



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:33 AM UTC

PDB ID : 6TP4 / pdb_00006tp4
Title : Crystal structure of the Orexin-1 receptor in complex with ACT-462206
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 : 2019-12-12
Resolution : 3.01 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

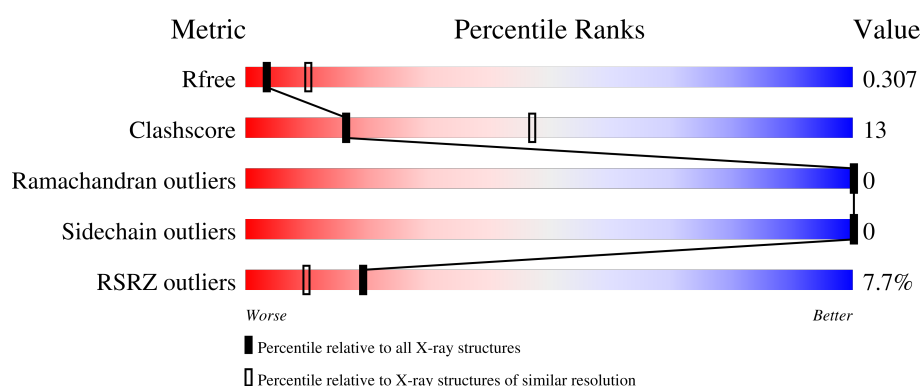
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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	336	
1	B	336	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5035 atoms, of which 24 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	298	Total	C	N	O	S	0	0	0
			2397	1594	394	392	17			
1	B	300	Total	C	N	O	S	0	0	0
			2374	1572	398	387	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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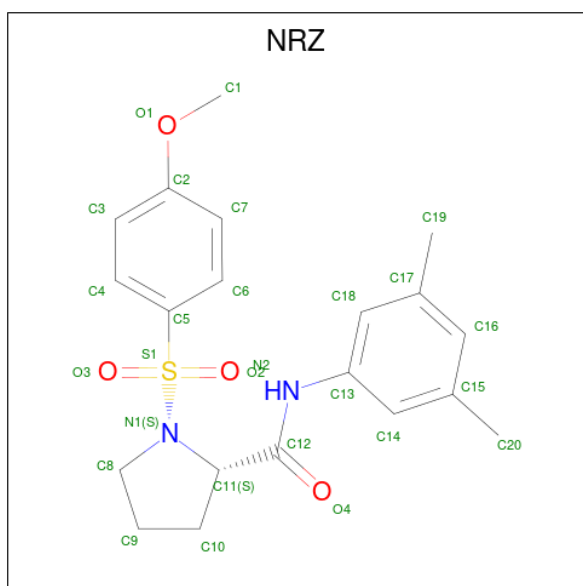
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613
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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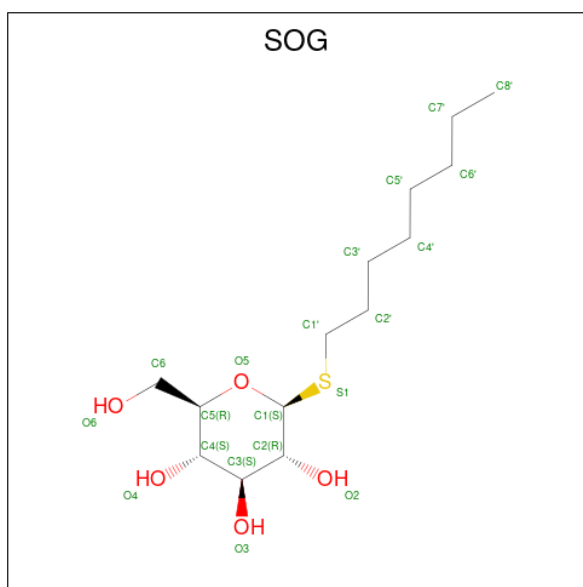
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is (2 {S})- {N}-(3,5-dimethylphenyl)-1-(4-methoxyphenyl)sulfonyl-pyrrolidine-2-carboxamide (CCD ID: NRZ) (formula: C₂₀H₂₄N₂O₄S) (labeled as "Ligand of Interest" by depositor).



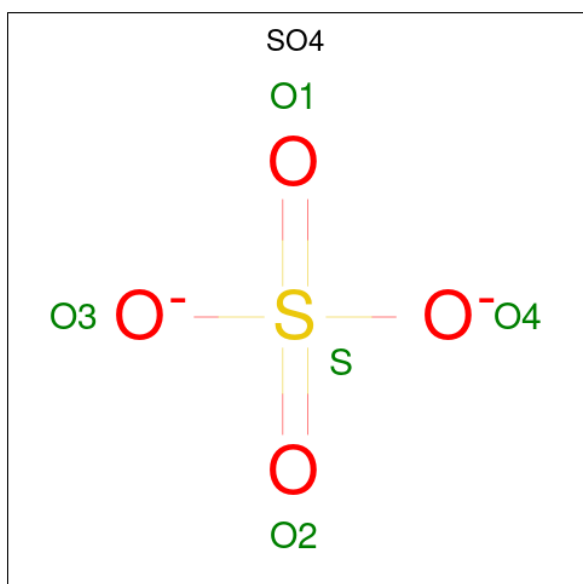
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	
			51	20	24	2	4	1	0

- Molecule 3 is octyl 1-thio-beta-D-glucopyranoside (CCD ID: SOG) (formula: C₁₄H₂₈O₅S).



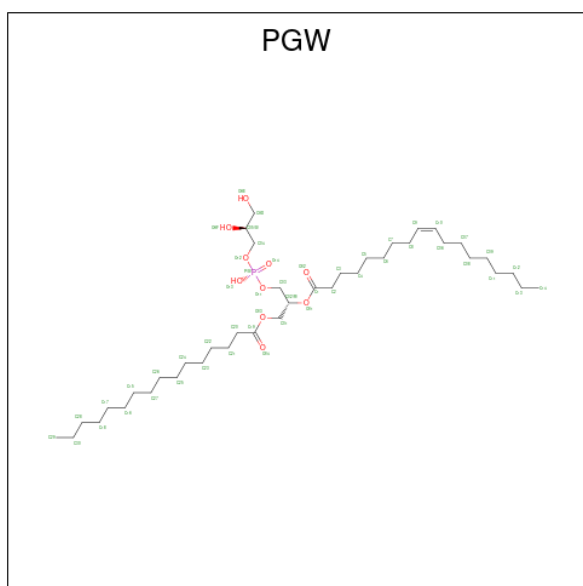
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	O	S	0	0
			12	6	5	1		

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



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

- Molecule 5 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
5	A	1	Total C O P 51 40 10 1	0	0
5	B	1	Total C O P 51 40 10 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	4	Total O 4 4	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.72Å 146.67Å 73.75Å 90.00° 108.29° 90.00°	Depositor
Resolution (Å)	34.62 – 3.01 34.62 – 3.01	Depositor EDS
% Data completeness (in resolution range)	54.9 (34.62-3.01) 78.0 (34.62-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.57 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.226 , 0.264 0.283 , 0.307	Depositor DCC
R_{free} test set	4026 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	5.4	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 24.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5035	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 7.25% 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: PGW, NRZ, SOG, SO4

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	0.29	0/2464	0.68	0/3356
1	B	0.30	0/2439	0.68	0/3327
All	All	0.30	0/4903	0.68	0/6683

There are no bond length outliers.

There are no bond angle outliers.

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	2397	0	2441	54	0
1	B	2374	0	2444	72	0
2	A	27	24	0	0	0
3	A	60	0	84	14	0
3	B	32	0	39	7	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
5	A	51	0	76	3	0
5	B	51	0	76	9	0
6	A	4	0	0	0	0
All	All	5011	24	5160	131	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 13.

