2 (4%)	53,56,56	1.01	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SOG	B	407	-	16,16,20	1.04	1 (6%)	20,21,25	0.96	1 (5%)
3	PG4	A	402	-	12,12,12	0.19	0	11,11,11	0.12	0
5	SOG	B	405	-	12,13,20	0.69	0	17,18,25	1.09	1 (5%)
4	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.14	0
2	NRK	B	401	-	31,33,33	1.45	5 (16%)	38,48,48	2.28	13 (34%)
5	SOG	A	405	-	20,20,20	0.85	1 (5%)	24,25,25	1.13	1 (4%)
5	SOG	A	408	-	20,20,20	0.96	1 (5%)	24,25,25	1.03	1 (4%)

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
5	SOG	A	406	-	-	9/11/31/31	0/1/1/1
5	SOG	B	404	-	-	9/11/31/31	0/1/1/1
5	SOG	B	406	-	-	7/11/31/31	0/1/1/1
2	NRK	A	401	-	-	5/20/28/28	0/4/4/4
6	PGW	A	409	-	-	30/55/55/55	-
5	SOG	B	408	-	-	5/11/31/31	0/1/1/1
5	SOG	A	407	-	-	4/4/24/31	0/1/1/1
6	PGW	A	410	-	-	21/55/55/55	-
5	SOG	B	407	-	-	3/7/27/31	0/1/1/1
3	PG4	A	402	-	-	2/10/10/10	-
5	SOG	B	405	-	-	1/4/24/31	0/1/1/1
2	NRK	B	401	-	-	5/20/28/28	0/4/4/4
5	SOG	A	405	-	-	6/11/31/31	0/1/1/1
5	SOG	A	408	-	-	5/11/31/31	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	409	PGW	O01-C1	4.64	1.47	1.34
6	A	410	PGW	O01-C1	4.58	1.47	1.34
6	A	409	PGW	O03-C19	4.53	1.46	1.33
6	A	410	PGW	O03-C19	4.30	1.45	1.33
5	B	406	SOG	C1'-S1	-4.01	1.75	1.81
5	B	408	SOG	C1'-S1	-3.40	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	408	SOG	C1'-S1	-3.10	1.77	1.81
5	A	406	SOG	C1'-S1	-3.09	1.77	1.81
5	B	407	SOG	C1'-S1	-3.05	1.77	1.81
2	B	401	NRK	C18-C13	2.95	1.43	1.38
5	A	405	SOG	C1'-S1	-2.94	1.77	1.81
5	B	404	SOG	C1'-S1	-2.87	1.77	1.81
2	A	401	NRK	C04-C03	2.67	1.57	1.53
2	A	401	NRK	C18-C13	2.54	1.43	1.38
2	B	401	NRK	C04-C03	2.42	1.57	1.53
5	B	408	SOG	C1-S1	-2.36	1.76	1.80
2	B	401	NRK	C14-N15	2.33	1.37	1.34
2	A	401	NRK	C21-N26	2.26	1.38	1.34
2	B	401	NRK	C01-C05	2.15	1.56	1.51
2	B	401	NRK	C23-C24	2.15	1.41	1.37
5	B	404	SOG	C1-S1	-2.02	1.77	1.80
2	A	401	NRK	C23-C24	2.02	1.41	1.37

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NRK	C23-C24-C25	-6.94	117.90	121.55
2	A	401	NRK	C23-C24-C25	-6.38	118.20	121.55
2	A	401	NRK	O19-C05-C01	-5.91	110.86	122.10
2	B	401	NRK	C01-C05-N20	5.11	128.95	114.72
2	B	401	NRK	O19-C05-C01	-4.63	113.29	122.10
2	A	401	NRK	C01-C05-N20	4.58	127.47	114.72
6	A	410	PGW	O01-C1-C2	4.31	120.81	111.48
6	A	409	PGW	O01-C1-C2	4.05	120.24	111.48
2	B	401	NRK	C02-C01-C05	3.85	131.50	119.56
2	A	401	NRK	C02-C01-C05	3.49	130.37	119.56
6	A	409	PGW	O03-C19-C20	3.27	121.82	111.83
5	A	406	SOG	C1-O5-C5	3.19	118.29	112.56
5	B	406	SOG	C3-C4-C5	3.19	116.02	110.23
5	A	405	SOG	C1'-S1-C1	3.17	107.29	100.45
2	A	401	NRK	C02-C03-C06	3.07	125.48	118.80
2	B	401	NRK	F29-C24-C23	3.07	123.46	118.55
5	B	405	SOG	C1-O5-C5	3.04	118.01	112.56
5	A	407	SOG	C4-C3-C2	2.96	116.02	110.83
2	B	401	NRK	O19-C05-N20	-2.96	117.68	123.92
5	A	407	SOG	C3-C4-C5	2.95	115.58	110.23
2	B	401	NRK	C09-C08-C07	-2.72	119.64	123.23
5	B	406	SOG	C4-C3-C2	2.70	115.57	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	NRK	C06-C07-C08	2.67	121.22	118.35
6	A	410	PGW	O03-C19-C20	2.66	119.95	111.83
2	B	401	NRK	C02-C03-C04	-2.49	112.03	117.48
2	A	401	NRK	C22-C21-N26	-2.47	118.85	122.61
2	A	401	NRK	O12-C04-C03	2.46	111.38	108.07
2	A	401	NRK	C25-N26-C21	2.43	120.11	117.83
2	A	401	NRK	C28-C14-C13	2.40	124.29	120.15
2	B	401	NRK	C28-C14-C13	2.38	124.25	120.15
5	B	407	SOG	C4-C3-C2	2.35	114.95	110.83
2	B	401	NRK	C04-O12-C13	2.33	123.41	117.63
5	B	408	SOG	C1-O5-C5	2.29	116.67	112.56
2	A	401	NRK	O12-C13-C18	2.25	127.06	124.43
2	B	401	NRK	C22-C21-N26	-2.17	119.30	122.61
5	A	408	SOG	C1-C2-C3	-2.12	106.40	110.55
5	B	408	SOG	C3-C4-C5	2.10	114.03	110.23
2	A	401	NRK	F29-C24-C23	2.08	121.88	118.55
6	A	409	PGW	C03-C02-C01	-2.07	106.97	111.78
2	B	401	NRK	C02-C03-C06	2.06	123.27	118.80

There are no chirality outliers.

All (112) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	NRK	C03-C01-C05-N20
2	B	401	NRK	C03-C01-C05-O19
2	B	401	NRK	C03-C01-C05-N20
5	A	407	SOG	O5-C1-S1-C1'
5	B	404	SOG	O5-C1-S1-C1'
5	B	406	SOG	C2-C1-S1-C1'
5	B	406	SOG	O5-C1-S1-C1'
6	A	409	PGW	C03-O11-P-O12
6	A	409	PGW	C03-O11-P-O13
6	A	409	PGW	C04-O12-P-O14
6	A	410	PGW	C03-O11-P-O12
6	A	410	PGW	C03-O11-P-O13
5	A	408	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	O12-C04-C05-OAF
5	A	407	SOG	O5-C5-C6-O6
5	A	406	SOG	O5-C5-C6-O6
5	A	405	SOG	O5-C5-C6-O6
5	A	408	SOG	O5-C5-C6-O6
5	B	406	SOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	410	PGW	O12-C04-C05-CAD
6	A	410	PGW	C20-C19-O03-C01
6	A	410	PGW	O04-C19-O03-C01
6	A	409	PGW	C19-C20-C21-C22
5	B	404	SOG	O5-C5-C6-O6
5	A	406	SOG	C4-C5-C6-O6
5	B	408	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	C19-C20-C21-C22
5	A	406	SOG	S1-C1'-C2'-C3'
5	A	407	SOG	C4-C5-C6-O6
6	A	409	PGW	C05-C04-O12-P
6	A	409	PGW	C1-C2-C3-C4
5	A	406	SOG	C1'-C2'-C3'-C4'
5	A	406	SOG	C2'-C3'-C4'-C5'
5	B	404	SOG	C2'-C3'-C4'-C5'
5	B	404	SOG	C3'-C4'-C5'-C6'
5	B	404	SOG	C4'-C5'-C6'-C7'
6	A	409	PGW	C5-C6-C7-C8
6	A	410	PGW	O02-C1-O01-C02
5	A	405	SOG	C1'-C2'-C3'-C4'
5	B	404	SOG	C1'-C2'-C3'-C4'
5	A	406	SOG	C3'-C4'-C5'-C6'
6	A	410	PGW	C6-C7-C8-C9
6	A	409	PGW	C2-C1-O01-C02
6	A	410	PGW	C2-C1-O01-C02
5	B	407	SOG	S1-C1'-C2'-C3'
6	A	410	PGW	C21-C22-C23-C24
5	A	405	SOG	C4'-C5'-C6'-C7'
6	A	409	PGW	C2-C3-C4-C5
6	A	410	PGW	C22-C23-C24-C25
6	A	409	PGW	C16-C15-C27-C26
5	A	408	SOG	C4'-C5'-C6'-C7'
5	B	407	SOG	O5-C5-C6-O6
6	A	410	PGW	C08-C09-C11-C12
6	A	409	PGW	O02-C1-O01-C02
6	A	410	PGW	C09-C11-C12-C13
6	A	409	PGW	C08-C09-C11-C12
5	B	406	SOG	C4-C5-C6-O6
6	A	410	PGW	C27-C15-C16-C17
5	B	408	SOG	O5-C5-C6-O6
5	A	405	SOG	C2'-C3'-C4'-C5'
5	A	405	SOG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
6	A	409	PGW	C25-C26-C27-C15
6	A	410	PGW	C2-C3-C4-C5
5	A	405	SOG	C5'-C6'-C7'-C8'
5	B	404	SOG	S1-C1'-C2'-C3'
6	A	409	PGW	C11-C12-C13-C14
6	A	409	PGW	C3-C4-C5-C6
5	A	406	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	C01-C02-C03-O11
6	A	410	PGW	O03-C01-C02-C03
6	A	409	PGW	C6-C7-C8-C9
5	A	406	SOG	C4'-C5'-C6'-C7'
2	A	401	NRK	C02-C01-C05-O19
6	A	410	PGW	C16-C15-C27-C26
2	A	401	NRK	C02-C01-C05-N20
3	A	402	PG4	C3-C4-O3-C5
6	A	409	PGW	C20-C19-O03-C01
5	A	408	SOG	C4-C5-C6-O6
6	A	409	PGW	O01-C02-C03-O11
6	A	410	PGW	O03-C01-C02-O01
6	A	409	PGW	C4-C5-C6-C7
6	A	409	PGW	C15-C16-C17-C18
6	A	409	PGW	O04-C19-O03-C01
5	B	404	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	C23-C24-C25-C26
5	B	408	SOG	C3'-C4'-C5'-C6'
2	A	401	NRK	C03-C01-C05-O19
6	A	409	PGW	C04-O12-P-O11
6	A	409	PGW	C04-O12-P-O13
6	A	410	PGW	C05-C04-O12-P
5	B	406	SOG	C2'-C3'-C4'-C5'
6	A	410	PGW	C24-C25-C26-C27
5	B	408	SOG	C4'-C5'-C6'-C7'
5	A	408	SOG	C1'-C2'-C3'-C4'
5	B	408	SOG	C2'-C3'-C4'-C5'
6	A	409	PGW	C03-C02-O01-C1
6	A	409	PGW	C20-C21-C22-C23
2	B	401	NRK	C02-C01-C05-O19
5	B	404	SOG	C4-C5-C6-O6
2	B	401	NRK	C02-C01-C05-N20
6	A	409	PGW	C7-C8-C9-C10
2	B	401	NRK	C03-C04-O12-C13
3	A	402	PG4	C6-C5-O3-C4

