



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:04 PM UTC

PDB ID : 6TQ9 / pdb_00006tq9
Title : Crystal structure of the Orexin-1 receptor in complex with SB-408124
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 : 2019-12-16
Resolution : 2.65 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

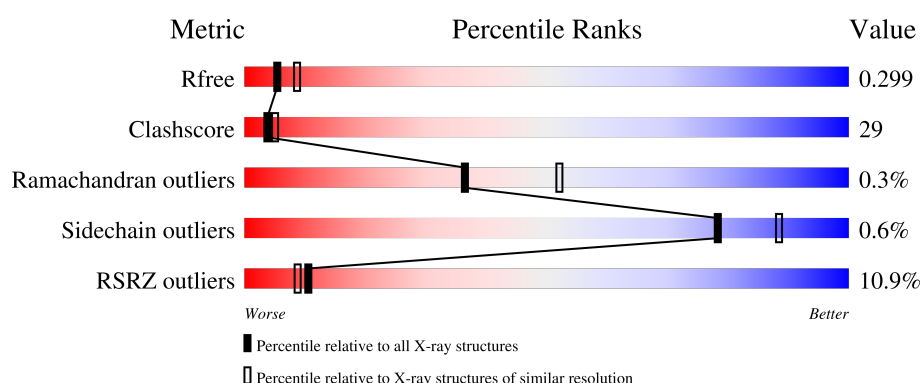
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SOG	A	403	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5287 atoms, of which 54 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	304	Total	C	N	O	S	0	0	0
			2440	1621	401	401	17			
1	B	302	Total	C	N	O	S	0	0	0
			2393	1586	400	390	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	GLY	conflict	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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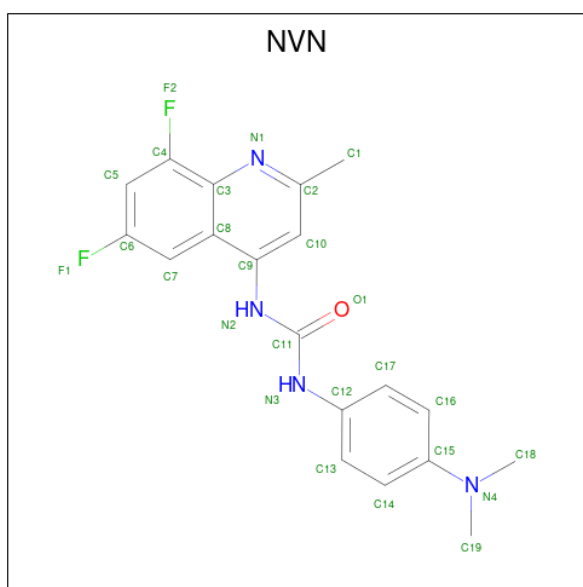
Chain	Residue	Modelled	Actual	Comment	Reference
B	211	ALA	TYR	engineered mutation	UNP O43613
B	?	-	ALA	deletion	UNP O43613
B	?	-	LEU	deletion	UNP O43613
B	?	-	VAL	deletion	UNP O43613
B	?	-	ARG	deletion	UNP O43613
B	?	-	ASN	deletion	UNP O43613
B	?	-	TRP	deletion	UNP O43613
B	?	-	LYS	deletion	UNP O43613
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	GLY	conflict	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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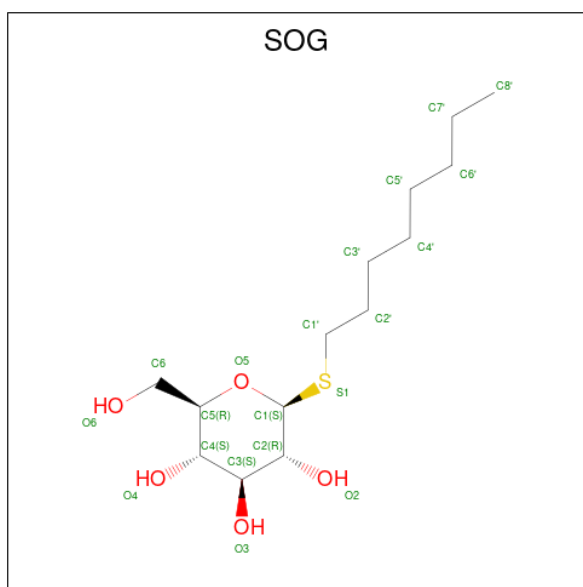
Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	expression tag	UNP O43613
B	387	HIS	-	expression tag	UNP O43613
B	388	HIS	-	expression tag	UNP O43613
B	389	HIS	-	expression tag	UNP O43613
B	390	HIS	-	expression tag	UNP O43613
B	391	HIS	-	expression tag	UNP O43613
B	392	HIS	-	expression tag	UNP O43613

- Molecule 2 is 1-[6,8-bis(fluoranyl)-2-methyl-quinolin-4-yl]-3-[4-(dimethylamino)phenyl]urea (CCD ID: NVN) (formula: C₁₉H₁₈F₂N₄O) (labeled as "Ligand of Interest" by depositor).



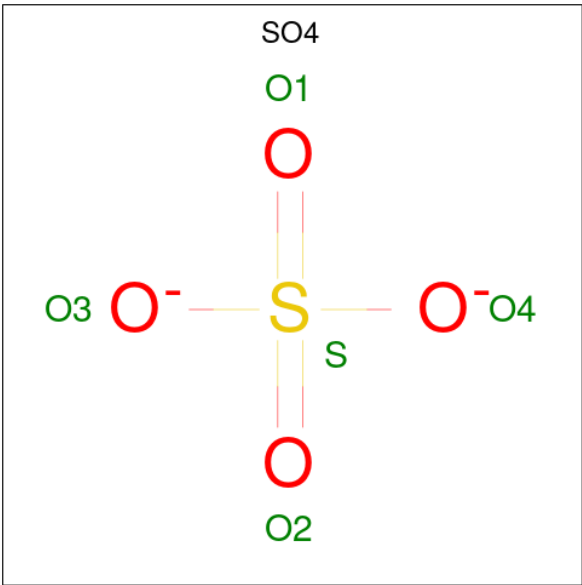
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	0	0
			44	19	2	18	4	1		
2	A	1	Total	C	F	H	N	O	0	0
			44	19	2	18	4	1		
2	B	1	Total	C	F	H	N	O	0	0
			44	19	2	18	4	1		

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



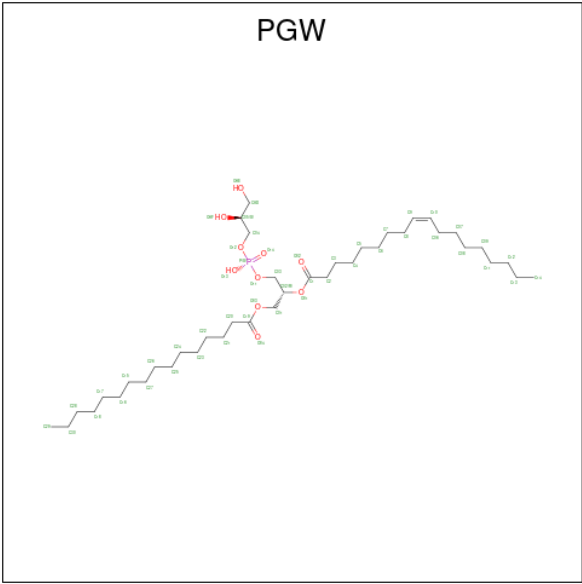
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	A	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	S		0	0
			9	8	1			
3	B	1	Total	C	O	S	0	0
			20	14	5	1		
3	B	1	Total	C	O	S	0	0
			20	14	5	1		

- 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		

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

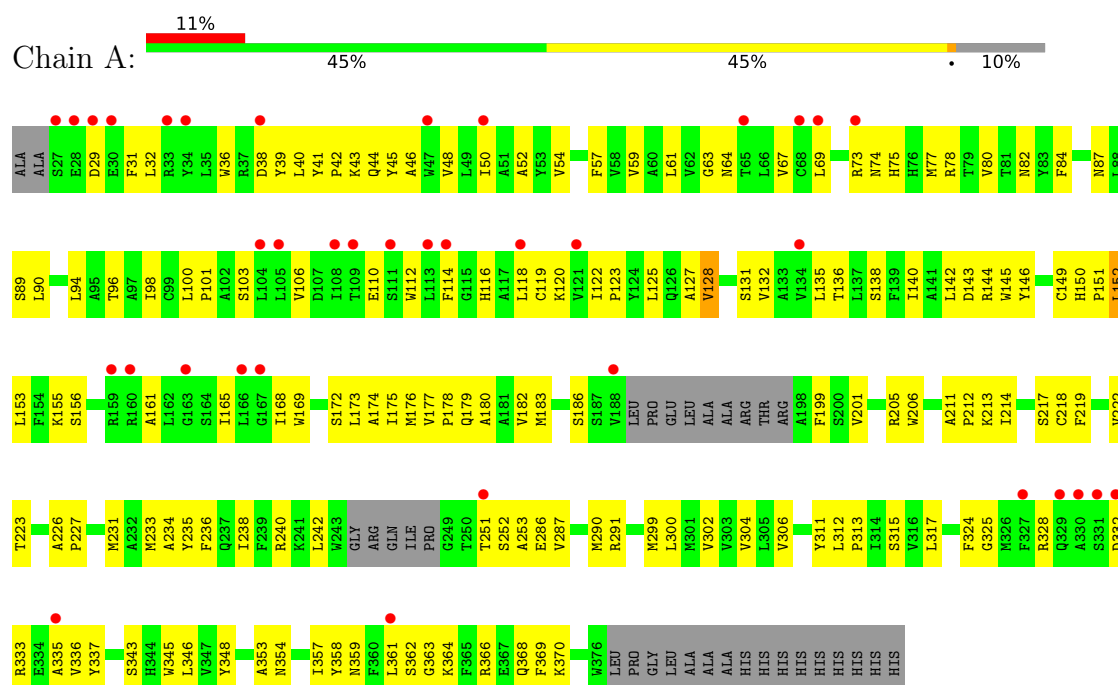
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	8	Total	O	0	0
			8	8		