All (131) 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:50:ILE:HD11	1:A:108:ILE:HD11	1.30	1.14
1:A:234:ALA:HB2	5:A:406:PGW:H7A	1.31	1.06
1:A:159:ARG:HG2	3:A:403:SOG:H1'2	1.50	0.94
1:B:50:ILE:HD13	1:B:104:LEU:HD11	1.55	0.87
1:A:38:ASP:HA	3:A:402:SOG:H62	1.57	0.85
1:B:108:ILE:HG13	1:B:109:THR:HG23	1.59	0.83
1:A:50:ILE:HD11	1:A:108:ILE:CD1	2.10	0.82
1:A:73:ARG:HH22	1:A:372:ALA:HB2	1.43	0.81
1:B:83:TYR:O	1:B:86:VAL:HG12	1.80	0.81
1:A:50:ILE:CD1	1:A:108:ILE:HD11	2.09	0.81
1:B:234:ALA:HB2	5:B:405:PGW:H24A	1.66	0.77
1:A:50:ILE:HD13	1:A:104:LEU:HD11	1.68	0.76
1:B:247:ILE:HG13	1:B:248:PRO:HD2	1.66	0.75
1:B:138:SER:HB3	5:B:405:PGW:H16A	1.69	0.72
1:B:332:ASP:OD1	1:B:335:ALA:HB3	1.91	0.71
1:A:287:VAL:HG12	1:A:291:ARG:HE	1.56	0.70
1:B:191:GLU:O	1:B:191:GLU:HG3	1.89	0.70
1:A:369:PHE:O	1:A:373:PHE:HB2	1.92	0.70
1:A:39:TYR:C	1:A:42:PRO:HD2	2.18	0.69
1:B:105:LEU:HD23	1:B:108:ILE:HD11	1.77	0.66
1:A:53:TYR:CD2	1:A:104:LEU:HB2	2.31	0.66
1:B:53:TYR:CD2	1:B:104:LEU:HB2	2.31	0.66
1:B:247:ILE:HG23	1:B:250:THR:HG22	1.79	0.65
1:B:207:ALA:CB	3:B:401:SOG:H2	2.27	0.65
1:A:73:ARG:NH2	1:A:372:ALA:HB2	2.12	0.64
3:A:403:SOG:H6'2	1:B:160:ARG:HD3	1.80	0.63
1:A:36:TRP:HA	1:A:40:LEU:HB2	1.81	0.62
1:B:306:VAL:HG21	1:B:357:ILE:HD11	1.81	0.62
1:A:105:LEU:HD22	1:A:114:PHE:CZ	2.35	0.60
1:A:83:TYR:O	1:A:86:VAL:HG22	2.00	0.60
1:A:206:TRP:HA	3:A:404:SOG:O3	2.02	0.59
1:B:120:LYS:HG2	1:B:183:MET:HB2	1.85	0.59
1:B:120:LYS:HE2	1:B:183:MET:O	2.03	0.59
1:B:120:LYS:NZ	3:B:401:SOG:H8'2	2.18	0.59
1:B:120:LYS:HZ1	3:B:401:SOG:H6'1	1.68	0.58
1:B:230:LEU:HB3	5:B:405:PGW:H25	1.85	0.58
1:B:120:LYS:HZ1	3:B:401:SOG:H8'2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ALA:HB2	3:B:401:SOG:H2	1.85	0.58
1:A:100:LEU:HD13	1:A:348:TYR:CG	2.38	0.58
1:B:187:SER:HB2	1:B:193:ALA:HB2	1.86	0.57
1:B:184:GLU:HG3	1:B:205:ARG:HD3	1.86	0.57
1:B:144:ARG:NH1	1:B:148:ILE:HD11	2.20	0.57
1:A:138:SER:HB3	5:A:406:PGW:H07	1.87	0.56
3:A:404:SOG:H61	5:B:405:PGW:HADA	1.87	0.56
1:A:144:ARG:O	1:A:148:ILE:HD13	2.06	0.56
1:B:325:GLY:HA2	1:B:328:ARG:NH2	2.20	0.56
3:A:404:SOG:C6	5:B:405:PGW:HADA	2.37	0.56
1:B:134:VAL:HG22	1:B:307:PHE:CZ	2.41	0.56
1:A:299:MET:HA	1:A:361:LEU:HD13	1.88	0.55
1:A:147:ALA:HB3	1:A:148:ILE:HD12	1.88	0.55
1:A:159:ARG:HD3	3:A:403:SOG:O5	2.06	0.55
1:A:370:LYS:HA	1:A:373:PHE:HB3	1.88	0.55
1:B:98:ILE:HG22	1:B:122:ILE:HD12	1.89	0.55
1:B:114:PHE:HB3	1:B:118:LEU:HD12	1.89	0.55
1:B:376:TRP:O	1:B:377:LEU:HG	2.07	0.54
1:B:67:VAL:HG22	1:B:369:PHE:HZ	1.71	0.54
1:A:112:TRP:O	1:A:200:SER:OG	2.23	0.54
1:A:177:VAL:N	1:A:178:PRO:HD2	2.22	0.53
1:B:147:ALA:HB3	1:B:148:ILE:HD12	1.89	0.53
1:B:108:ILE:HG13	1:B:109:THR:N	2.24	0.53
1:A:184:GLU:HG3	1:A:205:ARG:HD3	1.91	0.53
1:B:148:ILE:O	1:B:241:LYS:NZ	2.41	0.53
1:A:105:LEU:HD22	1:A:114:PHE:HZ	1.75	0.52
1:A:287:VAL:HG12	1:A:291:ARG:HH21	1.75	0.52
1:B:122:ILE:HB	1:B:123:PRO:HD3	1.90	0.52
1:A:314:ILE:HB	1:A:343:SER:HB2	1.92	0.51
1:B:150:HIS:HB3	1:B:153:LEU:HD12	1.92	0.51
1:B:313:PRO:HG3	1:B:346:LEU:HD12	1.93	0.51
1:A:41:TYR:OH	3:A:402:SOG:H6'1	2.11	0.50
1:B:329:GLN:HG3	1:B:331:SER:H	1.76	0.50
1:B:177:VAL:N	1:B:178:PRO:HD2	2.28	0.49
1:B:321:LYS:HB2	1:B:327:PHE:HD2	1.78	0.49
1:B:321:LYS:HB2	1:B:327:PHE:CD2	2.47	0.49
1:A:152:LEU:HD12	1:A:152:LEU:N	2.27	0.49
3:A:404:SOG:H61	5:B:405:PGW:CAD	2.43	0.48
1:B:235:TYR:CE2	1:B:304:VAL:HG21	2.48	0.48
1:B:226:ALA:HA	5:B:405:PGW:H08A	1.97	0.47
1:B:134:VAL:HG22	1:B:307:PHE:HZ	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ARG:O	1:B:148:ILE:HD13	2.14	0.47
1:B:130:VAL:O	1:B:134:VAL:HG23	2.15	0.47
1:A:122:ILE:HB	1:A:123:PRO:HD3	1.97	0.47
1:A:38:ASP:CA	3:A:402:SOG:H62	2.38	0.46
1:B:159:ARG:O	1:B:162:LEU:HG	2.16	0.46
1:B:150:HIS:HB3	1:B:153:LEU:CD1	2.46	0.46
1:B:142:LEU:HD23	3:B:402:SOG:H2	1.97	0.46
1:A:114:PHE:HB3	1:A:118:LEU:HD12	1.98	0.46
1:B:105:LEU:CD2	1:B:108:ILE:HD11	2.45	0.45
1:A:53:TYR:CE1	1:A:345:TRP:HB2	2.51	0.45
1:A:359:ASN:O	1:A:366:ARG:HB2	2.17	0.45
1:B:325:GLY:HA2	1:B:328:ARG:CZ	2.47	0.45
1:B:233:MET:HB3	5:B:405:PGW:H20A	1.99	0.45
1:A:100:LEU:HB3	1:A:101:PRO:HD3	1.97	0.45
1:A:230:LEU:HA	1:A:233:MET:HE3	1.98	0.45
1:A:287:VAL:HG12	1:A:291:ARG:NE	2.26	0.45
1:A:138:SER:OG	1:A:231:MET:HE2	2.16	0.45