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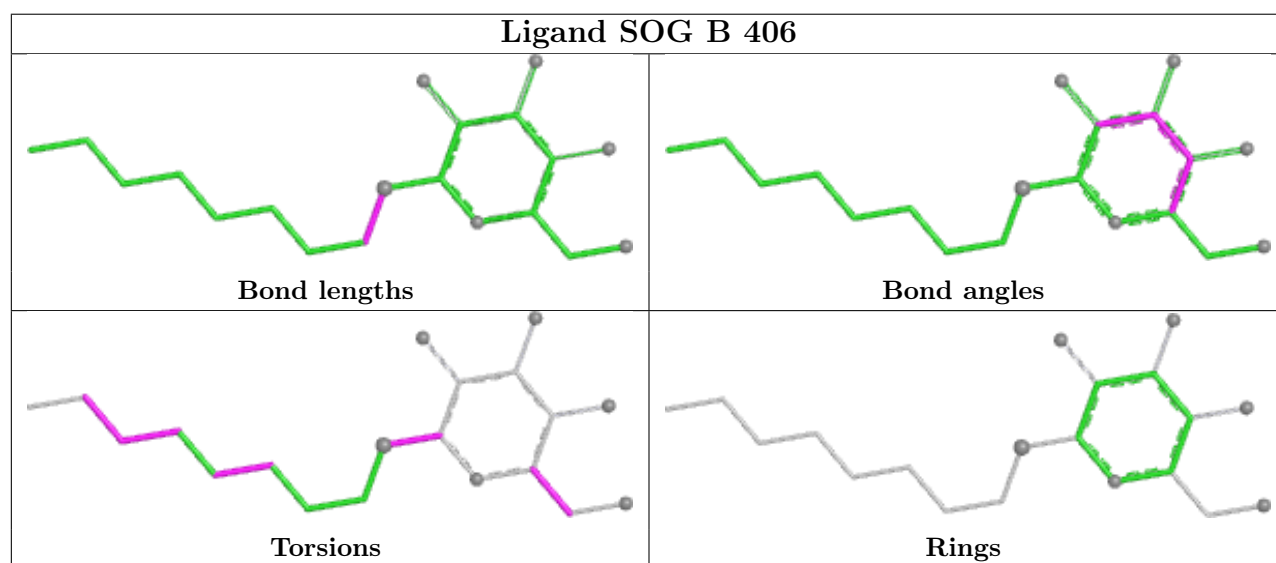
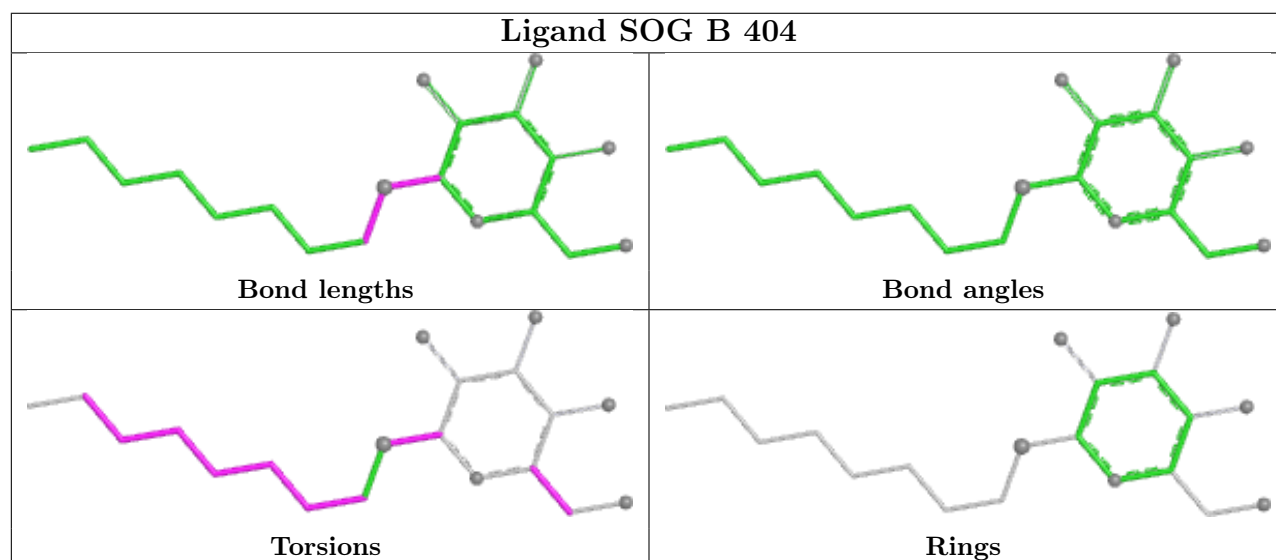
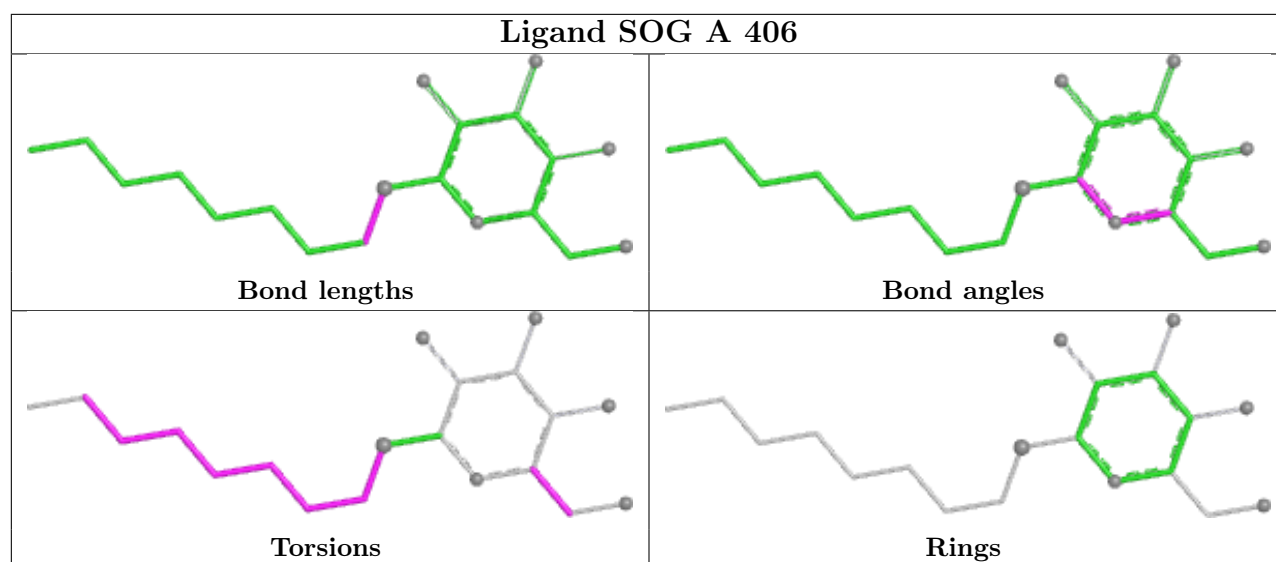
Mol	Chain	Res	Type	Atoms
5	B	406	SOG	C5'-C6'-C7'-C8'
6	A	409	PGW	O01-C1-C2-C3
5	A	406	SOG	C2'-C1'-S1-C1
5	B	407	SOG	C2'-C1'-S1-C1
2	A	401	NRK	C03-C04-O12-C13
5	B	406	SOG	C4'-C5'-C6'-C7'
6	A	409	PGW	O02-C1-C2-C3
5	A	407	SOG	C2-C1-S1-C1'
5	B	405	SOG	C2-C1-S1-C1'