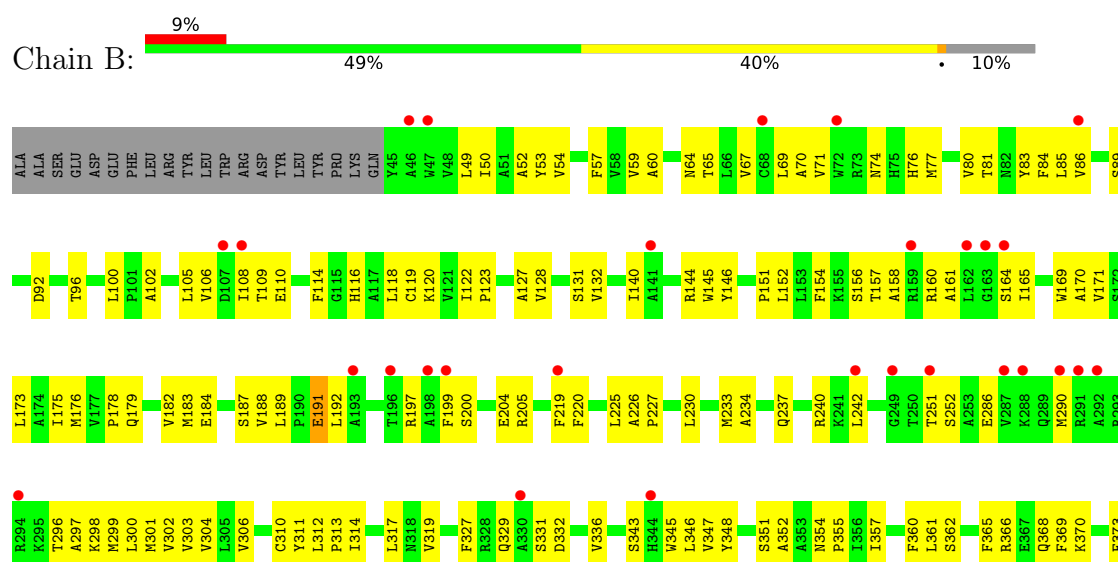
3 Residue-property plots

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



S374			
L377			
P378			
GLY			
LEU			
ALA			
ALA			
ALA			
HIS			
HIS			
HIS			
HIS			
HIS			
HIS			
HIS			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	60.37Å 147.07Å 72.54Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	44.71 – 2.65 44.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	58.3 (44.71-2.65) 78.2 (44.71-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.02 (at 1.75Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.240 , 0.269 0.270 , 0.299	Depositor DCC
R_{free} test set	4752 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	-8.1	Xtriage
Anisotropy	-0.566	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	5287	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.69% 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: NVN, SO4, SOG, 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	0.25	0/2509	0.48	0/3419
1	B	0.22	0/2460	0.43	0/3357
All	All	0.24	0/4969	0.46	0/6776

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	2440	0	2478	163	0
1	B	2393	0	2460	128	0
2	A	52	36	0	3	0
2	B	26	18	0	2	0
3	A	100	0	140	26	0
3	B	89	0	129	14	0
4	A	10	0	0	0	0
4	B	5	0	0	0	0
5	A	102	0	152	33	0
6	A	8	0	0	0	0
6	B	8	0	0	0	0
All	All	5233	54	5359	303	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 29.