1:A:207:ALA:H	3:A:404:SOG:H3	1.82	0.45
1:B:247:ILE:CG2	1:B:250:THR:HG22	2.45	0.44
1:B:191:GLU:O	1:B:191:GLU:CG	2.61	0.44
1:A:160:ARG:CZ	3:A:403:SOG:H1'1	2.48	0.44
1:B:143:ASP:HA	3:B:402:SOG:O3	2.18	0.44
1:B:376:TRP:O	1:B:376:TRP:CG	2.71	0.44
1:B:50:ILE:O	1:B:54:VAL:HG23	2.17	0.44
1:B:363:GLY:HA2	1:B:366:ARG:HG2	2.00	0.44
1:A:94:LEU:HD23	1:A:94:LEU:C	2.42	0.44
1:A:150:HIS:O	1:A:153:LEU:HD13	2.17	0.44
1:B:325:GLY:CA	1:B:328:ARG:NH2	2.80	0.44
1:B:100:LEU:HB3	1:B:101:PRO:HD3	2.00	0.44
1:A:369:PHE:O	1:A:373:PHE:N	2.49	0.43
1:A:100:LEU:HD13	1:A:348:TYR:CD2	2.54	0.43
1:B:184:GLU:HG3	1:B:205:ARG:CD	2.48	0.43
1:A:162:LEU:HD23	1:A:166:LEU:HD13	2.00	0.43
1:B:235:TYR:HE2	1:B:304:VAL:HG21	1.84	0.43
1:B:346:LEU:HD23	1:B:346:LEU:HA	1.78	0.43
1:A:287:VAL:HA	1:A:290:MET:HB2	2.00	0.42
1:A:162:LEU:HD23	1:A:162:LEU:O	2.20	0.42
1:B:124:TYR:HB2	1:B:180:ALA:HB2	2.01	0.42
5:A:406:PGW:H26A	5:A:406:PGW:H16A	1.70	0.42
1:B:69:LEU:HD23	1:B:69:LEU:HA	1.78	0.42
1:B:77:MET:O	1:B:82:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:GLY:HA2	1:A:328:ARG:CZ	2.50	0.42
1:B:105:LEU:HD12	1:B:114:PHE:HZ	1.83	0.41
1:B:148:ILE:HD12	1:B:148:ILE:N	2.35	0.41
1:A:159:ARG:CG	3:A:403:SOG:H3'2	2.50	0.41
1:B:119:CYS:O	1:B:123:PRO:HG2	2.20	0.41
1:B:314:ILE:N	1:B:343:SER:OG	2.53	0.41
1:A:145:TRP:O	1:A:149:CYS:HB2	2.20	0.41
1:B:88:LEU:HD23	1:B:88:LEU:C	2.46	0.41
1:B:240:ARG:HA	1:B:240:ARG:HD2	1.73	0.41
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.81	0.41
3:A:404:SOG:H62	5:B:405:PGW:HADA	2.03	0.40
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	292/336 (87%)	289 (99%)	3 (1%)	0	100	100
1	B	298/336 (89%)	296 (99%)	2 (1%)	0	100	100
All	All	590/672 (88%)	585 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	252/279 (90%)	252 (100%)	0	100	100
1	B	249/279 (89%)	249 (100%)	0	100	100
All	All	501/558 (90%)	501 (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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	359	ASN
1	B	75	HIS
1	B	150	HIS
1	B	350	ASN
1	B	368	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NRZ	A	401	-	29,29,29	0.35	0	42,42,42	0.61	0
3	SOG	B	402	-	11,12,20	0.16	0	15,17,25	0.33	0
5	PGW	A	406	-	50,50,50	0.30	0	53,56,56	0.46	0
5	PGW	B	405	-	50,50,50	0.27	0	53,56,56	0.41	0
3	SOG	A	404	-	20,20,20	0.37	0	24,25,25	0.24	0
4	SO4	B	403	-	4,4,4	0.26	0	6,6,6	0.08	0
3	SOG	B	401	-	20,20,20	0.35	0	24,25,25	0.35	0
3	SOG	A	403	-	20,20,20	0.35	0	24,25,25	0.38	0
4	SO4	B	404	-	4,4,4	0.22	0	6,6,6	0.11	0
3	SOG	A	402	-	20,20,20	0.29	0	24,25,25	0.30	0
4	SO4	A	405	-	4,4,4	0.24	0	6,6,6	0.09	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NRZ	A	401	-	-	7/22/32/32	0/3/3/3
3	SOG	B	402	-	-	2/2/22/31	0/1/1/1
5	PGW	A	406	-	-	20/55/55/55	-
5	PGW	B	405	-	-	15/55/55/55	-
3	SOG	A	404	-	-	1/11/31/31	0/1/1/1
3	SOG	B	401	-	-	1/11/31/31	0/1/1/1
3	SOG	A	403	-	-	4/11/31/31	0/1/1/1
3	SOG	A	402	-	-	1/11/31/31	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	PGW	C04-O12-P-O11
5	A	406	PGW	C04-O12-P-O13
5	B	405	PGW	O12-C04-C05-CAD
3	B	402	SOG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	405	PGW	O12-C04-C05-OAF
3	B	402	SOG	C4-C5-C6-O6
2	A	401	NRZ	C11-N1-S1-O3
5	A	406	PGW	C02-C01-O03-C19
5	A	406	PGW	C16-C15-C27-C26
5	B	405	PGW	C19-C20-C21-C22
5	B	405	PGW	C08-C09-C11-C12
5	B	405	PGW	C27-C15-C16-C17
3	A	403	SOG	C3'-C4'-C5'-C6'
3	A	403	SOG	O5-C5-C6-O6
5	B	405	PGW	C22-C23-C24-C25
2	A	401	NRZ	C11-N1-S1-C5
5	A	406	PGW	C2-C1-O01-C02
3	A	402	SOG	O5-C5-C6-O6
5	B	405	PGW	C5-C6-C7-C8
5	A	406	PGW	C15-C16-C17-C18
5	A	406	PGW	O02-C1-O01-C02
3	A	404	SOG	O5-C5-C6-O6
5	A	406	PGW	O03-C01-C02-C03
5	A	406	PGW	C25-C26-C27-C15
3	A	403	SOG	C2'-C3'-C4'-C5'
5	A	406	PGW	C6-C7-C8-C9
3	A	403	SOG	C4'-C5'-C6'-C7'
3	B	401	SOG	C2'-C3'-C4'-C5'
5	B	405	PGW	C01-C02-C03-O11
5	A	406	PGW	C07-C08-C09-C11
5	B	405	PGW	O03-C01-C02-C03
5	B	405	PGW	O03-C01-C02-O01
5	B	405	PGW	C15-C16-C17-C18
5	B	405	PGW	O01-C02-C03-O11
5	A	406	PGW	C21-C22-C23-C24
2	A	401	NRZ	C11-N1-S1-O2
2	A	401	NRZ	C6-C5-S1-O3
2	A	401	NRZ	C4-C5-S1-O3
5	A	406	PGW	C27-C15-C16-C17
5	B	405	PGW	C05-C04-O12-P
5	B	405	PGW	C7-C8-C9-C10
5	A	406	PGW	C24-C25-C26-C27
5	A	406	PGW	C16-C17-C18-C28
5	A	406	PGW	C7-C8-C9-C10
5	A	406	PGW	C07-C06-C10-C9
5	A	406	PGW	C10-C06-C07-C08