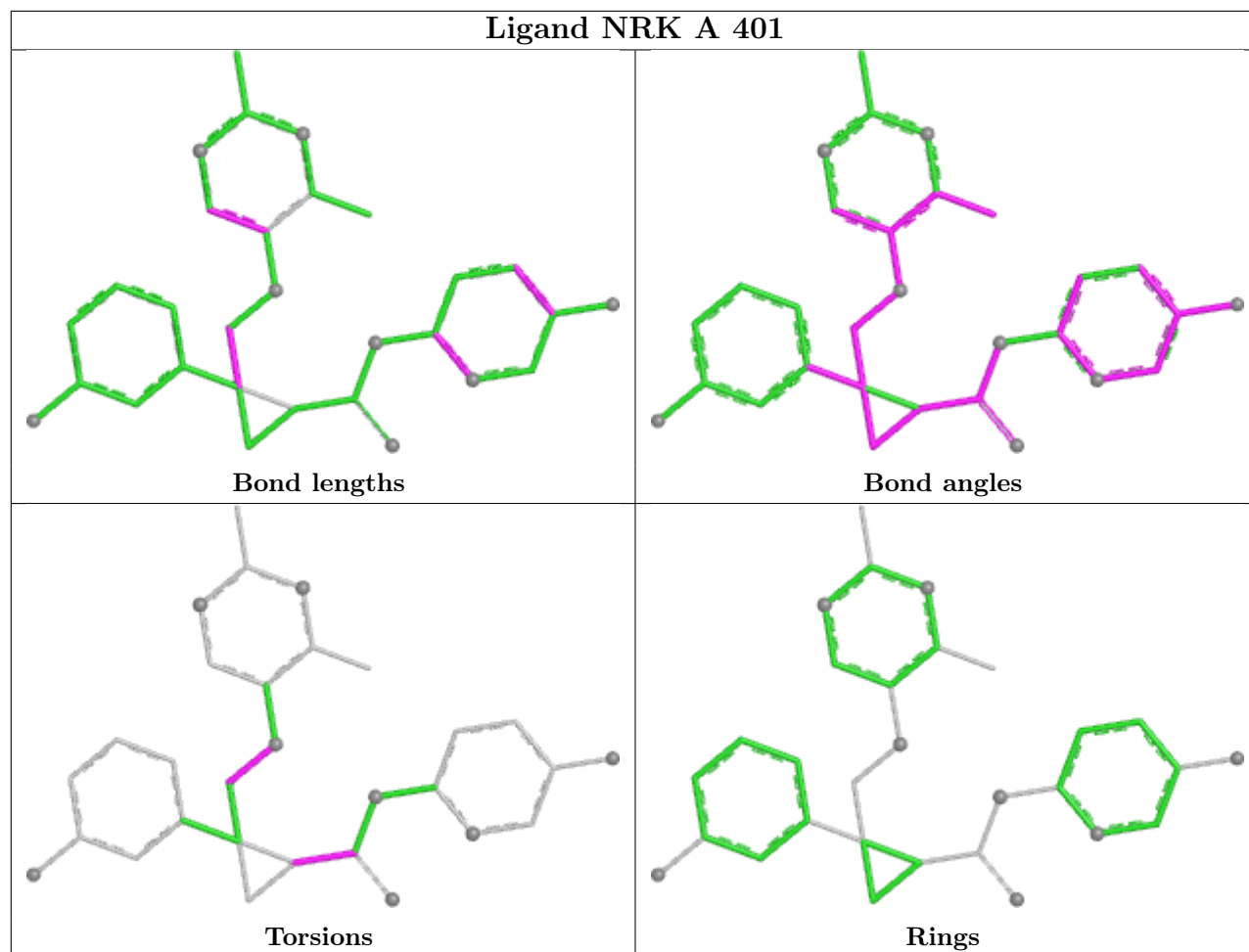
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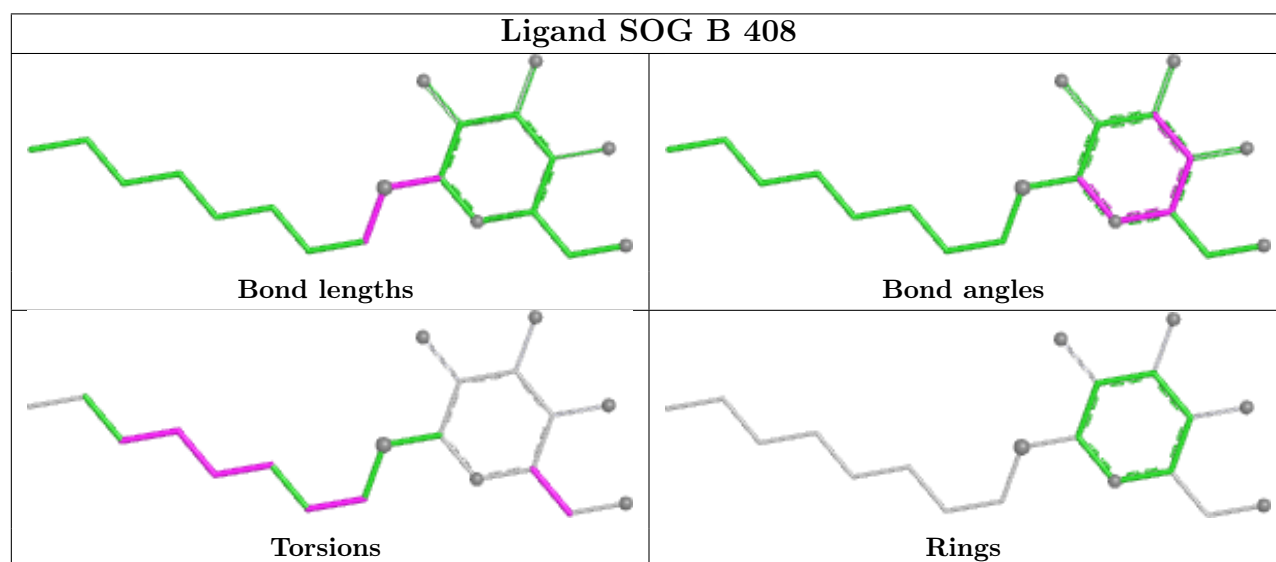
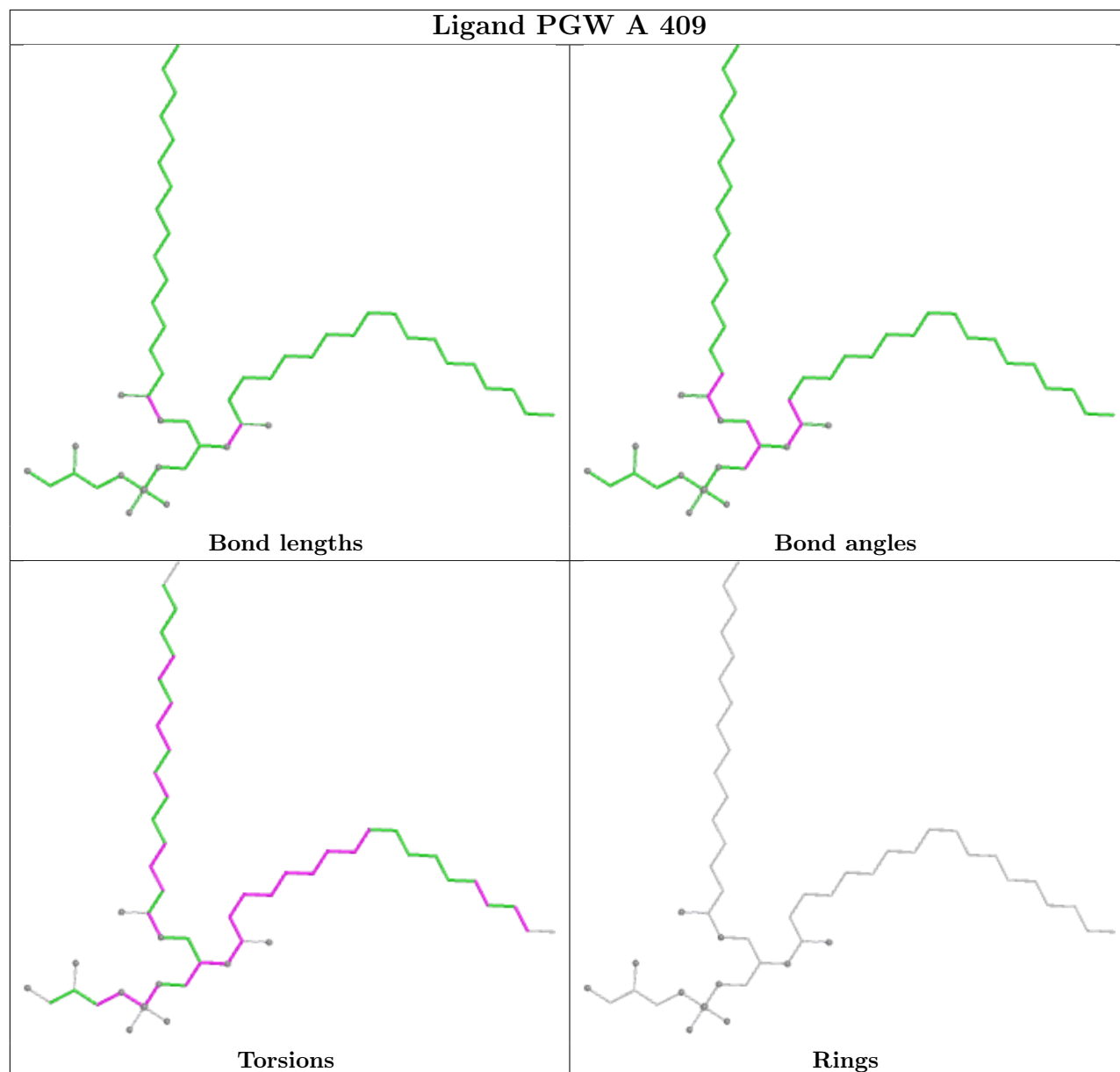
4 monomers are involved in 8 short contacts:

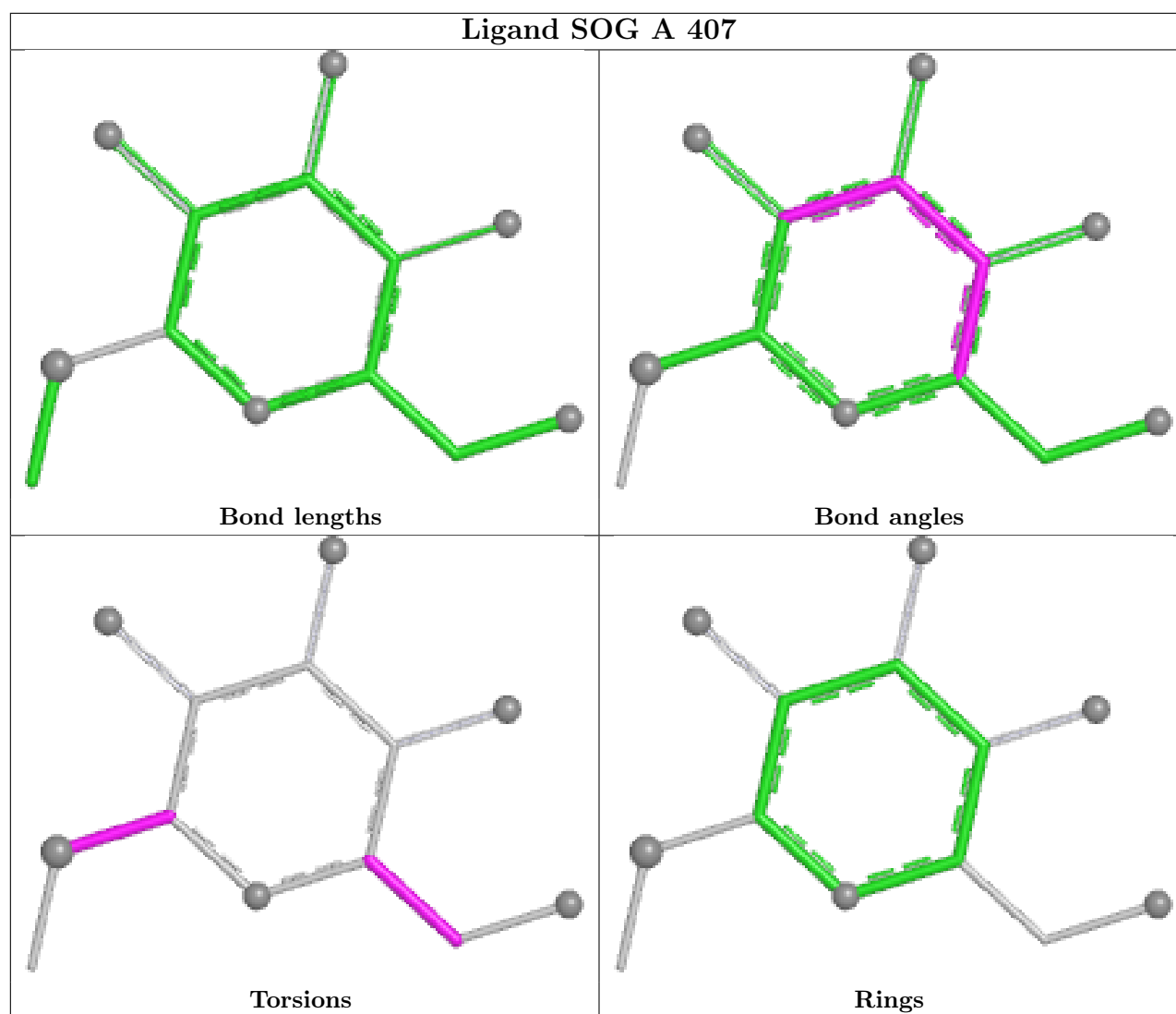
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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6	A	409	PGW	2	0
6	A	410	PGW	4	0
3	A	402	PG4	1	0

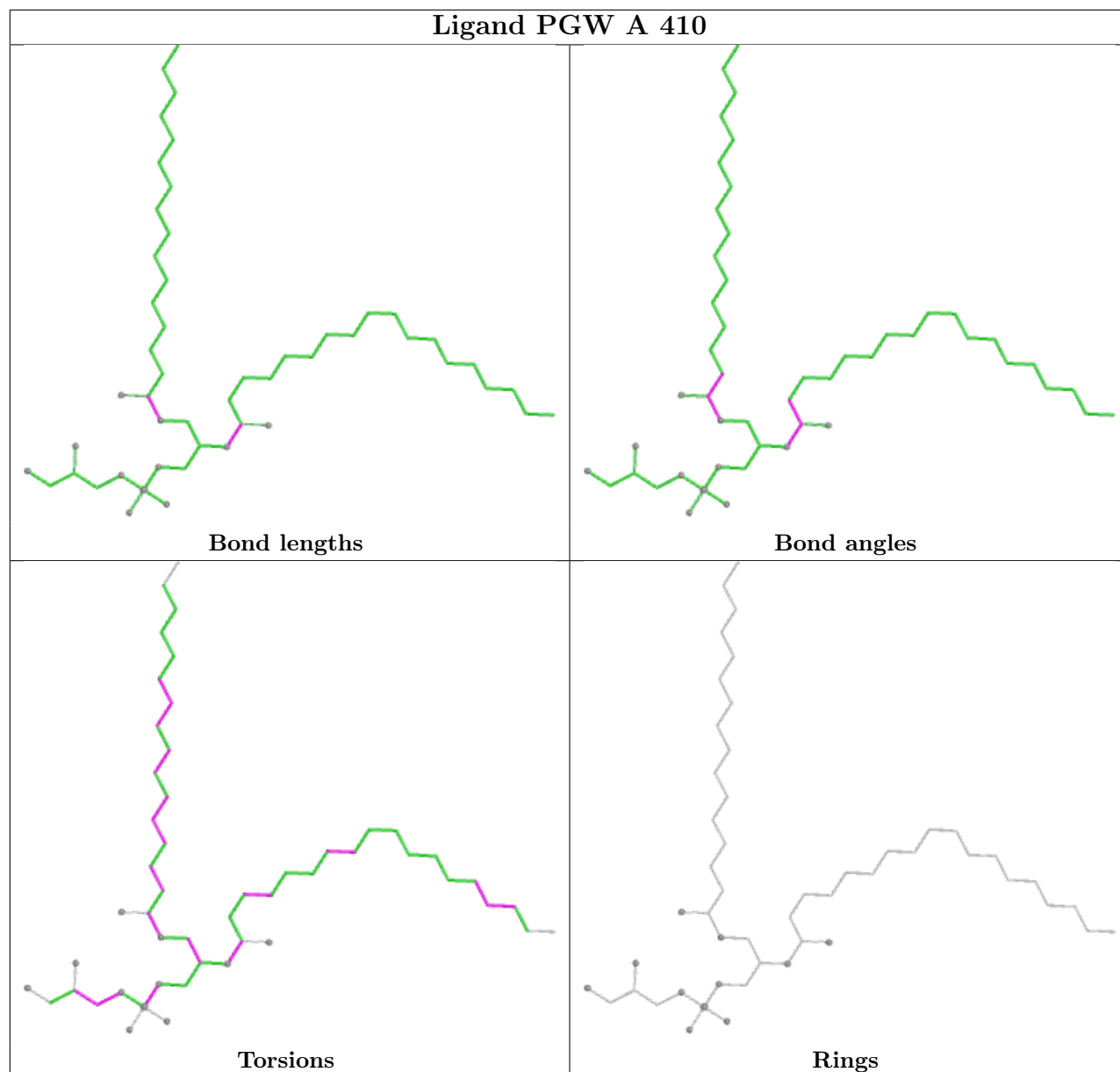
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