All (303) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLU:HG3	1:B:205:ARG:HD3	1.35	1.07
1:A:38:ASP:HA	3:A:403:SOG:H62	1.37	1.03
1:A:214:ILE:HG12	3:A:405:SOG:H5	1.42	1.00
1:A:186:SER:HB2	1:A:201:VAL:HG22	1.42	0.99
1:A:152:LEU:HD11	1:A:155:LYS:HE2	1.43	0.97
1:A:138:SER:HB3	5:A:410:PGW:H15	1.47	0.97
1:A:75:HIS:HA	1:A:78:ARG:HE	1.34	0.93
1:B:297:ALA:HB1	1:B:301:MET:HE3	1.49	0.93
1:B:251:THR:OG1	1:B:286:GLU:HG2	1.71	0.89
1:B:83:TYR:HE2	1:B:158:ALA:HB1	1.36	0.89
1:A:29:ASP:HA	1:A:32:LEU:HD12	1.56	0.88
1:B:116:HIS:HB2	3:B:403:SOG:S1	2.17	0.85
1:A:80:VAL:HG13	1:A:161:ALA:HB2	1.56	0.84
1:B:377:LEU:HB3	1:B:378:PRO:HD3	1.60	0.84
1:A:333:ARG:HD3	1:A:337:TYR:OH	1.78	0.83
1:A:80:VAL:HG13	1:A:161:ALA:CB	2.12	0.80
3:A:406:SOG:H1	5:A:411:PGW:O04	1.81	0.79
1:A:325:GLY:O	1:A:328:ARG:NE	2.16	0.78
1:A:45:TYR:HD2	3:A:403:SOG:H7'1	1.50	0.77
5:A:410:PGW:H29A	5:A:411:PGW:C13	2.16	0.76
1:A:87:ASN:HA	1:A:90:LEU:HD12	1.66	0.76
1:B:114:PHE:HB3	1:B:118:LEU:HD12	1.68	0.76
1:B:197:ARG:HH21	3:B:403:SOG:H3	1.51	0.75
3:A:405:SOG:H7'1	3:A:405:SOG:H3'2	1.69	0.74
3:A:404:SOG:H1'1	1:B:164:SER:OG	1.86	0.74
1:A:150:HIS:HB3	1:A:153:LEU:CD1	2.18	0.74
1:A:131:SER:HB2	1:A:176:MET:HE2	1.70	0.74
5:A:411:PGW:C2	1:B:233:MET:HB3	2.18	0.73
1:A:100:LEU:HD12	1:A:348:TYR:CG	2.23	0.73
1:A:179:GLN:O	1:A:182:VAL:HG22	1.88	0.73
1:B:299:MET:SD	1:B:362:SER:HB2	2.28	0.73
1:B:300:LEU:O	1:B:304:VAL:HG23	1.88	0.73
1:A:64:ASN:HB3	1:A:89:SER:HB3	1.69	0.73
1:A:150:HIS:HB3	1:A:153:LEU:HD12	1.71	0.72
1:A:214:ILE:CG1	3:A:405:SOG:H5	2.17	0.72
1:B:65:THR:O	1:B:69:LEU:HG	1.89	0.72
2:A:402:NVN:O1	2:A:402:NVN:C7	2.39	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH2	3:B:403:SOG:H3	2.06	0.71
1:A:287:VAL:O	1:A:291:ARG:HG3	1.90	0.71
1:A:77:MET:HE1	1:A:368:GLN:HG3	1.70	0.71
5:A:410:PGW:H29A	5:A:411:PGW:H13	1.73	0.70
1:B:64:ASN:HB3	1:B:89:SER:HB3	1.74	0.70
1:B:205:ARG:O	3:B:405:SOG:O2	2.10	0.70
5:A:411:PGW:H2A	1:B:233:MET:HB3	1.74	0.69
1:B:184:GLU:HG3	1:B:205:ARG:CD	2.18	0.69
1:B:374:SER:HA	1:B:378:PRO:HD2	1.74	0.69
1:A:96:THR:O	1:A:101:PRO:HD3	1.93	0.69
1:A:94:LEU:HD11	1:A:125:LEU:HB3	1.75	0.68
1:B:59:VAL:HG12	1:B:352:ALA:HB1	1.76	0.68
1:A:103:SER:OG	1:A:348:TYR:OH	2.07	0.68
1:A:186:SER:HB2	1:A:201:VAL:CG2	2.22	0.68
1:A:74:ASN:ND2	1:A:77:MET:HE2	2.09	0.68
1:A:142:LEU:HD22	1:B:171:VAL:HG22	1.76	0.67
1:A:242:LEU:O	1:A:290:MET:HE2	1.95	0.66
1:A:38:ASP:CA	3:A:403:SOG:H62	2.22	0.66
1:B:377:LEU:HB3	1:B:378:PRO:CD	2.26	0.65
1:B:83:TYR:CE2	1:B:158:ALA:HB1	2.24	0.65
1:A:152:LEU:CD1	1:A:155:LYS:HG2	2.26	0.65
1:A:131:SER:HB2	1:A:176:MET:CE	2.27	0.65
1:A:234:ALA:HB2	5:A:410:PGW:H24A	1.79	0.65
1:A:94:LEU:HD11	1:A:125:LEU:HD13	1.79	0.65
1:A:142:LEU:CD2	1:B:171:VAL:HG22	2.27	0.64
1:A:57:PHE:O	1:A:61:LEU:HG	1.97	0.64
1:A:96:THR:O	1:A:100:LEU:HB3	1.97	0.64
1:A:205:ARG:O	3:A:406:SOG:O3	2.15	0.64
1:A:251:THR:HB	1:A:286:GLU:HG2	1.80	0.64
1:A:45:TYR:CD2	3:A:403:SOG:H7'1	2.33	0.63
5:A:411:PGW:H03A	1:B:237:GLN:HE21	1.63	0.63
1:B:242:LEU:O	1:B:290:MET:HE2	1.99	0.62
1:A:36:TRP:HA	1:A:40:LEU:HB2	1.79	0.62
1:A:251:THR:HG22	1:A:253:ALA:H	1.63	0.62
1:A:313:PRO:HG2	1:A:346:LEU:HD12	1.80	0.62
1:A:226:ALA:HB3	1:A:227:PRO:HD3	1.80	0.62
1:A:57:PHE:CD1	1:A:100:LEU:HD22	2.35	0.62
1:A:114:PHE:HB3	1:A:118:LEU:HD12	1.82	0.62
1:B:299:MET:O	1:B:303:VAL:HG23	1.99	0.61
1:A:41:TYR:HE2	3:A:403:SOG:H2'2	1.63	0.61
5:A:411:PGW:H2	1:B:233:MET:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:VAL:HG22	1:A:172:SER:O	2.01	0.61
1:A:128:VAL:HG21	1:A:173:LEU:HD23	1.83	0.61
1:A:332:ASP:HB2	1:A:335:ALA:HB3	1.82	0.61
1:A:175:ILE:O	1:A:178:PRO:HD2	2.01	0.61
5:A:410:PGW:H4	3:B:405:SOG:H5	1.83	0.61
1:A:29:ASP:HA	1:A:32:LEU:CD1	2.31	0.60
1:A:363:GLY:HA2	1:A:366:ARG:NH1	2.17	0.60
1:A:46:ALA:CB	3:A:403:SOG:H8'1	2.32	0.60
1:A:57:PHE:HD1	1:A:100:LEU:HD22	1.64	0.60
1:A:176:MET:O	1:A:179:GLN:HB3	2.03	0.59
5:A:411:PGW:HADA	1:B:240:ARG:HD3	1.85	0.59
1:B:127:ALA:HA	2:B:401:NVN:C13	2.33	0.59
1:B:314:ILE:HB	1:B:343:SER:HB3	1.84	0.59
3:A:404:SOG:C8'	1:B:156:SER:HB3	2.32	0.59
5:A:410:PGW:H13	1:B:219:PHE:CE2	2.38	0.58
1:B:116:HIS:CE1	3:B:403:SOG:H61	2.39	0.58
1:A:234:ALA:HB2	5:A:410:PGW:C24	2.33	0.58
1:A:39:TYR:C	1:A:42:PRO:HD2	2.29	0.58
1:B:119:CYS:O	1:B:123:PRO:HG2	2.04	0.58
1:B:297:ALA:O	1:B:301:MET:HG3	2.04	0.57
1:A:175:ILE:HG22	1:B:230:LEU:HD22	1.85	0.57
1:A:120:LYS:NZ	1:A:183:MET:O	2.37	0.57
1:B:100:LEU:HD12	1:B:348:TYR:HB3	1.86	0.57
1:B:50:ILE:O	1:B:54:VAL:HG23	2.05	0.57
1:B:175:ILE:O	1:B:178:PRO:HD2	2.04	0.57
5:A:410:PGW:H3	3:B:405:SOG:H1'2	1.87	0.57
1:B:114:PHE:HB3	1:B:118:LEU:CD1	2.34	0.57
1:B:74:ASN:HB3	1:B:77:MET:HB2	1.86	0.57
1:B:92:ASP:HB3	1:B:351:SER:HB3	1.85	0.57
1:B:332:ASP:O	1:B:336:VAL:HG23	2.05	0.56
5:A:410:PGW:OAE	3:B:404:SOG:H8'3	2.04	0.56
1:A:213:LYS:O	1:A:217:SER:OG	2.24	0.56
1:B:184:GLU:CG	1:B:205:ARG:HD3	2.25	0.56
5:A:410:PGW:H28	5:A:411:PGW:H14	1.88	0.56
1:B:131:SER:HB2	1:B:176:MET:CE	2.35	0.56
1:A:77:MET:HE1	1:A:368:GLN:CG	2.36	0.56
1:B:374:SER:O	1:B:378:PRO:HD2	2.06	0.55
1:A:145:TRP:O	1:A:149:CYS:HB2	2.06	0.55
1:A:313:PRO:HG2	1:A:346:LEU:CD1	2.36	0.55
1:A:122:ILE:HB	1:A:123:PRO:HD3	1.88	0.55
1:A:324:PHE:HD2	3:A:407:SOG:H2'2	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:LEU:CB	1:B:378:PRO:HD3	2.35	0.55
1:A:143:ASP:OD1	1:A:156:SER:OG	2.15	0.55
1:A:219:PHE:CD2	5:A:411:PGW:H29B	2.42	0.54
1:A:300:LEU:O	1:A:304:VAL:HG23	2.08	0.54
1:B:226:ALA:HB3	1:B:227:PRO:HD3	1.89	0.54
1:B:59:VAL:CG1	1:B:352:ALA:HB1	2.36	0.54
1:B:74:ASN:OD1	1:B:76:HIS:HB2	2.08	0.54
1:A:50:ILE:O	1:A:54:VAL:HG23	2.07	0.54
1:B:184:GLU:OE2	3:B:405:SOG:H4'1	2.08	0.54
1:B:219:PHE:HB3	2:B:401:NVN:C18	2.37	0.53
1:A:152:LEU:HD11	1:A:155:LYS:HG2	1.89	0.53
1:B:105:LEU:O	1:B:109:THR:HG23	2.09	0.53
1:A:46:ALA:HB2	3:A:403:SOG:H8'1	1.90	0.53
1:B:116:HIS:O	1:B:119:CYS:HB3	2.09	0.53
1:B:297:ALA:HB1	1:B:301:MET:CE	2.29	0.53
1:A:333:ARG:HD3	1:A:337:TYR:CZ	2.42	0.53
1:A:42:PRO:HG3	3:A:403:SOG:S1	2.49	0.53
1:A:75:HIS:HA	1:A:78:ARG:NE	2.15	0.53
1:B:312:LEU:HB3	1:B:313:PRO:HD3	1.89	0.53
1:B:179:GLN:O	1:B:182:VAL:HG22	2.09	0.52
1:B:317:LEU:HD12	1:B:343:SER:OG	2.10	0.52
1:A:358:TYR:O	1:A:362:SER:HB3	2.09	0.52
5:A:410:PGW:H03A	5:A:410:PGW:H2A	1.91	0.52
1:A:152:LEU:HD11	1:A:155:LYS:CE	2.28	0.52
1:A:312:LEU:HB3	1:A:313:PRO:HD3	1.90	0.52
1:B:357:ILE:HG23	1:B:361:LEU:HD12	1.91	0.52
1:A:98:ILE:HG21	1:A:125:LEU:HD12	1.91	0.52
1:A:169:TRP:O	1:A:173:LEU:HG	2.09	0.52
1:A:84:PHE:HB3	1:A:140:ILE:HD11	1.90	0.52
1:A:94:LEU:CD1	1:A:125:LEU:HD13	2.39	0.52
1:B:70:ALA:HB1	1:B:368:GLN:HG3	1.91	0.51
1:A:132:VAL:HG23	1:A:172:SER:CB	2.40	0.51
1:A:84:PHE:O	1:A:136:THR:HG21	2.10	0.51
1:A:324:PHE:CE2	3:A:407:SOG:H61	2.45	0.51
1:B:161:ALA:O	1:B:165:ILE:HG13	2.11	0.51
1:A:218:CYS:SG	1:B:225:LEU:HD23	2.50	0.51
1:A:74:ASN:HD22	1:A:77:MET:HE2	1.76	0.51
1:B:80:VAL:HG21	1:B:156:SER:OG	2.11	0.51
1:B:329:GLN:HG3	1:B:331:SER:H	1.76	0.51
1:A:132:VAL:HA	1:A:168:ILE:CG2	2.41	0.50
1:B:50:ILE:HG12	1:B:108:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD21	1:B:199:PHE:CD2	2.46	0.50
1:B:187:SER:HA	1:B:200:SER:HA	1.93	0.50
1:A:219:PHE:CE2	5:A:411:PGW:H30	2.47	0.50
1:A:127:ALA:C	1:A:176:MET:HG3	2.36	0.50
1:A:236:PHE:CZ	1:A:240:ARG:HD2	2.47	0.50
1:B:96:THR:O	1:B:100:LEU:HB3	2.12	0.50
1:A:173:LEU:O	1:A:177:VAL:HG23	2.10	0.50
1:A:233:MET:HB3	5:A:410:PGW:H20	1.93	0.50
1:B:84:PHE:HB3	1:B:140:ILE:HD11	1.94	0.50
1:A:52:ALA:HB1	1:A:345:TRP:NE1	2.27	0.50
1:A:146:TYR:CE2	1:B:170:ALA:HB1	2.47	0.50
5:A:410:PGW:C4	3:B:405:SOG:H5	2.42	0.50
1:B:296:THR:O	1:B:300:LEU:HG	2.12	0.50
1:A:333:ARG:HD3	1:A:337:TYR:HH	1.74	0.49
1:B:169:TRP:O	1:B:173:LEU:HG	2.11	0.49
1:A:364:LYS:O	1:A:368:GLN:HG2	2.12	0.49
1:B:140:ILE:O	1:B:144:ARG:HG2	2.12	0.49
1:B:102:ALA:O	1:B:106:VAL:HG23	2.13	0.49
1:B:252:SER:HB3	3:B:406:SOG:H1	1.95	0.49
1:B:49:LEU:HD11	1:B:53:TYR:HE2	1.77	0.49
1:B:302:VAL:O	1:B:306:VAL:HG23	2.13	0.49
1:A:150:HIS:CB	1:A:153:LEU:HD12	2.42	0.49
1:A:77:MET:O	1:A:82:ASN:ND2	2.42	0.48
1:B:120:LYS:HG2	1:B:183:MET:HB2	1.95	0.48
1:B:131:SER:HB2	1:B:176:MET:HE3	1.95	0.48
1:A:120:LYS:HE3	1:A:180:ALA:O	2.14	0.48
1:A:44:GLN:O	1:A:48:VAL:HG23	2.14	0.48
3:A:405:SOG:H7'1	3:A:405:SOG:C3'	2.40	0.48
1:B:298:LYS:HE2	1:B:361:LEU:HD22	1.95	0.48
3:A:404:SOG:H6'1	1:B:154:PHE:HB3	1.96	0.47
1:B:370:LYS:HA	1:B:373:PHE:CD2	2.49	0.47
1:A:110:GLU:OE1	1:A:337:TYR:CZ	2.67	0.47
1:B:100:LEU:HD12	1:B:348:TYR:CB	2.44	0.47
1:A:214:ILE:HA	3:A:405:SOG:H3	1.97	0.47
1:B:100:LEU:C	1:B:100:LEU:HD23	2.40	0.47
1:B:122:ILE:HB	1:B:123:PRO:HD3	1.97	0.47
1:A:114:PHE:HB3	1:A:118:LEU:CD1	2.44	0.47
1:A:152:LEU:CD1	1:A:155:LYS:HE2	2.30	0.47
1:A:311:TYR:O	1:A:315:SER:OG	2.29	0.47
1:A:206:TRP:CZ3	5:A:411:PGW:H22	2.50	0.47
1:A:333:ARG:HG2	1:A:337:TYR:CZ	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:404:SOG:H8'2	1:B:156:SER:HB3	1.96	0.47
1:B:57:PHE:CD1	1:B:100:LEU:HD22	2.50	0.47
1:B:370:LYS:HA	1:B:373:PHE:HD2	1.78	0.47
5:A:410:PGW:H20A	1:B:178:PRO:HG3	1.98	0.46
1:A:41:TYR:HB3	1:A:42:PRO:HD3	1.97	0.46
1:A:140:ILE:O	1:A:144:ARG:HG2	2.16	0.46
1:A:174:ALA:O	1:A:177:VAL:HB	2.16	0.46
1:A:39:TYR:CE1	1:A:43:LYS:HD2	2.51	0.46
1:A:152:LEU:HD12	1:A:155:LYS:HG2	1.97	0.46
1:A:233:MET:CB	5:A:410:PGW:H20	2.46	0.46
5:A:410:PGW:C29	5:A:411:PGW:H13	2.44	0.46
1:A:59:VAL:O	1:A:63:GLY:N	2.39	0.46
1:A:151:PRO:C	1:A:153:LEU:H	2.23	0.46
1:A:199:PHE:CD1	1:A:199:PHE:C	2.94	0.46
1:A:332:ASP:O	1:A:336:VAL:HG23	2.16	0.46
1:B:151:PRO:C	1:B:152:LEU:HD12	2.41	0.46
1:B:191:GLU:H	1:B:191:GLU:CD	2.16	0.45
1:A:80:VAL:HG13	1:A:161:ALA:HB1	1.97	0.45
1:A:106:VAL:O	1:A:110:GLU:N	2.47	0.45
1:A:183:MET:HE1	2:A:401:NVN:C1	2.46	0.45
1:A:235:TYR:HA	1:A:238:ILE:HD12	1.97	0.45
1:A:366:ARG:HG2	1:A:370:LYS:HE3	1.98	0.45
1:B:360:PHE:O	1:B:366:ARG:NH2	2.49	0.45
1:A:74:ASN:CB	1:A:77:MET:HE2	2.46	0.45
1:B:377:LEU:CB	1:B:378:PRO:CD	2.95	0.45
1:A:87:ASN:CG	1:A:165:ILE:HG23	2.42	0.45
1:A:219:PHE:CG	5:A:411:PGW:H29B	2.52	0.45
3:A:406:SOG:H5'2	5:A:411:PGW:H04A	1.99	0.45
1:A:63:GLY:O	1:A:67:VAL:HG23	2.16	0.44
1:A:368:GLN:OE1	1:A:368:GLN:HA	2.17	0.44
1:A:138:SER:OG	1:A:231:MET:HE2	2.17	0.44
1:A:199:PHE:CD1	1:A:199:PHE:O	2.70	0.44
1:A:218:CYS:CB	5:A:411:PGW:H28	2.47	0.44
1:B:71:VAL:HG21	1:B:86:VAL:HG23	1.99	0.44
1:A:206:TRP:CH2	5:A:411:PGW:H22	2.52	0.44
1:A:222:VAL:HG12	1:A:223:THR:CG2	2.47	0.44
1:A:31:PHE:CD2	1:A:31:PHE:C	2.96	0.44
1:B:132:VAL:HG11	1:B:169:TRP:CZ2	2.52	0.44
1:B:116:HIS:CE1	3:B:403:SOG:C6	3.01	0.43
1:B:145:TRP:HZ3	1:B:146:TYR:CZ	2.36	0.43
1:B:188:VAL:HG23	1:B:189:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:ALA:O	1:B:64:ASN:ND2	2.44	0.43
1:A:353:ALA:O	1:A:357:ILE:HG13	2.18	0.43
1:A:214:ILE:HG12	3:A:405:SOG:C5	2.31	0.43
1:B:184:GLU:HB2	1:B:205:ARG:HB2	2.01	0.43
1:B:311:TYR:CZ	1:B:347:VAL:HG13	2.54	0.43
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.46	0.43
1:B:310:CYS:O	1:B:313:PRO:HD2	2.18	0.43
1:B:313:PRO:HG2	1:B:346:LEU:HD12	1.99	0.43
1:A:213:LYS:HD3	3:A:405:SOG:H2'1	2.01	0.43
1:B:171:VAL:O	1:B:175:ILE:HG12	2.17	0.43
1:B:365:PHE:HB3	1:B:369:PHE:CE2	2.53	0.43
1:B:242:LEU:C	1:B:290:MET:HE2	2.44	0.43
1:A:84:PHE:HB2	1:A:140:ILE:HG12	2.00	0.43
1:A:116:HIS:O	1:A:119:CYS:HB3	2.19	0.43
1:A:161:ALA:O	1:A:165:ILE:HG13	2.19	0.43
1:B:144:ARG:HA	1:B:144:ARG:NE	2.34	0.43
1:A:74:ASN:CG	1:A:77:MET:HE2	2.44	0.42
1:A:132:VAL:HG22	1:A:168:ILE:HG22	2.01	0.42
1:A:206:TRP:CD1	1:A:212:PRO:HB3	2.54	0.42
1:B:298:LYS:HE2	1:B:361:LEU:CD2	2.49	0.42
1:A:112:TRP:CZ2	1:A:119:CYS:HA	2.54	0.42
1:A:299:MET:HG3	1:A:361:LEU:HB2	2.02	0.42
1:B:354:ASN:HB2	1:B:355:PRO:HD3	2.01	0.42
1:B:182:VAL:HG23	1:B:204:GLU:HG2	2.01	0.42
1:B:327:PHE:HB3	1:B:336:VAL:HG11	2.01	0.42
1:B:67:VAL:HG13	1:B:365:PHE:CE1	2.54	0.42
1:B:157:THR:OG1	1:B:160:ARG:NH1	2.48	0.42
1:A:251:THR:HG22	1:A:252:SER:N	2.34	0.42
5:A:410:PGW:C1	5:A:410:PGW:H5A	2.49	0.42
1:B:83:TYR:HE2	1:B:158:ALA:CB	2.19	0.42
1:A:359:ASN:HB2	1:A:369:PHE:CD2	2.55	0.42
5:A:411:PGW:H7A	1:B:234:ALA:HB2	2.00	0.42
1:B:52:ALA:HB1	1:B:345:TRP:NE1	2.34	0.42
1:B:303:VAL:CG2	1:B:357:ILE:HG21	2.50	0.42
1:B:188:VAL:HG23	1:B:189:LEU:H	1.85	0.42
1:A:84:PHE:CB	1:A:140:ILE:CG1	2.98	0.41
1:A:211:ALA:N	1:A:212:PRO:HD2	2.34	0.41
1:A:46:ALA:HB2	3:A:403:SOG:C8'	2.49	0.41
1:B:81:THR:O	1:B:85:LEU:HG	2.19	0.41
1:A:36:TRP:O	1:A:41:TYR:N	2.27	0.41
1:A:302:VAL:O	1:A:306:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ASN:HB3	1:A:77:MET:CE	2.50	0.41
1:A:354:ASN:HA	1:A:357:ILE:HD12	2.02	0.41
1:B:131:SER:HB2	1:B:176:MET:HE2	2.01	0.41
1:A:57:PHE:CZ	1:A:61:LEU:HD11	2.54	0.41
5:A:410:PGW:H8A	5:A:410:PGW:H06A	1.79	0.41
1:B:197:ARG:HH21	3:B:403:SOG:C3	2.28	0.41
1:A:222:VAL:HG12	1:A:223:THR:HG22	2.03	0.41
1:B:374:SER:CA	1:B:378:PRO:HD2	2.47	0.41
1:A:84:PHE:HB3	1:A:140:ILE:CG1	2.51	0.41
1:A:131:SER:O	1:A:135:LEU:HB2	2.21	0.41
1:B:220:PHE:CG	1:B:319:VAL:HG21	2.56	0.41
5:A:410:PGW:H12A	5:A:410:PGW:H08	1.90	0.40
1:B:116:HIS:ND1	3:B:403:SOG:H61	2.36	0.40
1:B:345:TRP:CZ3	1:B:346:LEU:HD23	2.56	0.40
1:A:69:LEU:O	1:A:73:ARG:HB2	2.22	0.40
3:A:404:SOG:H1'1	1:B:164:SER:HG	1.83	0.40
1:A:74:ASN:HD22	1:A:368:GLN:NE2	2.19	0.40
1:A:112:TRP:HZ3	2:A:401:NVN:F2	1.95	0.40
1:A:317:LEU:HD12	1:A:343:SER:OG	2.22	0.40
1:B:109:THR:O	1:B:110:GLU:HB2	2.22	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	298/336 (89%)	288 (97%)	9 (3%)	1 (0%)	36	52
1	B	300/336 (89%)	288 (96%)	11 (4%)	1 (0%)	36	52
All	All	598/672 (89%)	576 (96%)	20 (3%)	2 (0%)	36	52