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Mol	Chain	Res	Type	Atoms
2	A	401	NRZ	C4-C5-S1-N1
2	A	401	NRZ	C6-C5-S1-N1
5	B	405	PGW	C4-C5-C6-C7
5	A	406	PGW	O01-C1-C2-C3
5	A	406	PGW	O02-C1-C2-C3

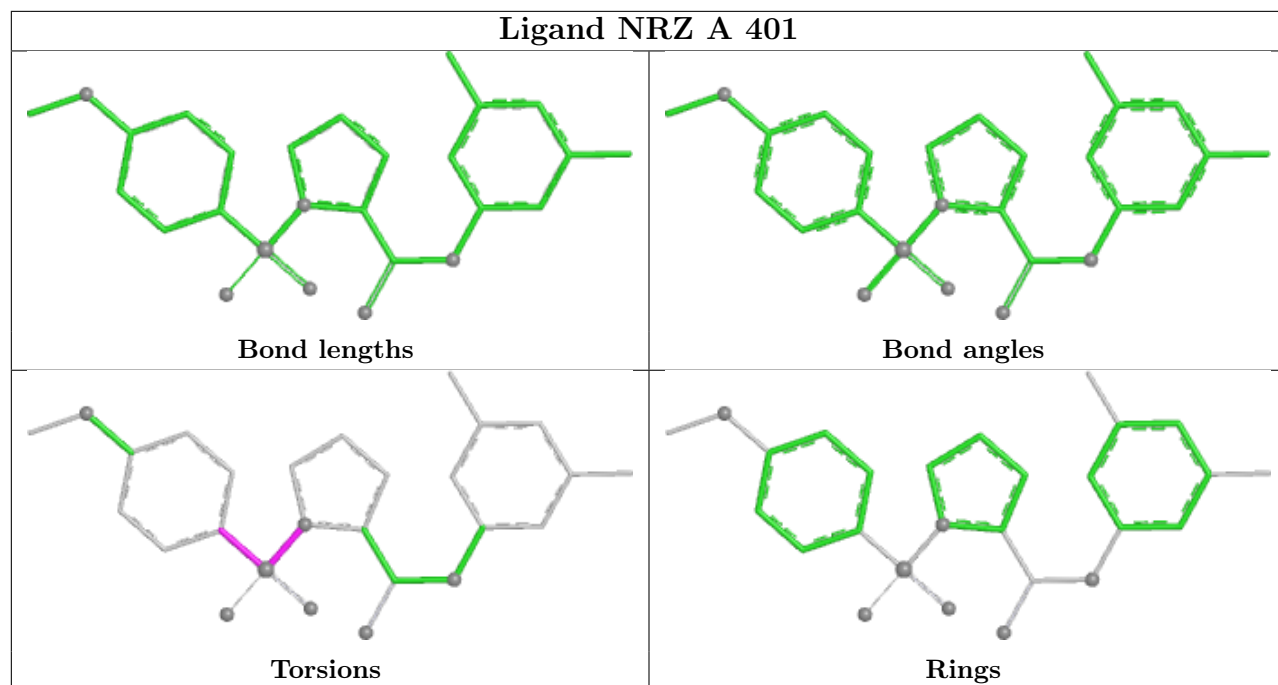
There are no ring outliers.

7 monomers are involved in 29 short contacts:

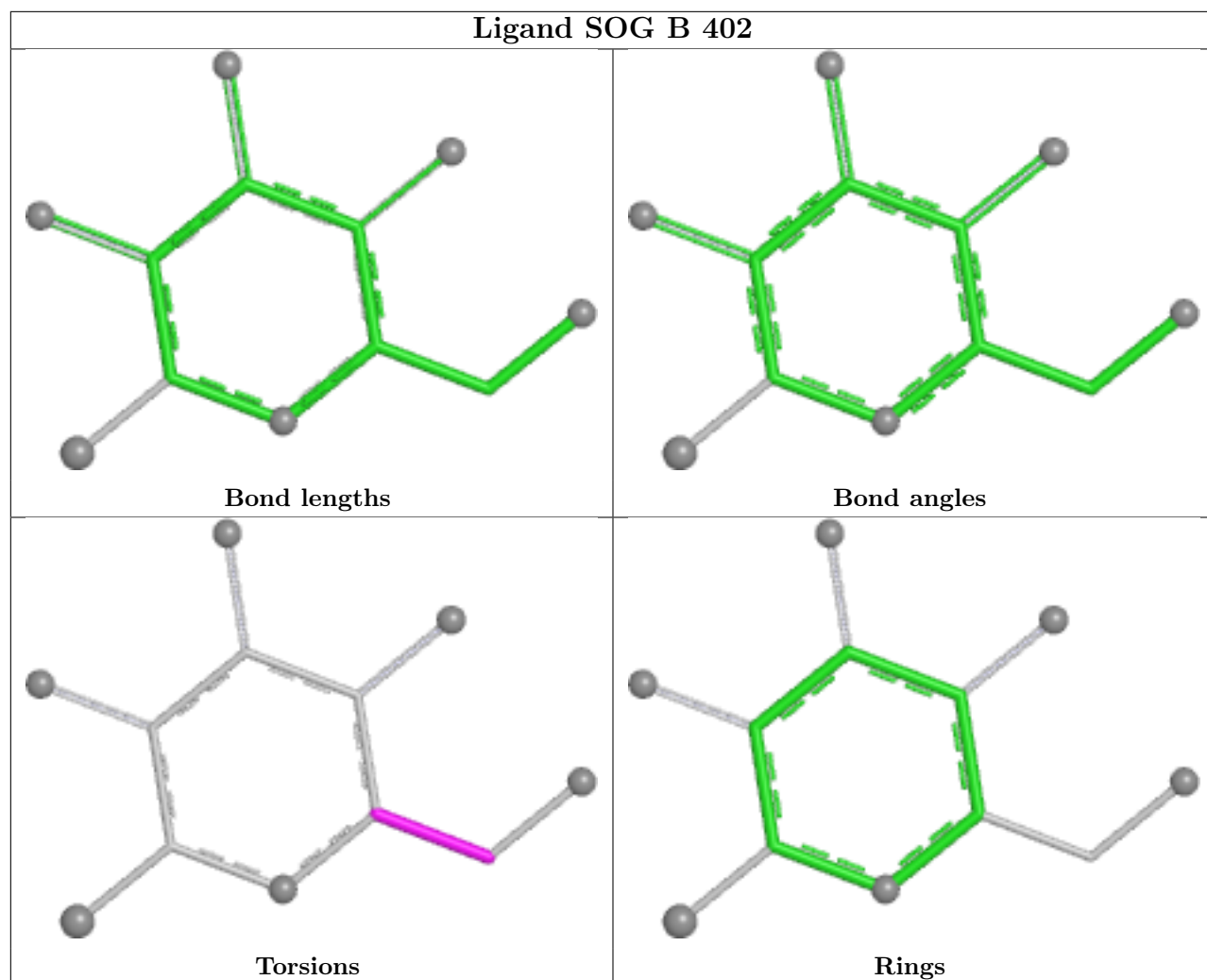
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	SOG	2	0
5	A	406	PGW	3	0
5	B	405	PGW	9	0
3	A	404	SOG	6	0
3	B	401	SOG	5	0
3	A	403	SOG	5	0
3	A	402	SOG	3	0