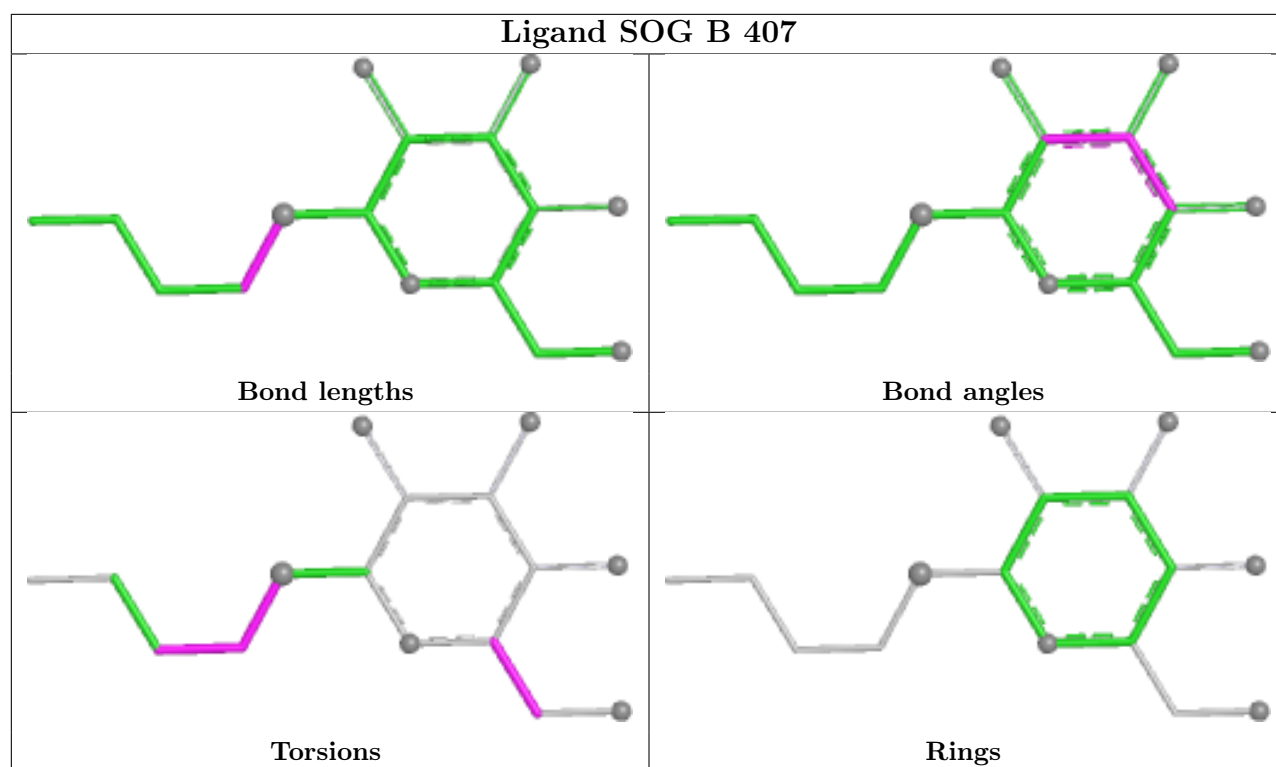


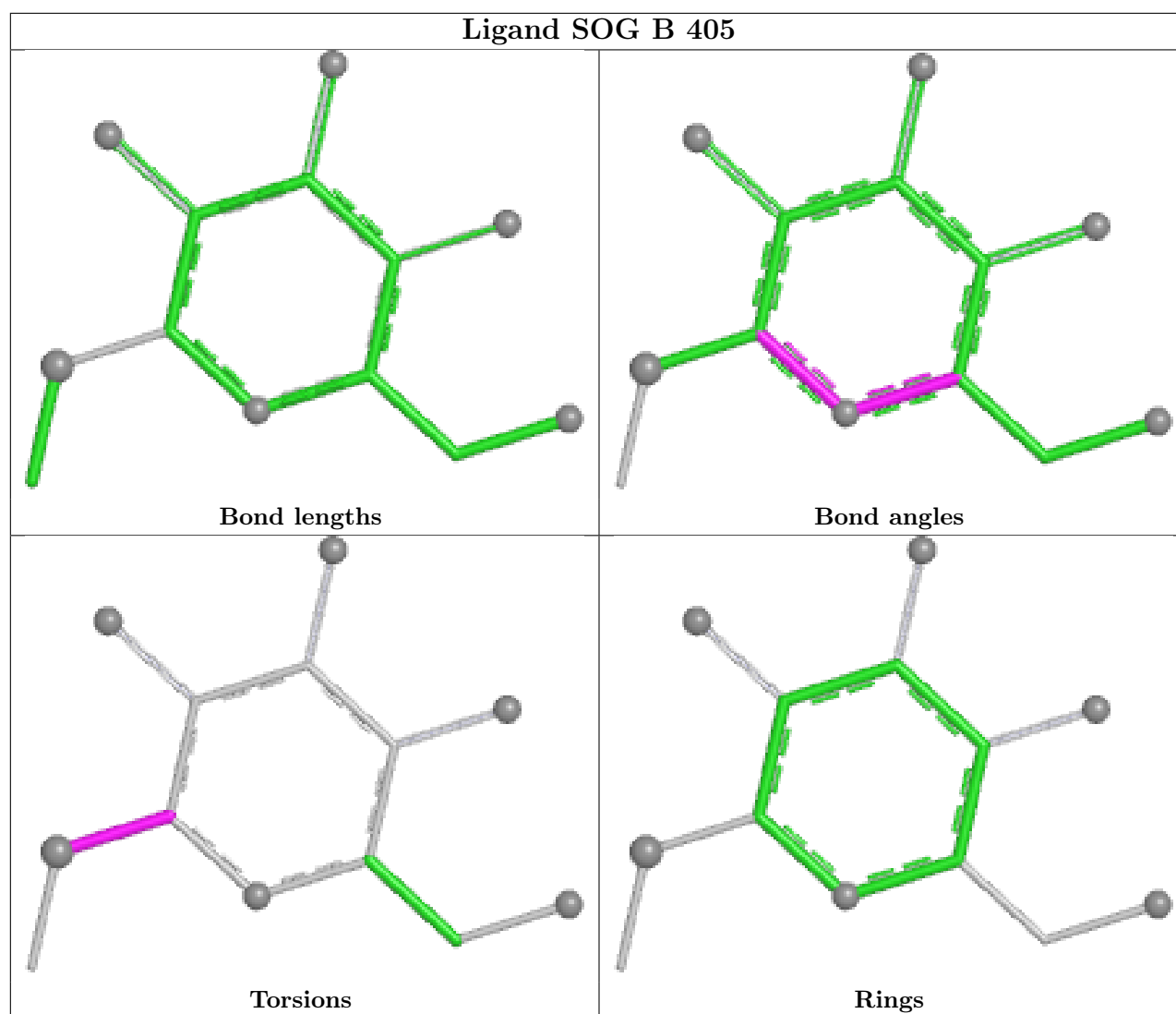


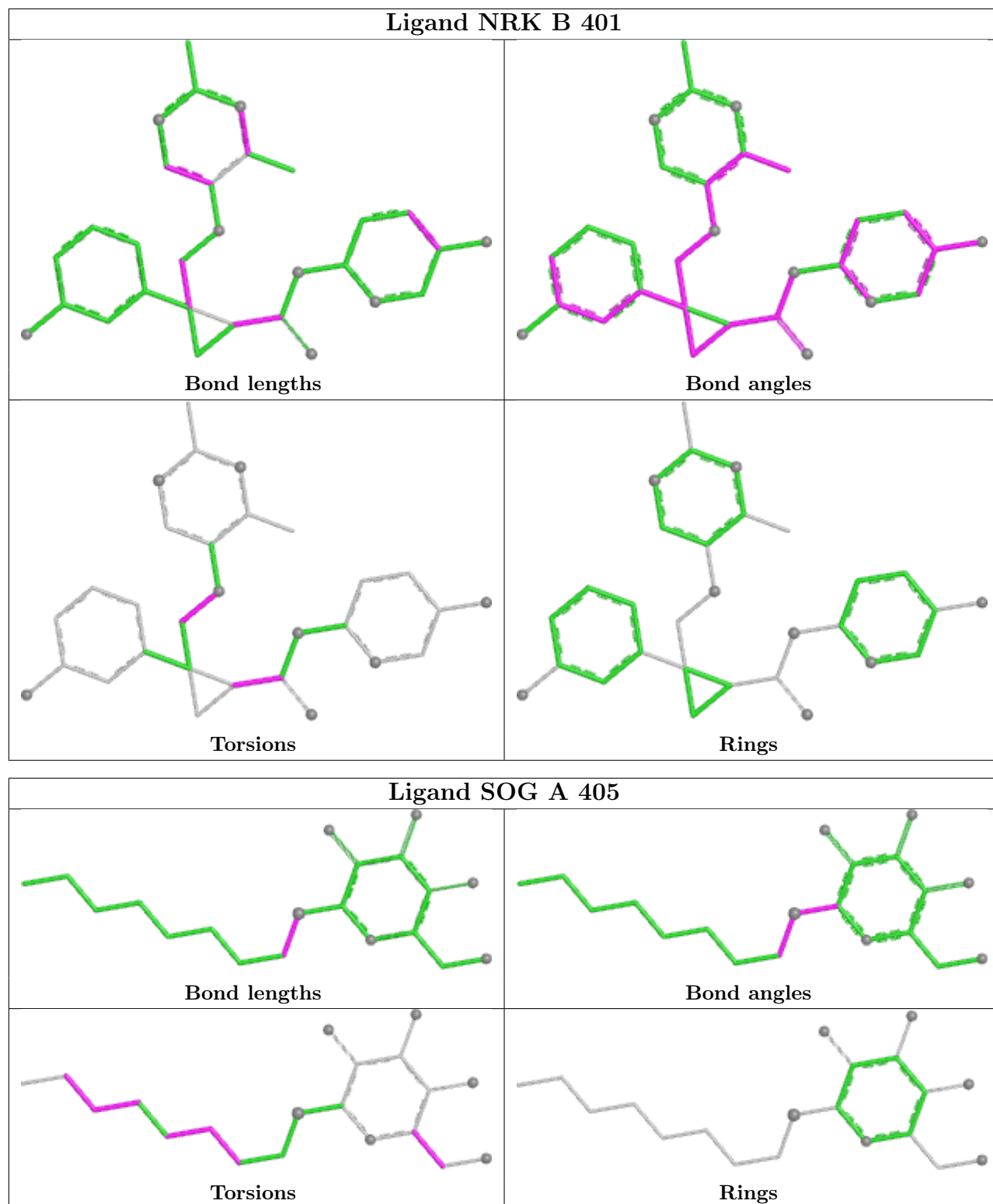


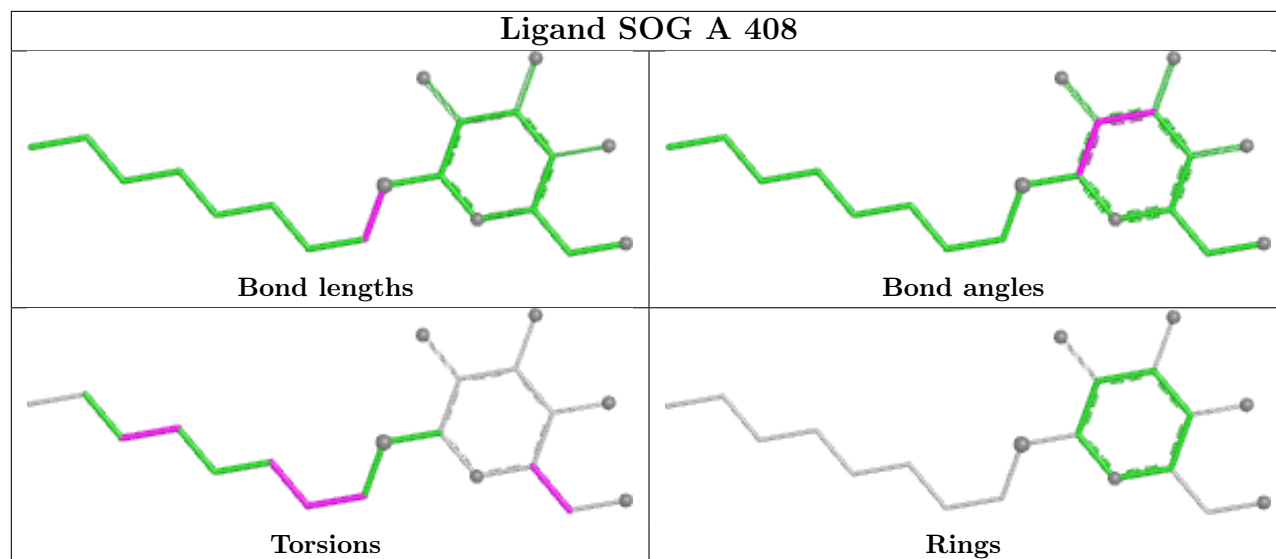












5.7 Other polymers [i](#)

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

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	300/336 (89%)	0.48	21 (7%) 22 19	38, 63, 119, 158	0
1	B	303/336 (90%)	0.38	13 (4%) 40 37	40, 61, 111, 159	0
All	All	603/672 (89%)	0.43	34 (5%) 30 27	38, 62, 116, 159	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	377	LEU	5.7
1	B	287	VAL	5.5
1	B	246	GLN	4.7
1	A	188	VAL	4.6
1	B	376	TRP	3.9
1	A	330	ALA	3.6
1	A	47	TRP	3.3
1	A	158	ALA	3.2
1	B	337	TYR	3.1
1	A	135	LEU	3.1
1	A	68	CYS	3.0
1	A	361	LEU	2.9
1	A	243	TRP	2.9
1	A	376	TRP	2.9
1	B	247	ILE	2.7
1	B	290	MET	2.7
1	B	162	LEU	2.7
1	A	329	GLN	2.7
1	A	333	ARG	2.6
1	A	332	ASP	2.5
1	A	83	TYR	2.5
1	A	209	ASP	2.5
1	A	115	GLY	2.4
1	B	45	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	75	HIS	2.4