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	LEU
1	B	377	LEU

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	256/279 (92%)	255 (100%)	1 (0%)	84	93
1	B	251/279 (90%)	249 (99%)	2 (1%)	73	85
All	All	507/558 (91%)	504 (99%)	3 (1%)	78	88

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	B	128	VAL
1	B	191	GLU

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	74	ASN
1	A	318	ASN
1	A	350	ASN
1	A	368	GLN
1	B	150	HIS

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	$\# Z > 2$
2	NVN	B	401	-	28,28,28	0.49	0	37,40,40	1.59	2 (5%)
5	PGW	A	411	-	50,50,50	0.29	0	53,56,56	0.38	0
4	SO4	A	409	-	4,4,4	0.23	0	6,6,6	0.34	0
3	SOG	A	407	-	20,20,20	0.20	0	24,25,25	0.36	0
3	SOG	B	404	-	8,8,20	0.31	0	7,7,25	0.48	0
4	SO4	A	408	-	4,4,4	0.23	0	6,6,6	0.17	0
4	SO4	B	407	-	4,4,4	0.25	0	6,6,6	0.28	0
5	PGW	A	410	-	50,50,50	0.27	0	53,56,56	0.51	0
2	NVN	A	402	-	28,28,28	0.51	0	37,40,40	1.89	6 (16%)
3	SOG	A	403	-	20,20,20	0.28	0	24,25,25	0.45	0
2	NVN	A	401	-	28,28,28	0.45	0	37,40,40	1.55	2 (5%)
3	SOG	B	402	-	20,20,20	0.34	0	24,25,25	0.36	0
3	SOG	B	405	-	20,20,20	0.21	0	24,25,25	0.35	0
3	SOG	B	406	-	20,20,20	0.30	0	24,25,25	0.63	1 (4%)
3	SOG	A	406	-	20,20,20	0.20	0	24,25,25	0.60	1 (4%)
3	SOG	A	405	-	20,20,20	0.31	0	24,25,25	0.42	0
3	SOG	B	403	-	20,20,20	0.20	0	24,25,25	0.36	0
3	SOG	A	404	-	20,20,20	0.28	0	24,25,25	0.49	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
2	NVN	B	401	-	-	0/12/12/12	0/3/3/3
5	PGW	A	411	-	-	19/55/55/55	-
3	SOG	A	407	-	-	3/11/31/31	0/1/1/1
3	SOG	B	404	-	-	0/6/6/31	-
5	PGW	A	410	-	-	14/55/55/55	-
2	NVN	A	402	-	-	2/12/12/12	0/3/3/3
3	SOG	A	403	-	-	3/11/31/31	0/1/1/1
2	NVN	A	401	-	-	0/12/12/12	0/3/3/3
3	SOG	B	402	-	-	4/11/31/31	0/1/1/1
3	SOG	B	405	-	-	1/11/31/31	0/1/1/1
3	SOG	B	406	-	-	0/11/31/31	0/1/1/1
3	SOG	A	406	-	-	4/11/31/31	0/1/1/1
3	SOG	A	405	-	-	1/11/31/31	0/1/1/1
3	SOG	B	403	-	-	2/11/31/31	0/1/1/1
3	SOG	A	404	-	-	3/11/31/31	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	402	NVN	F2-C4-C3	8.00	120.69	117.37
2	A	401	NVN	F2-C4-C3	7.78	120.60	117.37
2	B	401	NVN	F2-C4-C3	7.59	120.52	117.37
2	B	401	NVN	C4-C5-C6	4.53	120.44	116.66
2	A	402	NVN	C4-C5-C6	4.37	120.30	116.66
2	A	401	NVN	C4-C5-C6	4.36	120.29	116.66
2	A	402	NVN	C9-N2-C11	3.06	133.27	125.58
2	A	402	NVN	C8-C9-N2	2.64	122.75	118.35
2	A	402	NVN	C12-N3-C11	2.44	131.59	126.61
3	A	404	SOG	C2'-C1'-S1	2.16	119.64	112.36
3	A	406	SOG	C2'-C1'-S1	-2.10	105.29	112.36
3	B	406	SOG	C2'-C1'-S1	-2.04	105.49	112.36
2	A	402	NVN	C13-C12-N3	2.00	127.13	120.41

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	402	NVN	C10-C9-N2-C11
2	A	402	NVN	C8-C9-N2-C11
3	A	403	SOG	O5-C1-S1-C1'
3	A	403	SOG	C2'-C1'-S1-C1
3	A	406	SOG	O5-C1-S1-C1'
3	A	407	SOG	O5-C1-S1-C1'
3	B	403	SOG	C2-C1-S1-C1'
5	A	410	PGW	C2-C1-O01-C02
5	A	411	PGW	C03-O11-P-O12
5	A	411	PGW	C03-O11-P-O13
5	A	411	PGW	O12-C04-C05-CAD
5	A	410	PGW	O02-C1-O01-C02
5	A	411	PGW	O12-C04-C05-OAF
3	A	406	SOG	O5-C5-C6-O6
3	A	406	SOG	C4-C5-C6-O6
5	A	411	PGW	C05-C04-O12-P
5	A	410	PGW	C19-C20-C21-C22
3	A	406	SOG	S1-C1'-C2'-C3'
3	B	402	SOG	C1'-C2'-C3'-C4'
5	A	410	PGW	C24-C25-C26-C27
5	A	410	PGW	C16-C15-C27-C26
5	A	411	PGW	C24-C25-C26-C27
5	A	410	PGW	C17-C18-C28-C30
3	B	405	SOG	O5-C5-C6-O6
5	A	410	PGW	C25-C26-C27-C15
3	A	404	SOG	O5-C5-C6-O6
3	A	407	SOG	C3'-C4'-C5'-C6'
3	B	403	SOG	O5-C5-C6-O6
3	A	403	SOG	O5-C5-C6-O6
3	A	405	SOG	O5-C5-C6-O6
5	A	411	PGW	C20-C19-O03-C01
5	A	411	PGW	C4-C5-C6-C7
5	A	411	PGW	C25-C26-C27-C15
5	A	410	PGW	C5-C6-C7-C8
5	A	410	PGW	C20-C21-C22-C23
5	A	411	PGW	C11-C12-C13-C14
5	A	410	PGW	O12-C04-C05-CAD
3	A	404	SOG	C4'-C5'-C6'-C7'
5	A	410	PGW	C2-C3-C4-C5
5	A	411	PGW	C27-C15-C16-C17
3	A	404	SOG	C3'-C4'-C5'-C6'
5	A	411	PGW	O04-C19-O03-C01
3	B	402	SOG	C2'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
5	A	411	PGW	C02-C03-O11-P
3	B	402	SOG	C4-C5-C6-O6
5	A	411	PGW	C17-C18-C28-C30
5	A	411	PGW	C21-C22-C23-C24
5	A	411	PGW	C07-C06-C10-C9
3	A	407	SOG	C2'-C3'-C4'-C5'
5	A	411	PGW	C23-C24-C25-C26
5	A	411	PGW	C7-C8-C9-C10
5	A	410	PGW	C03-C02-O01-C1
5	A	410	PGW	O12-C04-C05-OAF
3	B	402	SOG	O5-C5-C6-O6
5	A	411	PGW	C15-C16-C17-C18
5	A	410	PGW	C07-C08-C09-C11