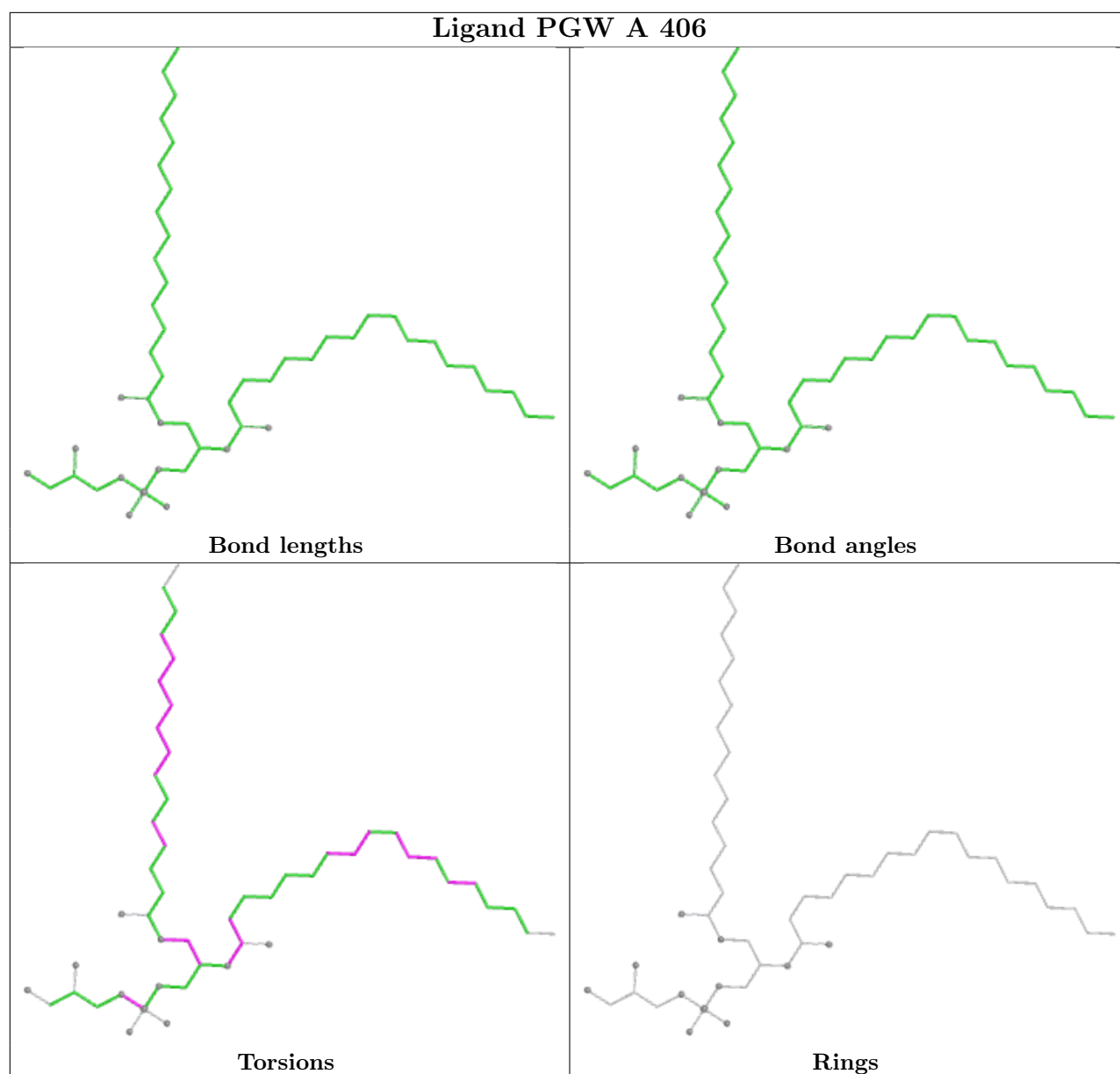
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

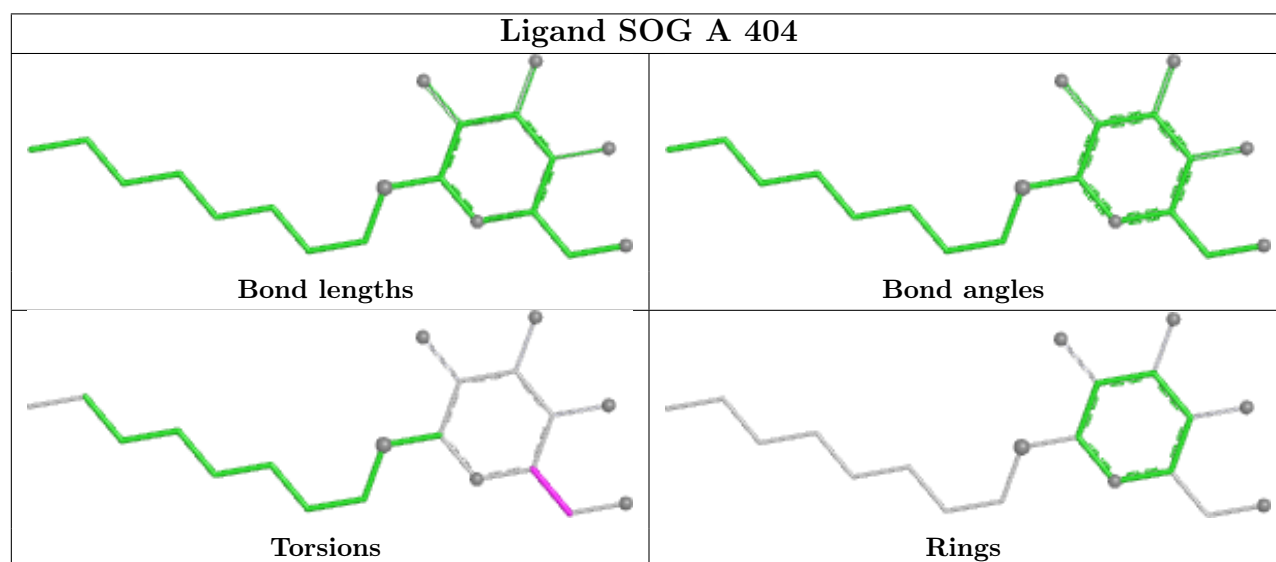
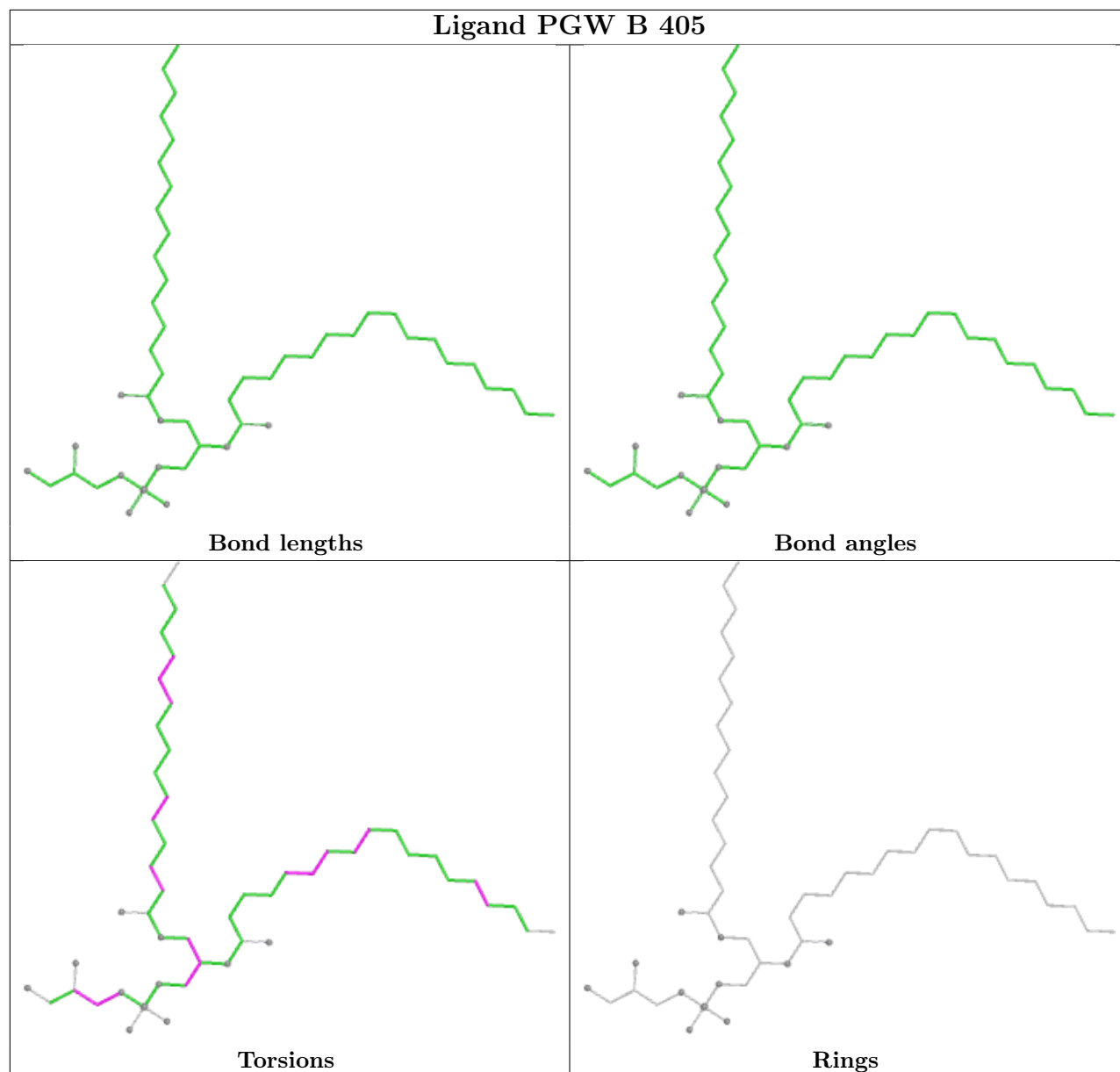
Ligand NRZ A 401