1	B	239	PHE	2.3
1	A	335	ALA	2.3
1	A	78	ARG	2.3
1	A	161	ALA	2.3
1	A	374	SER	2.3
1	A	147	ALA	2.2
1	B	124	TYR	2.2
1	B	252	SER	2.2
1	B	43	LYS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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.

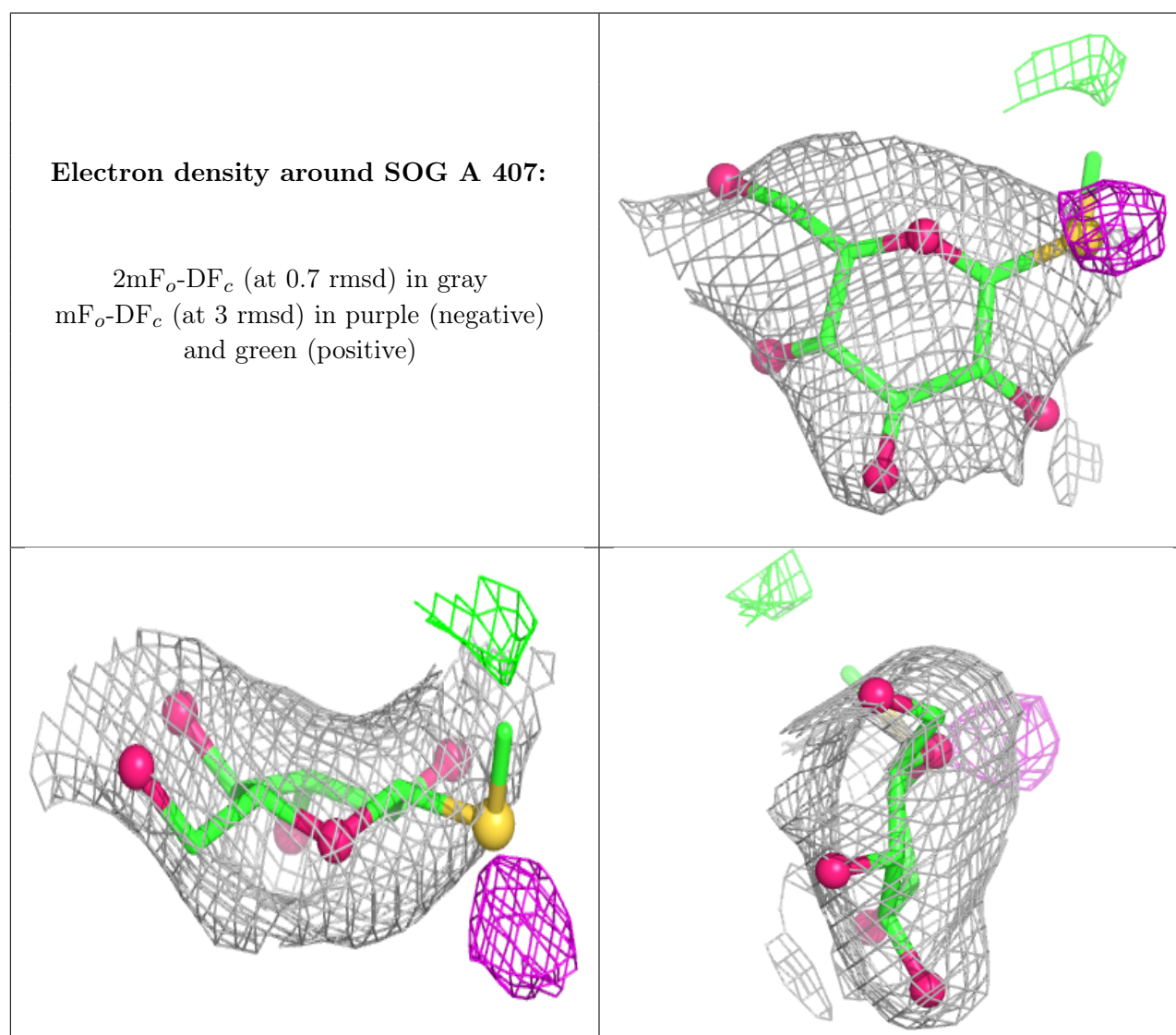
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SOG	A	407	13/20	0.52	0.17	126,128,132,132	0
4	SO4	A	404	5/5	0.57	0.13	138,139,139,140	0
3	PG4	A	402	13/13	0.60	0.27	87,94,102,102	0
5	SOG	B	405	13/20	0.67	0.17	113,116,118,119	0
4	SO4	B	403	5/5	0.72	0.14	119,120,122,122	0
5	SOG	A	406	20/20	0.73	0.16	57,102,108,109	0
5	SOG	A	408	20/20	0.74	0.20	98,116,120,121	0
5	SOG	B	407	16/20	0.77	0.19	105,125,128,129	0
6	PGW	A	410	51/51	0.78	0.20	42,74,115,118	0
5	SOG	B	408	20/20	0.79	0.14	65,101,106,107	0
5	SOG	B	404	20/20	0.82	0.16	94,100,102,103	0
6	PGW	A	409	51/51	0.83	0.17	47,72,119,120	0
5	SOG	B	406	20/20	0.84	0.13	58,89,93,95	0