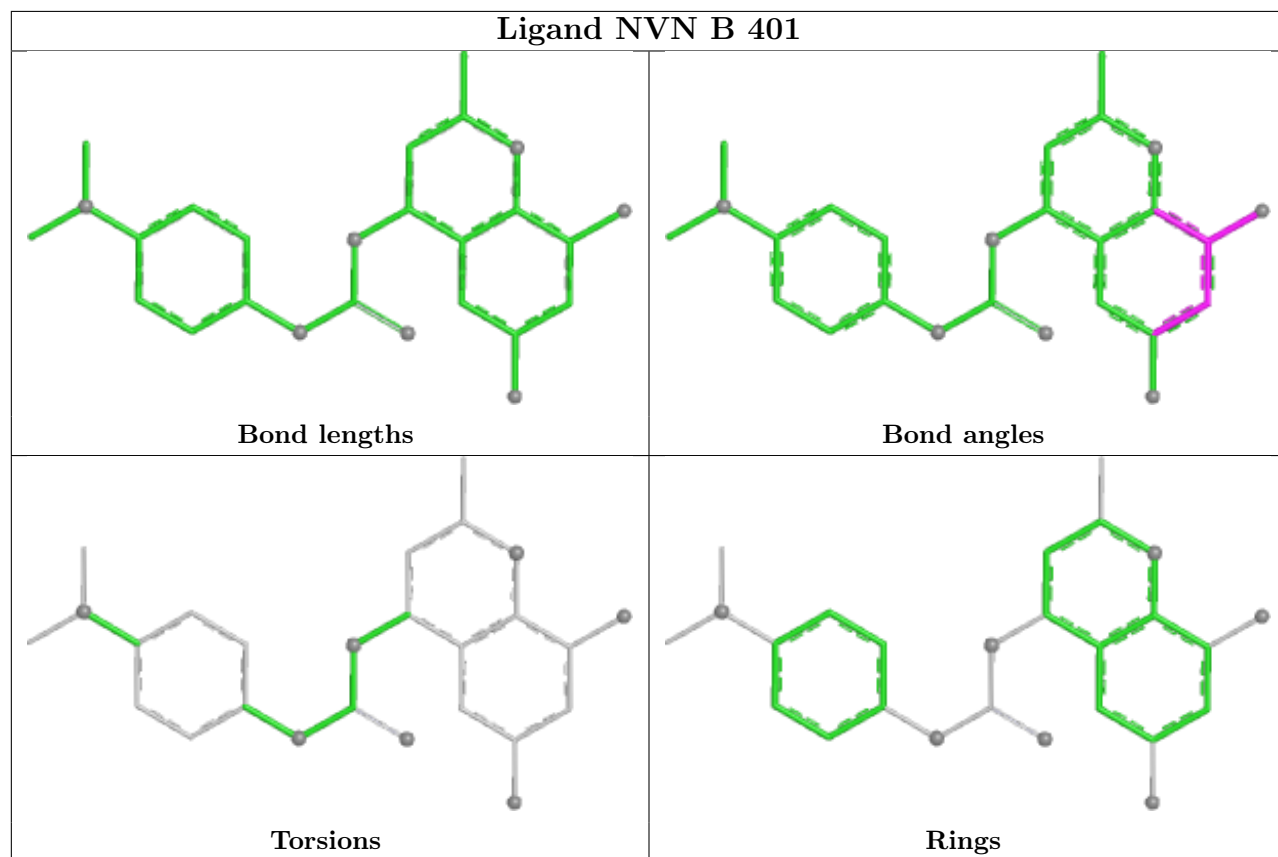
There are no ring outliers.

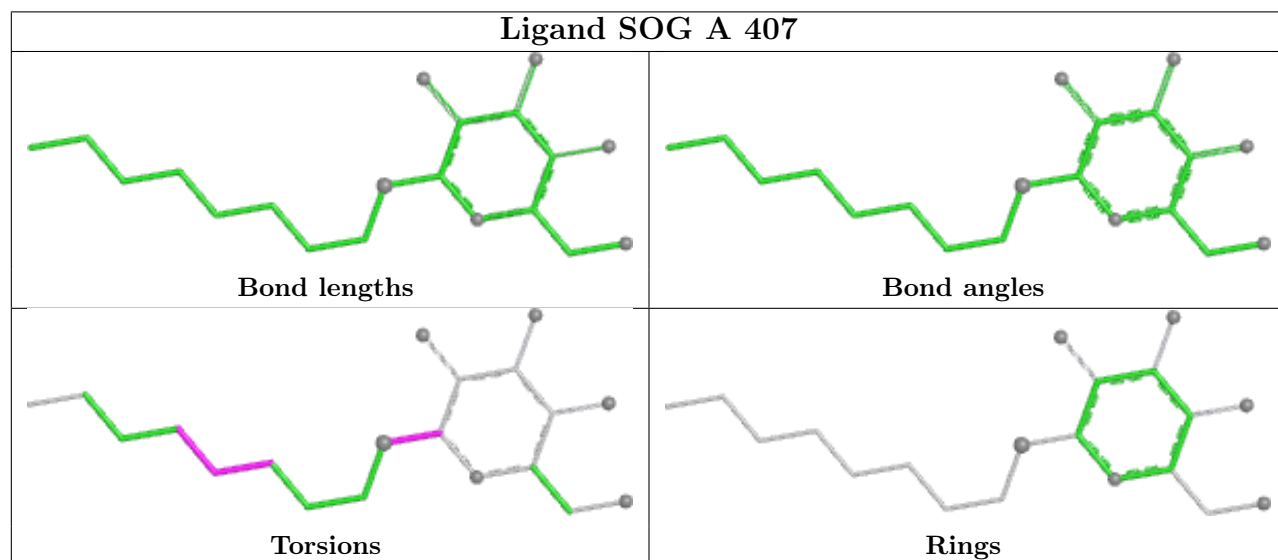
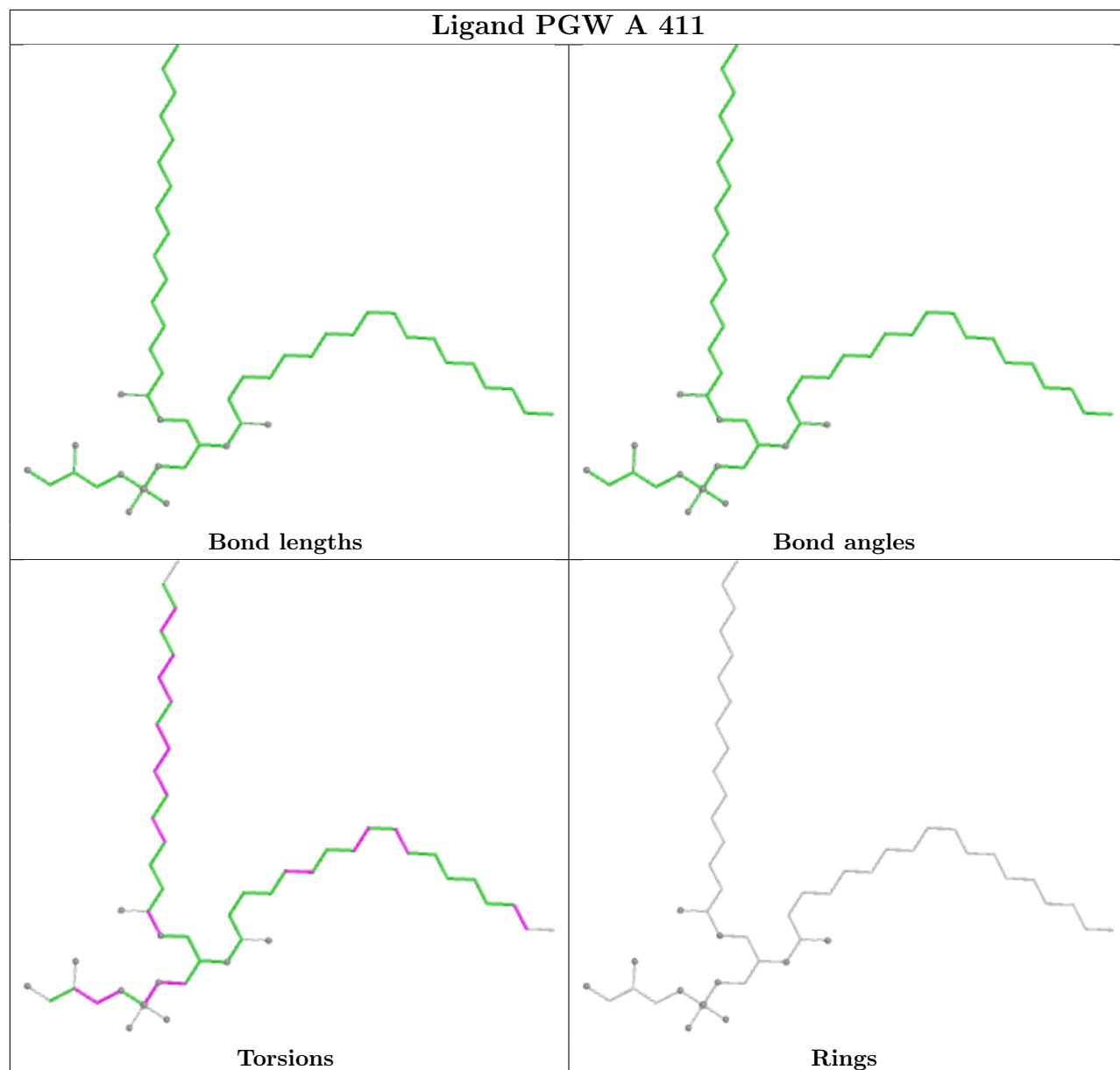
14 monomers are involved in 72 short contacts:

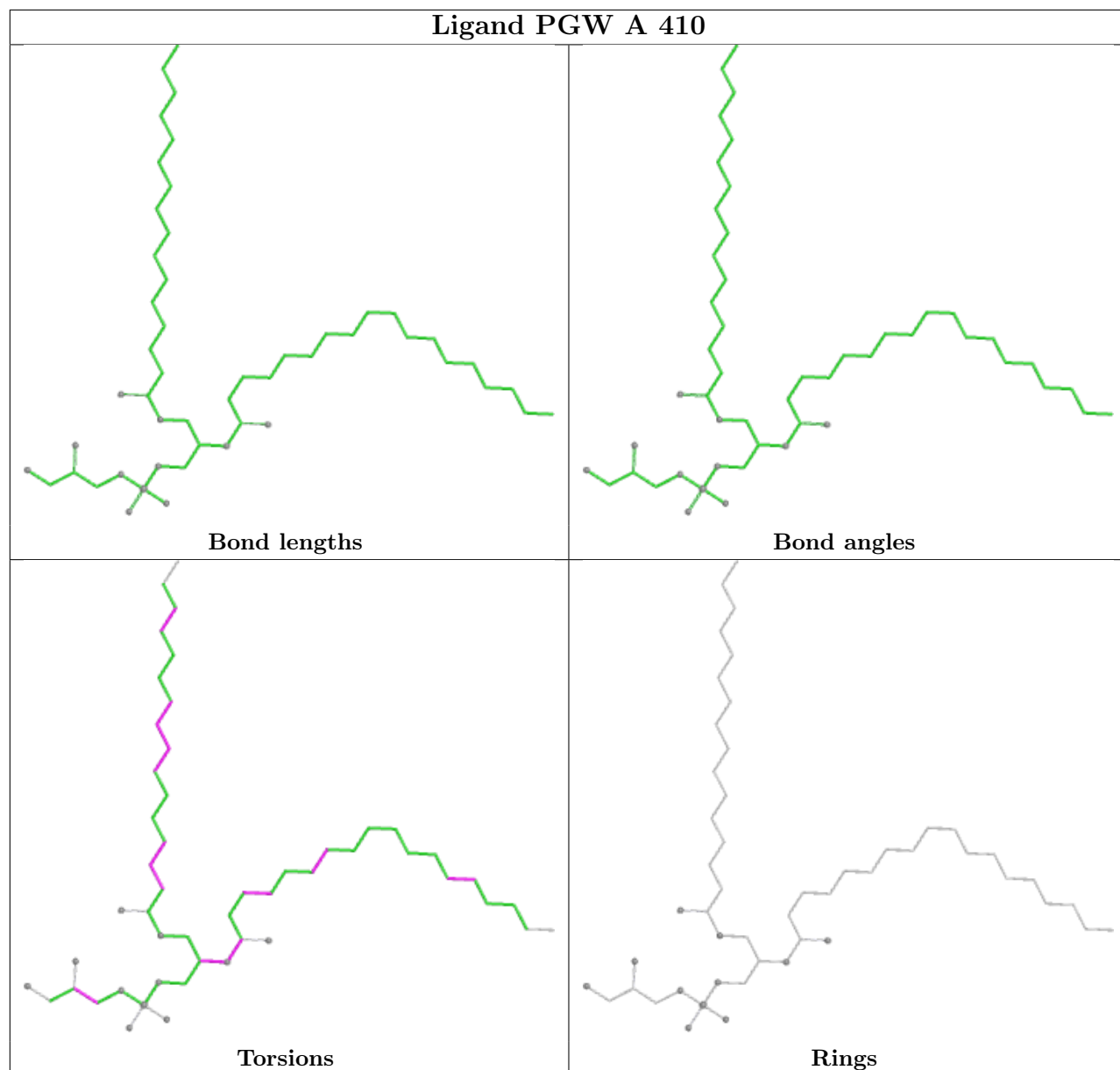
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	NVN	2	0
5	A	411	PGW	18	0
3	A	407	SOG	2	0
3	B	404	SOG	1	0
5	A	410	PGW	19	0
2	A	402	NVN	1	0
3	A	403	SOG	9	0
2	A	401	NVN	2	0
3	B	405	SOG	5	0
3	B	406	SOG	1	0
3	A	406	SOG	3	0
3	A	405	SOG	7	0
3	B	403	SOG	7	0
3	A	404	SOG	5	0

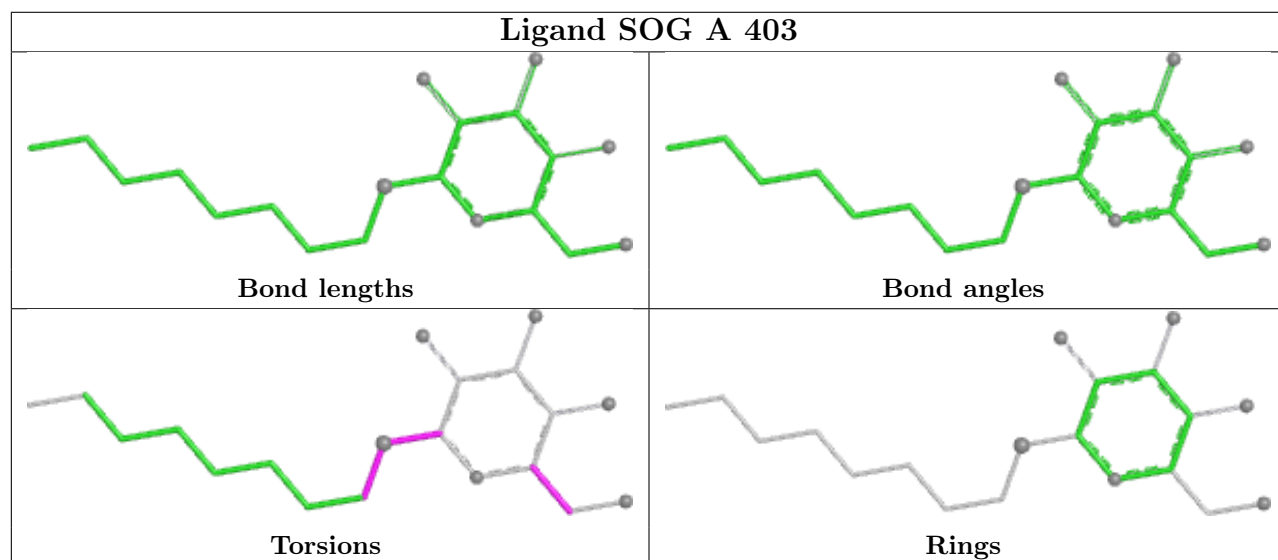
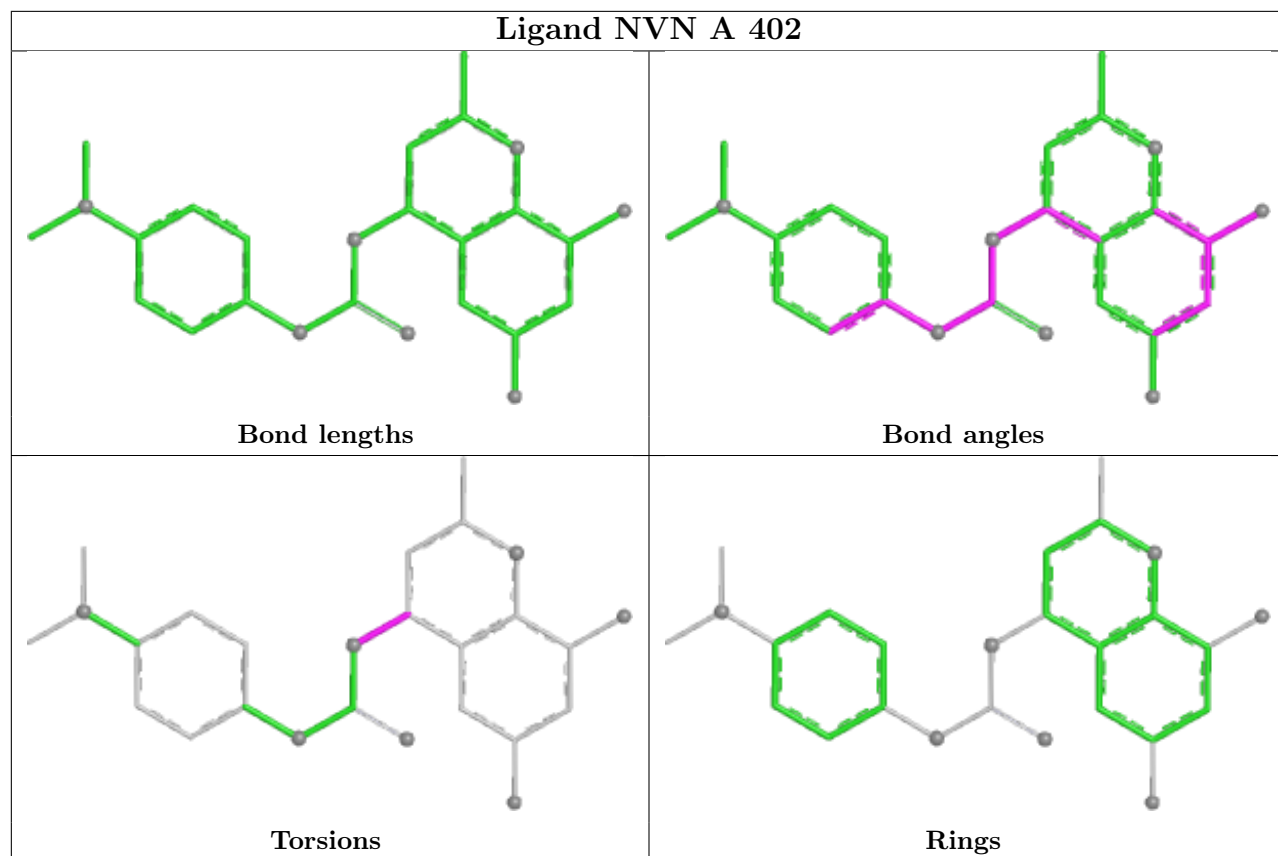
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