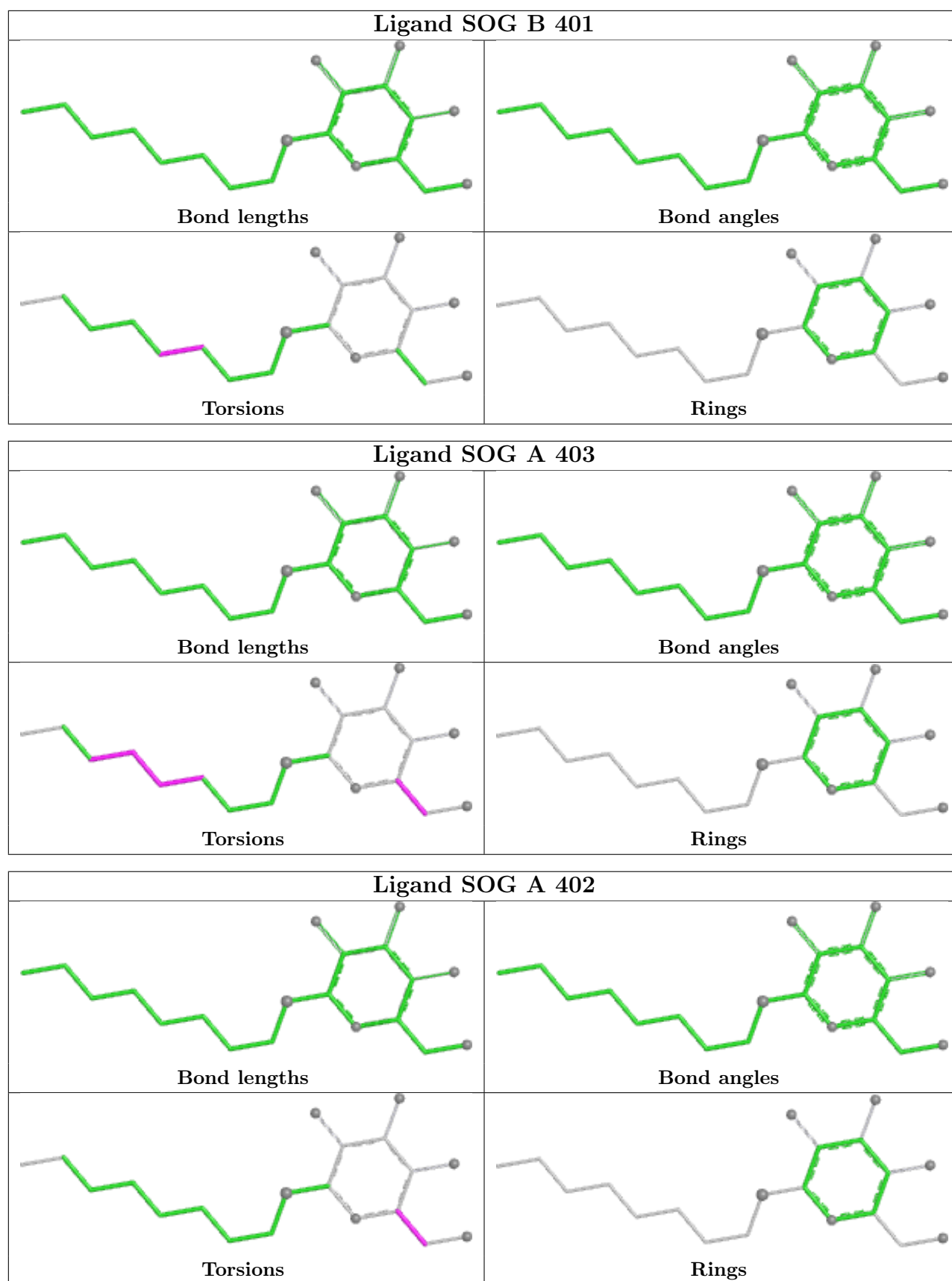


Ligand SOG B 402









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	298/336 (88%)	0.40	24 (8%) 18 9	29, 75, 145, 182	0
1	B	300/336 (89%)	0.30	22 (7%) 21 10	35, 80, 142, 170	0
All	All	598/672 (88%)	0.35	46 (7%) 19 10	29, 78, 144, 182	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	331	SER	15.6
1	A	332	ASP	10.6
1	A	152	LEU	9.7
1	A	329	GLN	7.9
1	A	330	ALA	7.8
1	B	86	VAL	7.3
1	A	334	GLU	5.6
1	A	153	LEU	5.2
1	B	53	TYR	4.4
1	A	151	PRO	4.3
1	B	71	VAL	4.1
1	B	201	VAL	4.0
1	B	114	PHE	4.0
1	A	335	ALA	4.0
1	B	242	LEU	3.8
1	B	202	CYS	3.7
1	A	134	VAL	3.6
1	B	103	SER	3.6
1	B	75	HIS	3.5
1	B	115	GLY	3.4
1	A	135	LEU	3.3
1	B	348	TYR	3.3
1	A	333	ARG	3.2
1	B	78	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	68	CYS	3.2
1	A	209	ASP	3.1
1	A	117	ALA	3.0
1	B	246	GLN	2.8
1	A	75	HIS	2.6
1	B	83	TYR	2.6
1	A	160	ARG	2.5
1	A	130	VAL	2.5
1	A	115	GLY	2.4
1	B	87	ASN	2.3
1	A	114	PHE	2.2
1	B	56	VAL	2.2
1	B	200	SER	2.2
1	A	76	HIS	2.2
1	B	100	LEU	2.1
1	A	118	LEU	2.1
1	A	105	LEU	2.1
1	B	84	PHE	2.1
1	B	72	TRP	2.1
1	B	322	ARG	2.1
1	A	121	VAL	2.0
1	A	78	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