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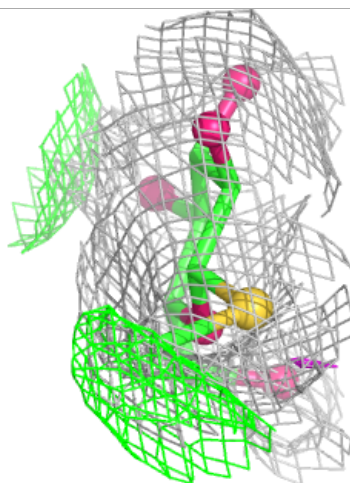
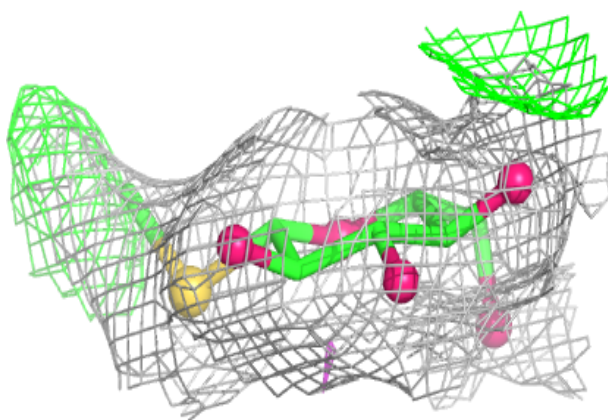
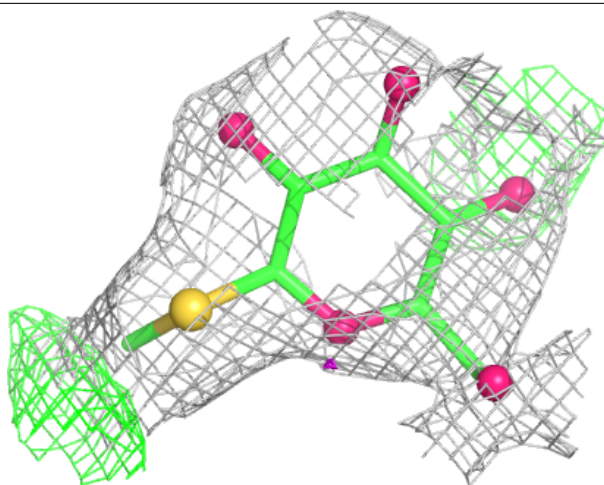
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NRK	B	401	30/30	0.90	0.09	44,45,49,60	0
2	NRK	A	401	30/30	0.90	0.10	44,45,51,66	0
4	SO4	A	403	5/5	0.92	0.10	112,112,113,114	0
5	SOG	A	405	20/20	0.92	0.10	55,63,73,73	0
4	SO4	B	402	5/5	0.93	0.07	89,90,91,93	0

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.



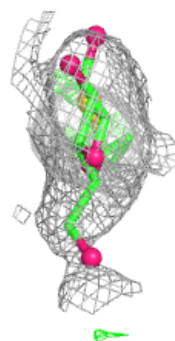
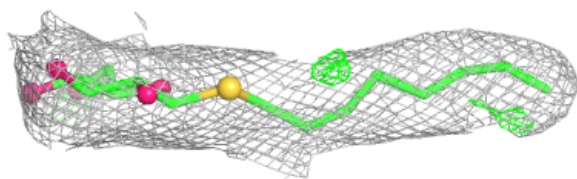
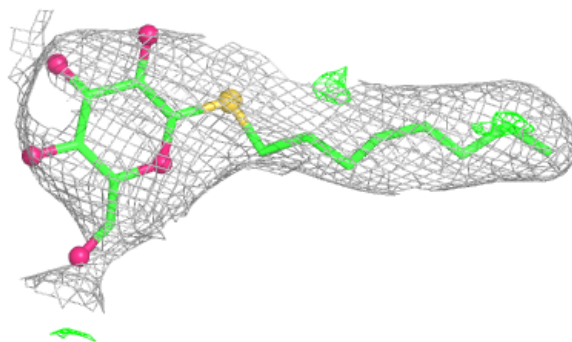
Electron density around SOG B 405:

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

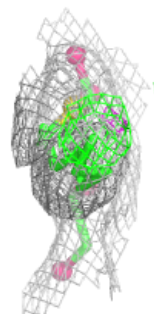
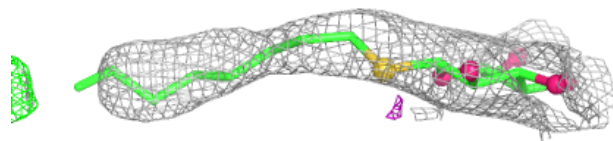
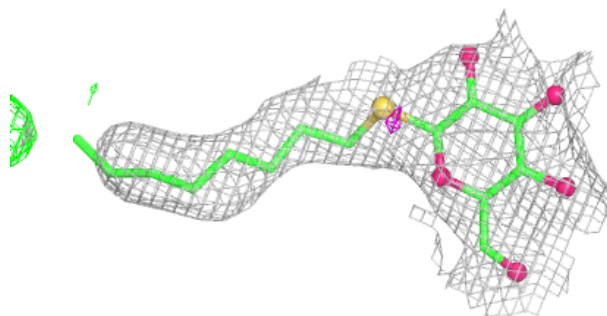


Electron density around SOG A 406:

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

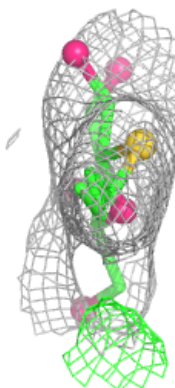
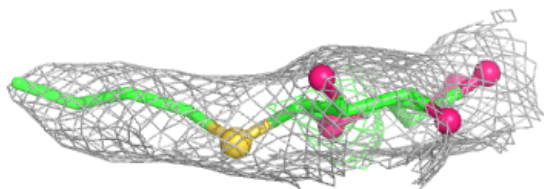
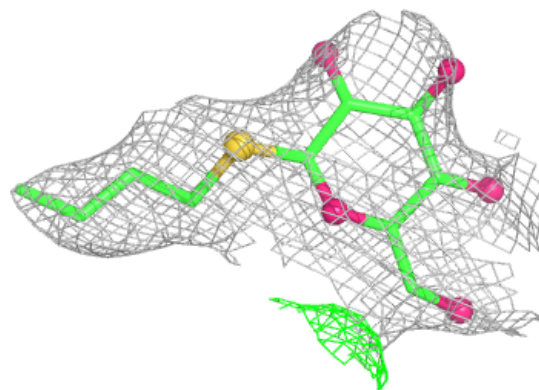
**Electron density around SOG A 408:**

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

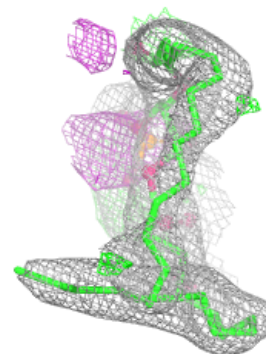
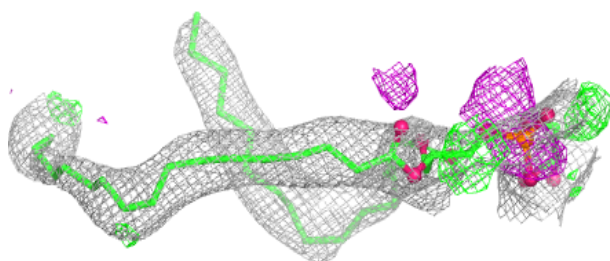
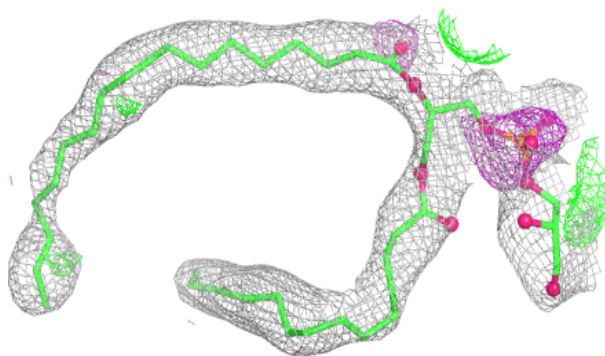


Electron density around SOG B 407:

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

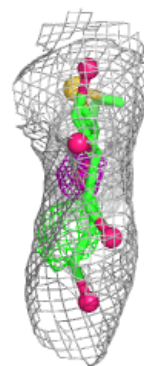
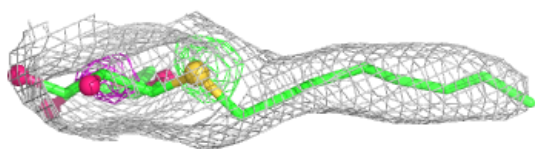
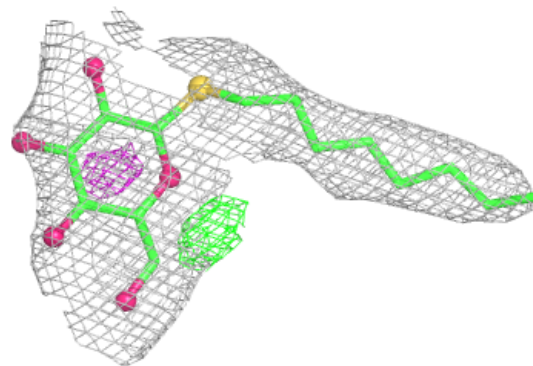
**Electron density around PGW A 410:**