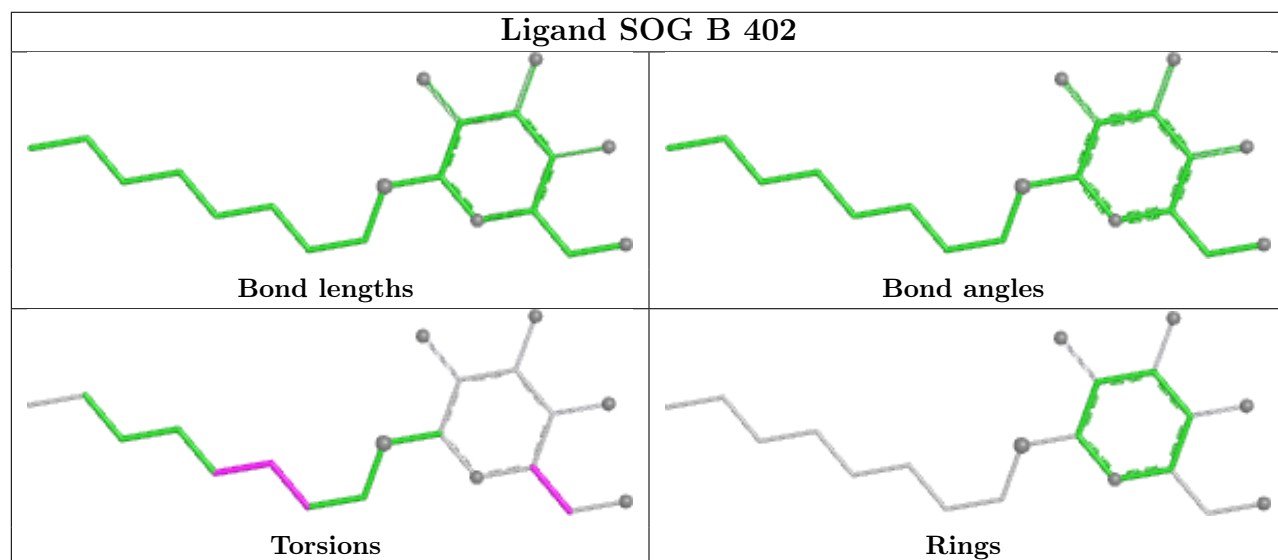
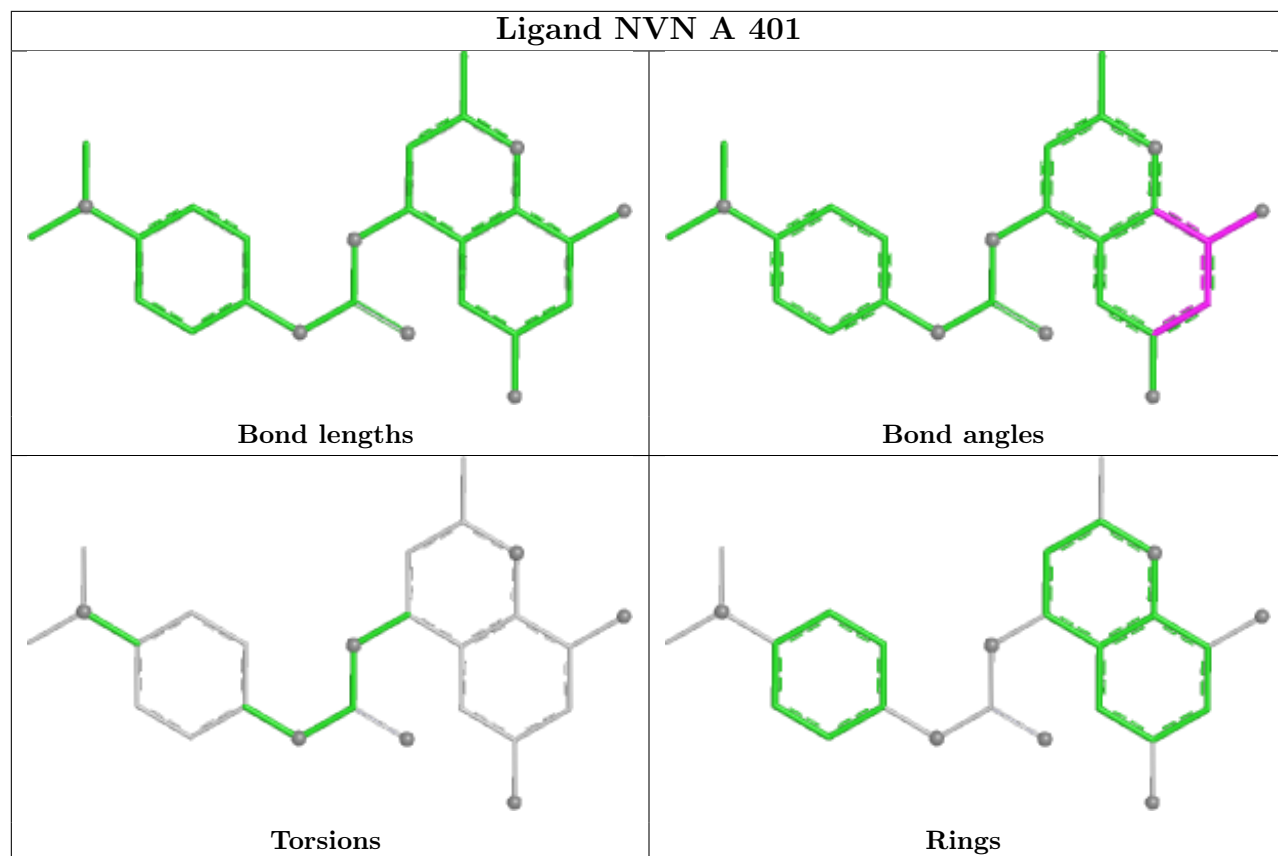
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

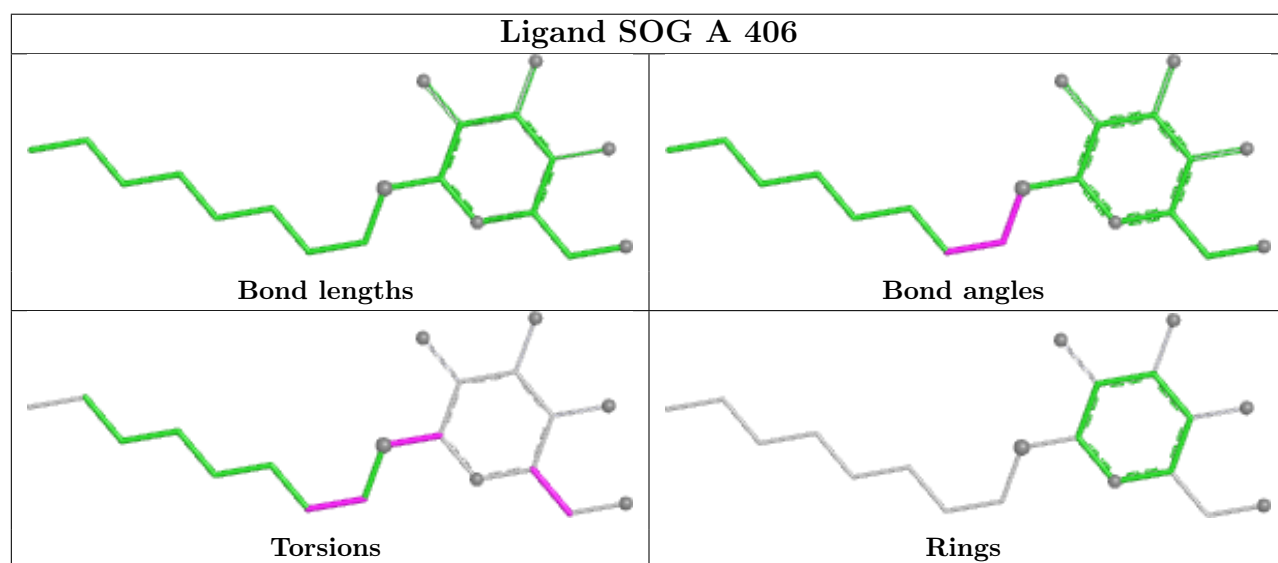
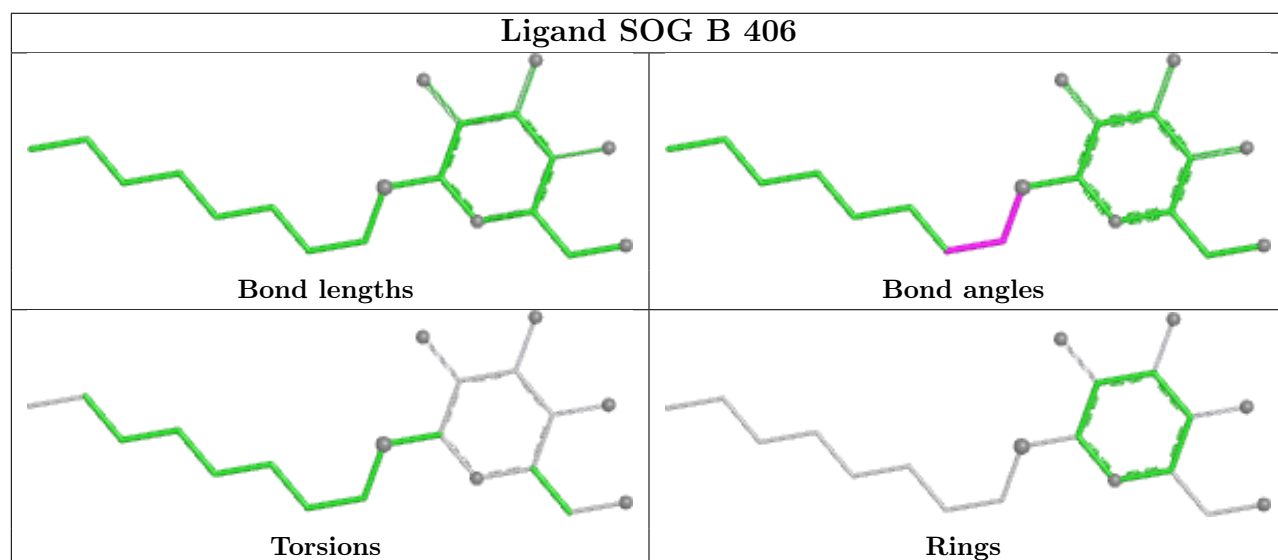
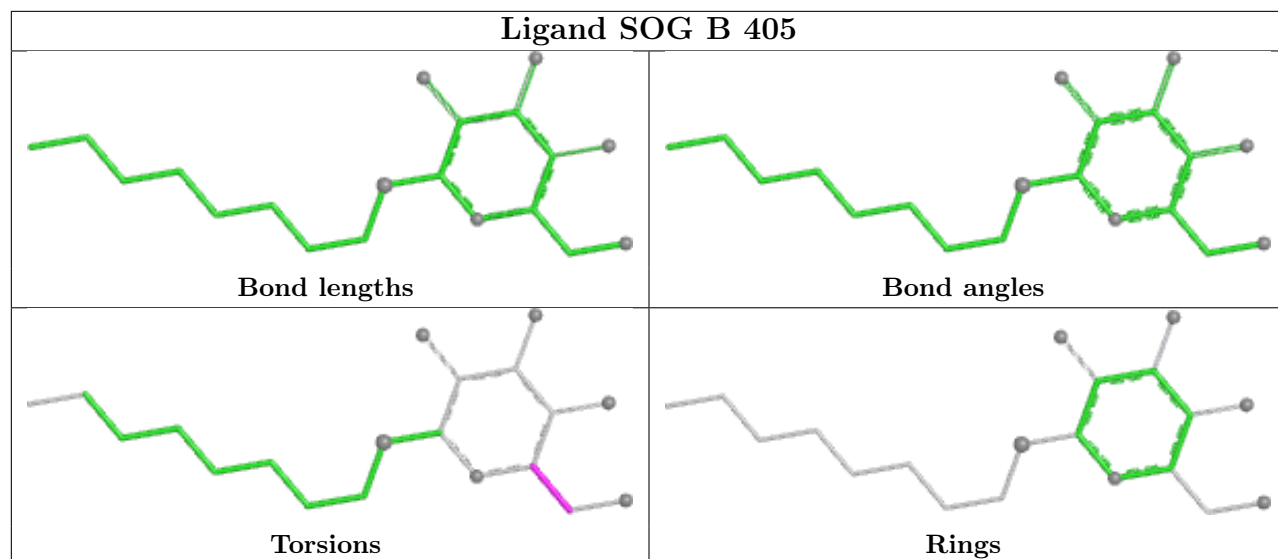