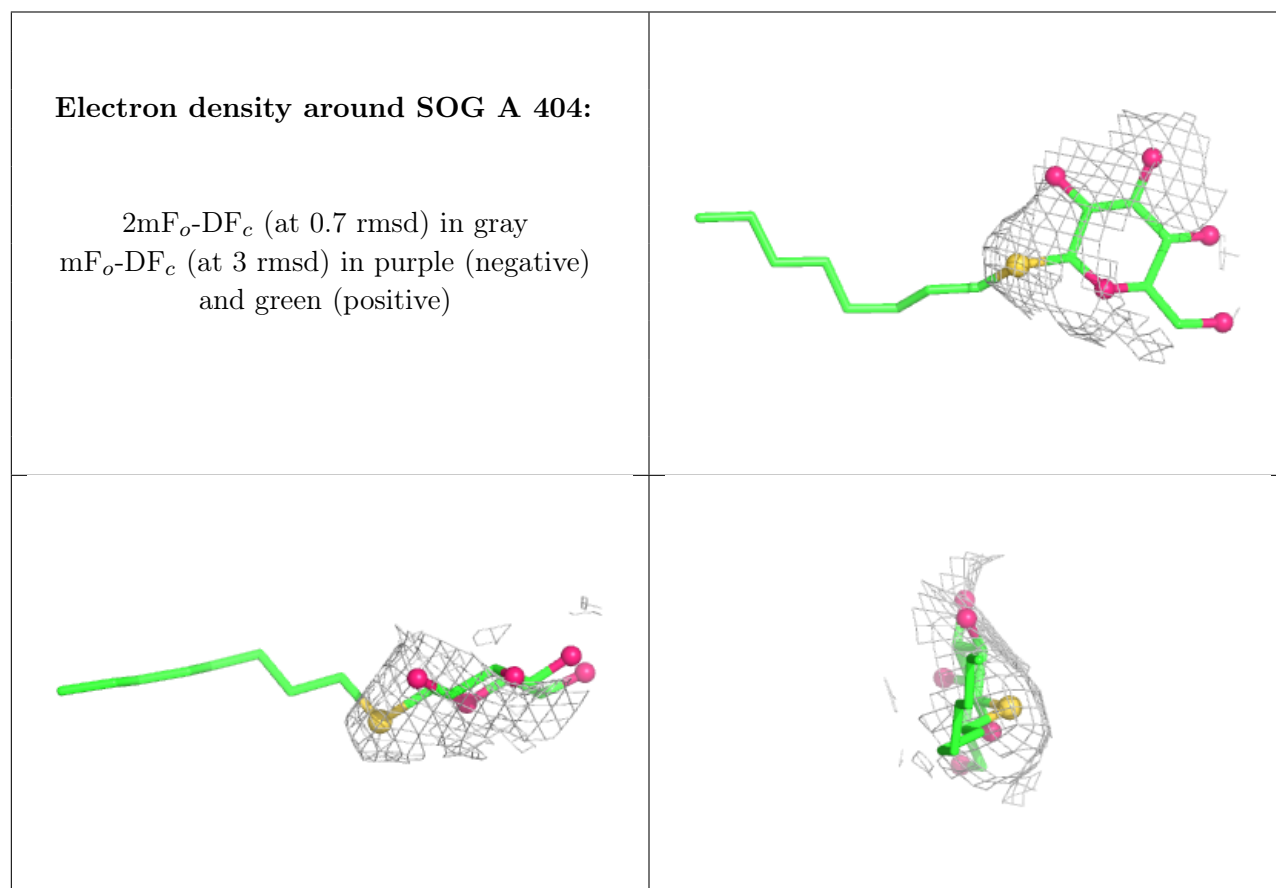
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	405	5/5	0.61	0.12	170,174,177,178	0

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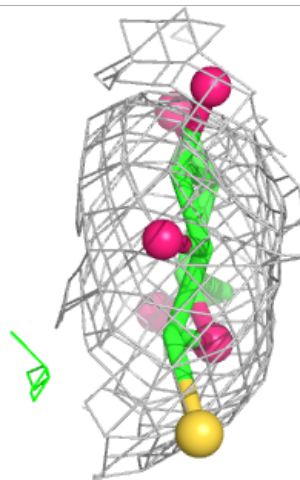
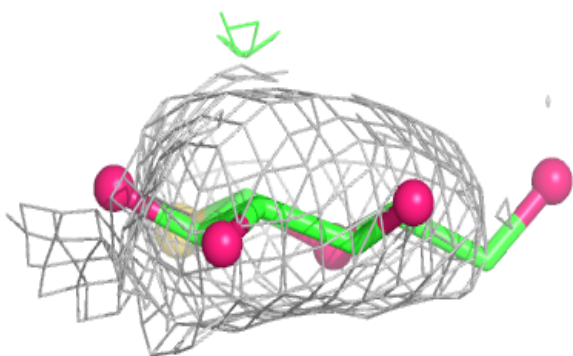
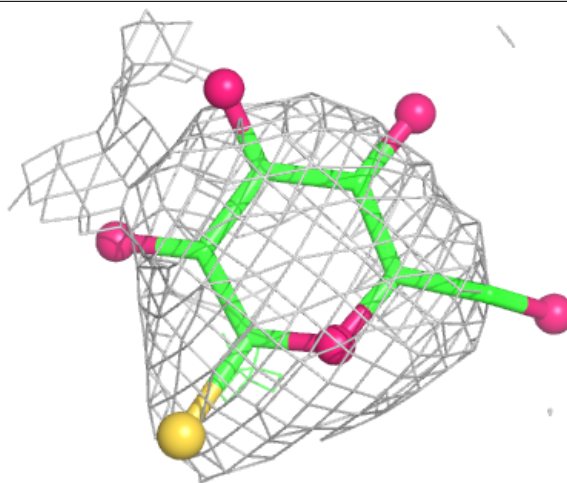
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SOG	A	404	20/20	0.68	0.14	92,133,151,152	0
3	SOG	B	402	12/20	0.69	0.21	125,144,156,164	0
3	SOG	B	401	20/20	0.71	0.14	95,112,133,134	0
3	SOG	A	403	20/20	0.76	0.11	104,125,153,156	0
4	SO4	B	403	5/5	0.82	0.07	104,105,109,117	0
5	PGW	B	405	51/51	0.85	0.18	20,68,139,146	0
4	SO4	B	404	5/5	0.86	0.08	170,172,173,174	0
5	PGW	A	406	51/51	0.89	0.18	23,74,167,170	0
3	SOG	A	402	20/20	0.89	0.13	58,100,112,123	0
2	NRZ	A	401	27/27	0.91	0.14	15,99,162,210	13

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.