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

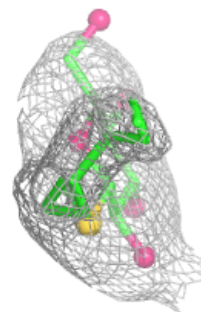
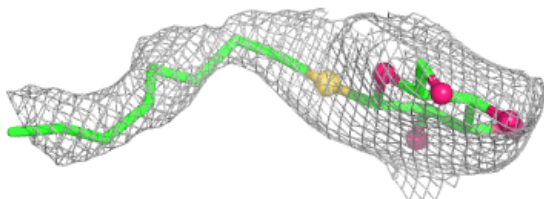
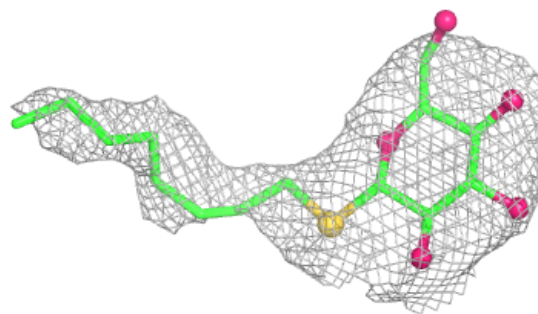


Electron density around SOG B 408:

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

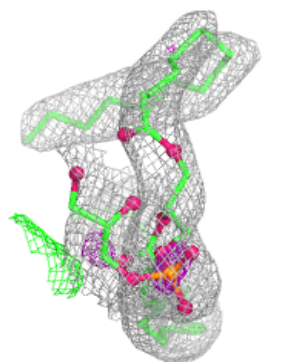
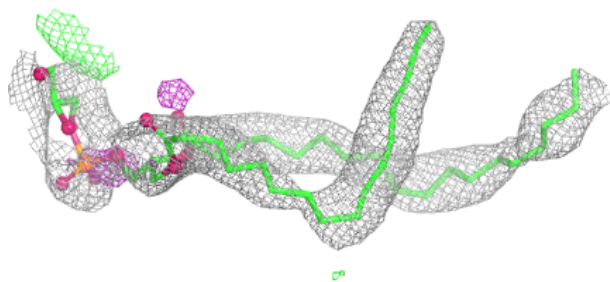
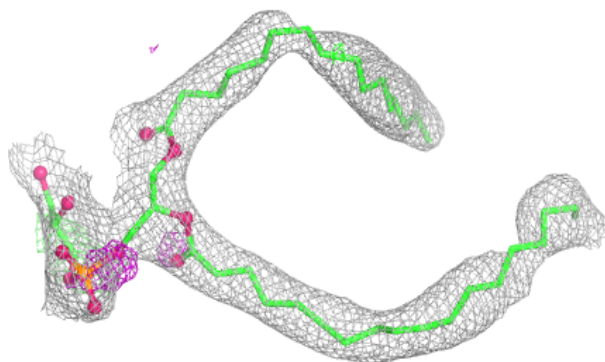
**Electron density around SOG B 404:**

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

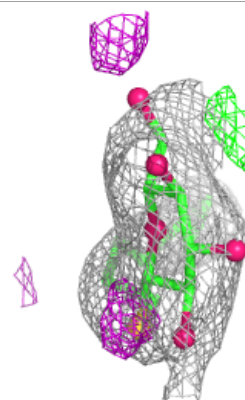
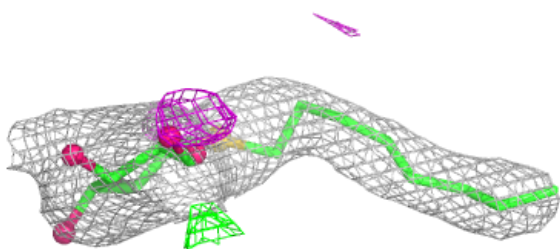
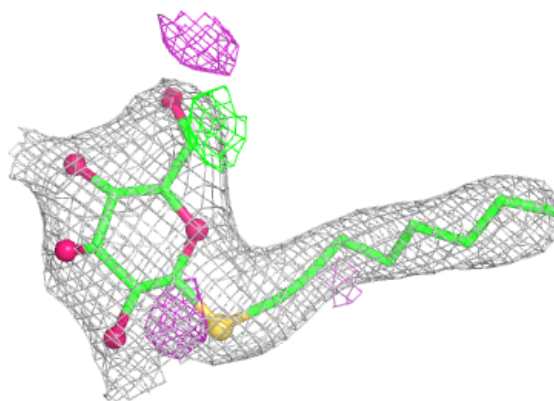


Electron density around PGW A 409:

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

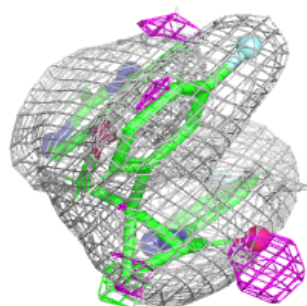
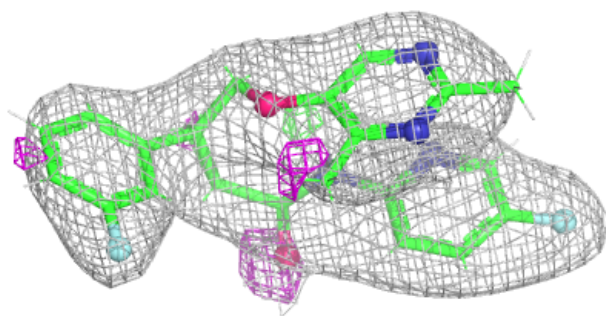
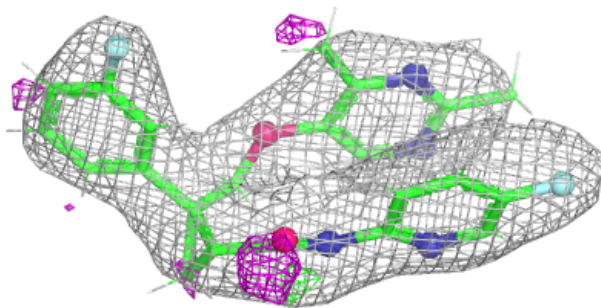
**Electron density around SOG B 406:**

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

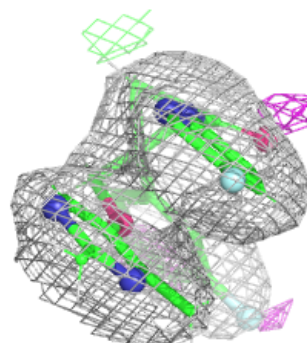
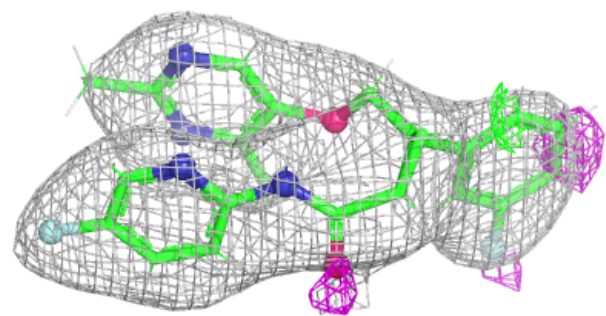
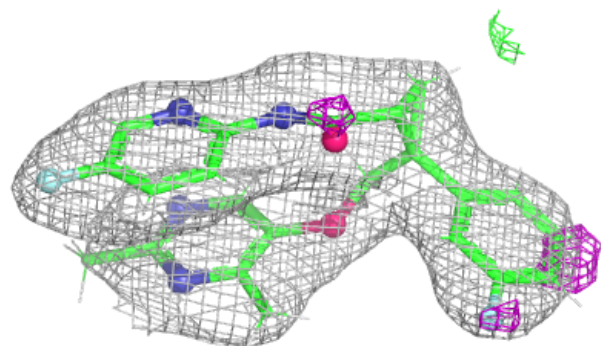


Electron density around NRK B 401:

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

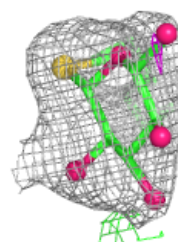
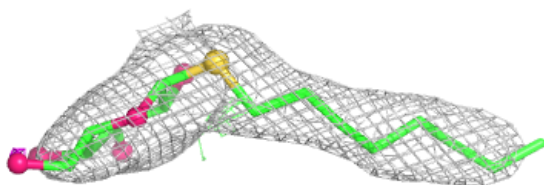
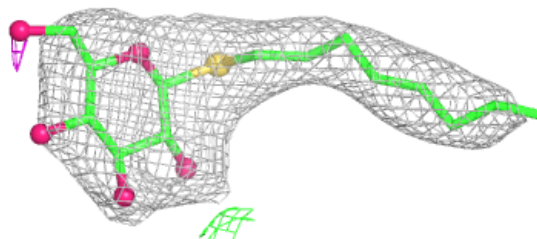
**Electron density around NRK A 401:**

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



Electron density around SOG A 405:

$2mF_o-DF_c$ (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.