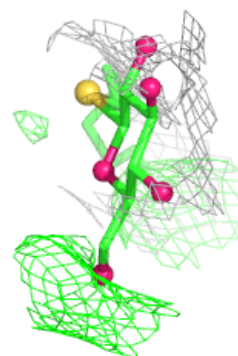
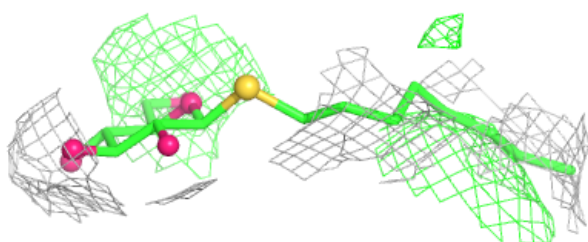
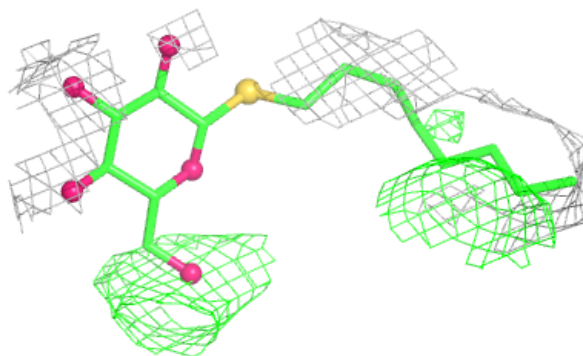
Electron density around SOG B 402:

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

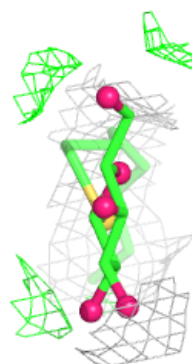
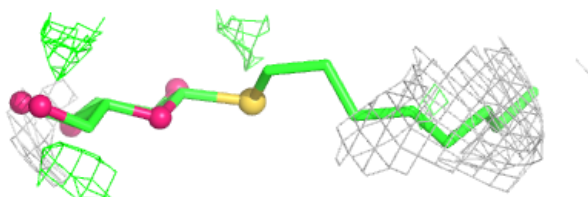
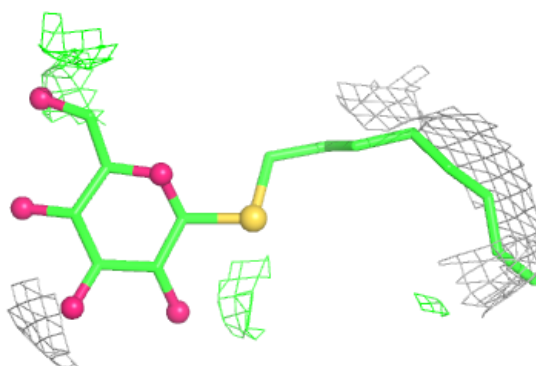


Electron density around SOG B 401:

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

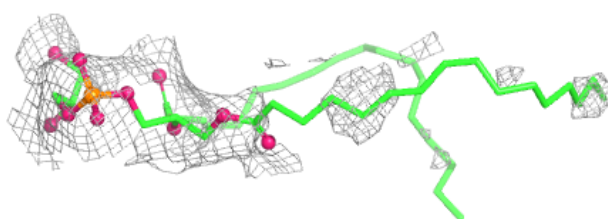
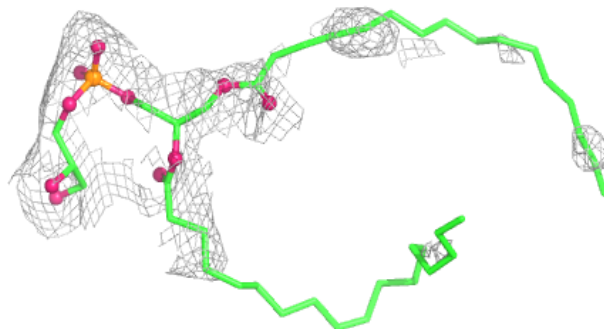
**Electron density around SOG A 403:**

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

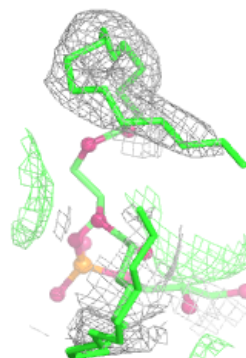
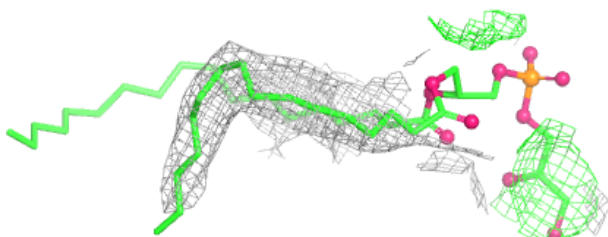
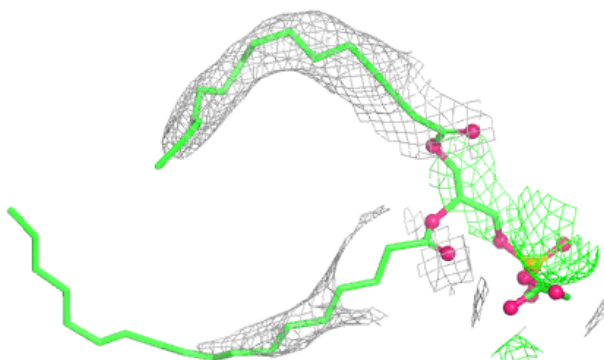


Electron density around PGW B 405:

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

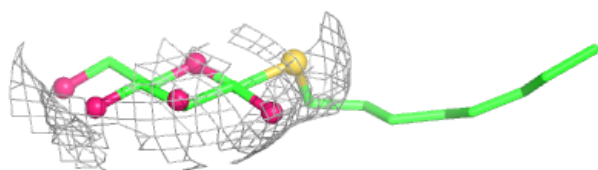
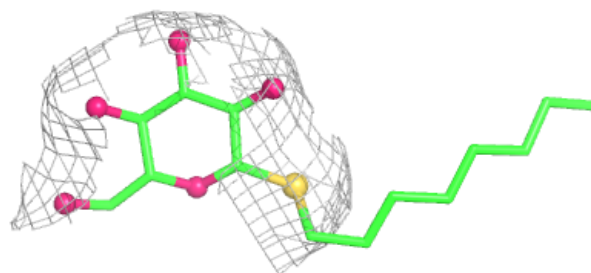
**Electron density around PGW A 406:**

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

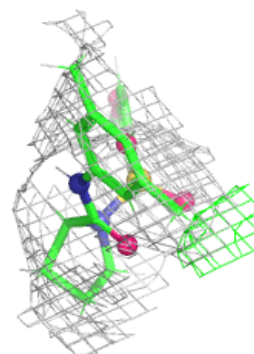
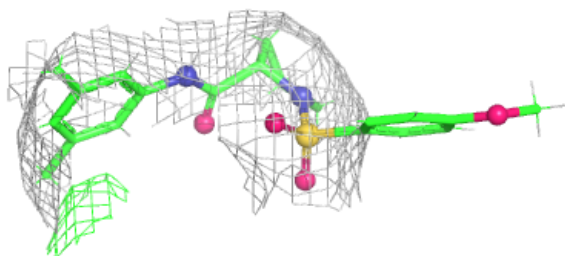
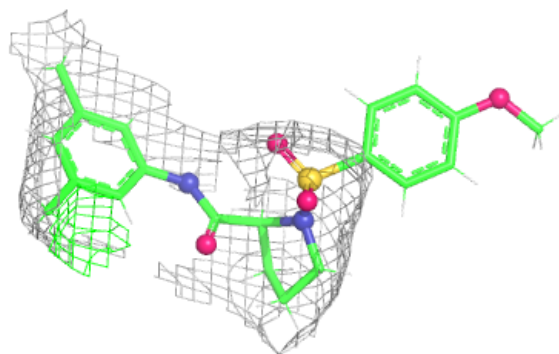


Electron density around SOG A 402:

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

**Electron density around NRZ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.