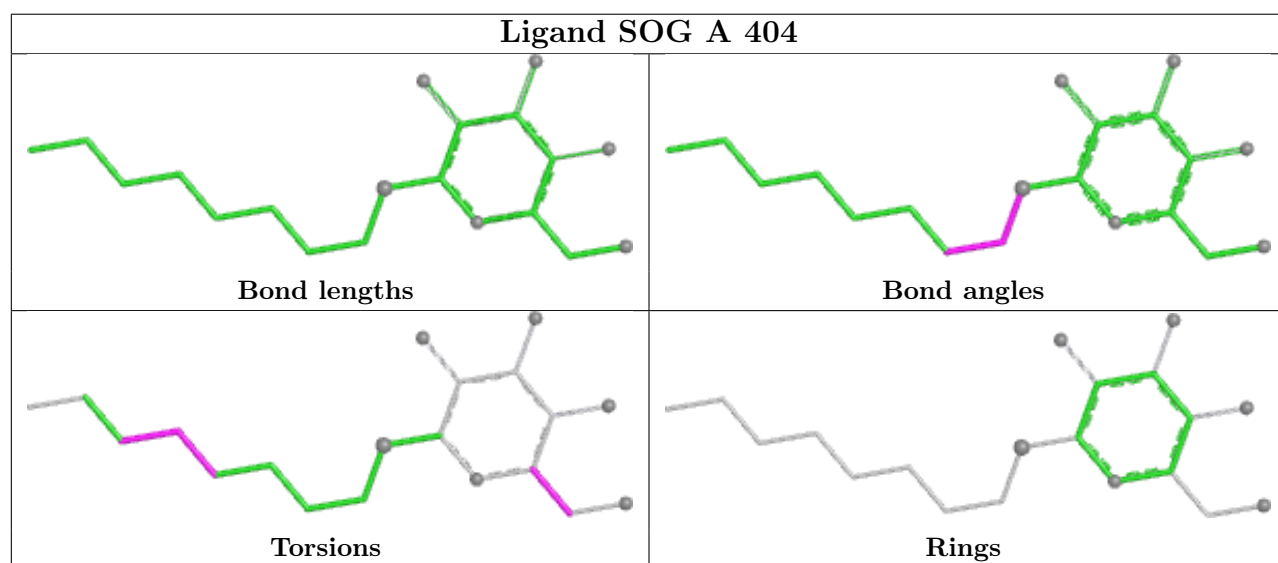
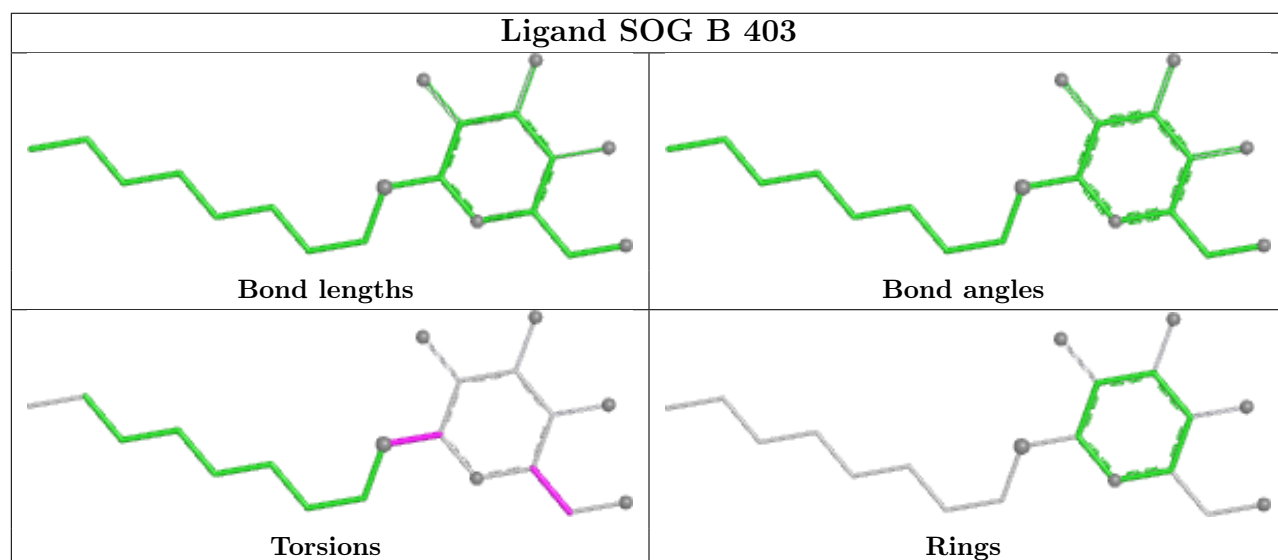
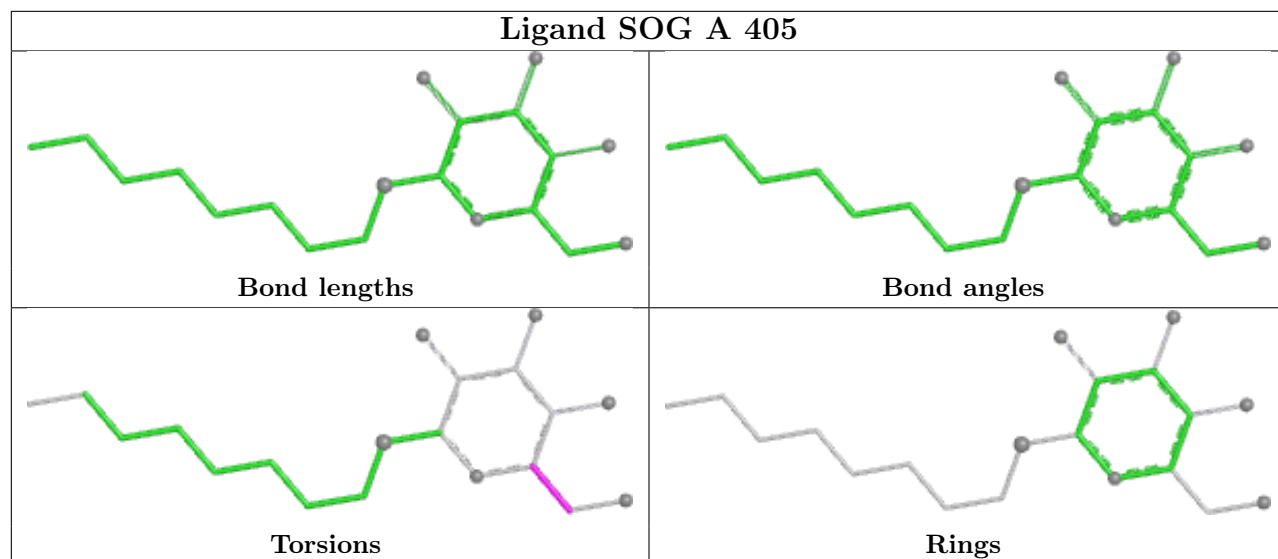












5.7 Other polymers [i](#)

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	304/336 (90%)	0.38	37 (12%) 8 7	33, 75, 139, 187	0
1	B	302/336 (89%)	0.35	29 (9%) 13 11	42, 79, 150, 191	0
All	All	606/672 (90%)	0.37	66 (10%) 10 9	33, 77, 146, 191	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	287	VAL	11.7
1	A	69	LEU	10.8
1	B	291	ARG	7.4
1	A	27	SER	7.2
1	A	105	LEU	6.7
1	A	28	GLU	5.8
1	B	290	MET	5.6
1	B	288	LYS	5.1
1	A	331	SER	5.0
1	B	108	ILE	4.9
1	B	196	THR	4.9
1	B	249	GLY	4.7
1	A	47	TRP	4.6
1	B	72	TRP	4.4
1	B	46	ALA	4.3
1	A	108	ILE	4.2
1	A	332	ASP	4.1
1	B	198	ALA	3.8
1	A	104	LEU	3.7
1	B	294	ARG	3.7
1	A	329	GLN	3.6
1	A	113	LEU	3.5
1	B	86	VAL	3.4
1	A	68	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	107	ASP	3.4
1	B	219	PHE	3.4
1	A	327	PHE	3.3
1	B	159	ARG	3.3
1	B	164	SER	3.2
1	A	29	ASP	3.1
1	A	114	PHE	3.1
1	A	30	GLU	3.0
1	A	34	TYR	3.0
1	A	73	ARG	3.0
1	A	167	GLY	2.9
1	A	159	ARG	2.9
1	B	199	PHE	2.8
1	B	292	ALA	2.8
1	A	109	THR	2.7
1	A	330	ALA	2.7
1	A	65	THR	2.7
1	A	121	VAL	2.7
1	A	160	ARG	2.6
1	A	166	LEU	2.6
1	A	33	ARG	2.5
1	B	251	THR	2.5
1	A	163	GLY	2.5
1	A	118	LEU	2.4
1	B	141	ALA	2.4
1	B	377	LEU	2.4
1	A	111	SER	2.4
1	A	335	ALA	2.3
1	A	134	VAL	2.3
1	B	193	ALA	2.2
1	A	361	LEU	2.2
1	B	162	LEU	2.2
1	B	242	LEU	2.2
1	B	68	CYS	2.2
1	A	251	THR	2.2
1	A	38	ASP	2.2
1	B	47	TRP	2.1
1	B	330	ALA	2.1
1	B	163	GLY	2.1
1	A	50	ILE	2.1
1	A	188	VAL	2.0
1	B	344	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

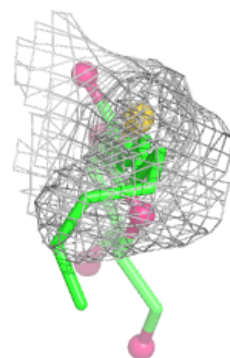
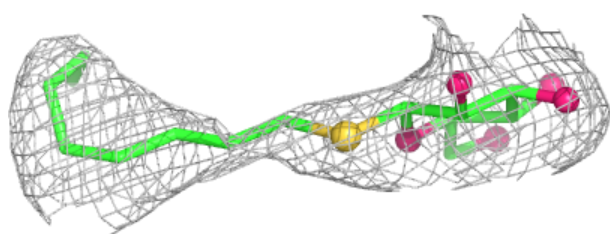
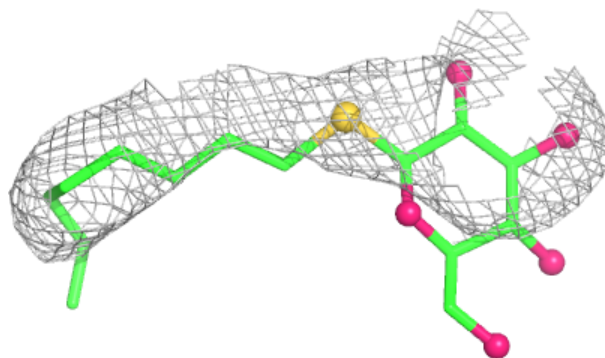
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SOG	A	405	20/20	0.68	0.20	59,107,137,142	0
3	SOG	A	406	20/20	0.72	0.11	89,118,134,135	0
3	SOG	B	403	20/20	0.72	0.14	110,144,156,163	0
3	SOG	A	407	20/20	0.76	0.15	109,120,130,132	0
3	SOG	B	405	20/20	0.76	0.12	113,123,140,144	0
4	SO4	A	409	5/5	0.76	0.07	131,139,140,143	0
3	SOG	B	406	20/20	0.77	0.13	113,134,154,155	0
4	SO4	A	408	5/5	0.80	0.06	146,148,151,159	0
3	SOG	B	404	9/20	0.80	0.22	70,75,94,100	0
2	NVN	B	401	26/26	0.81	0.14	61,103,130,137	0
2	NVN	A	402	26/26	0.84	0.12	69,88,106,109	0
5	PGW	A	411	51/51	0.84	0.17	37,89,169,170	0
5	PGW	A	410	51/51	0.87	0.17	41,82,155,163	0
3	SOG	A	404	20/20	0.88	0.11	75,125,138,138	0
2	NVN	A	401	26/26	0.89	0.10	48,73,97,101	0
4	SO4	B	407	5/5	0.90	0.05	97,98,101,116	0
3	SOG	B	402	20/20	0.92	0.09	64,97,108,112	0
3	SOG	A	403	20/20	0.93	0.08	45,80,87,98	0

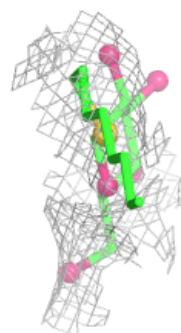
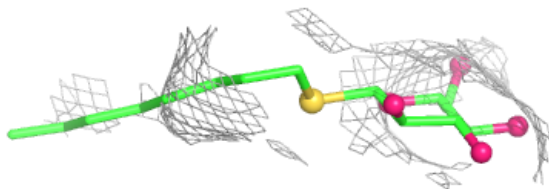
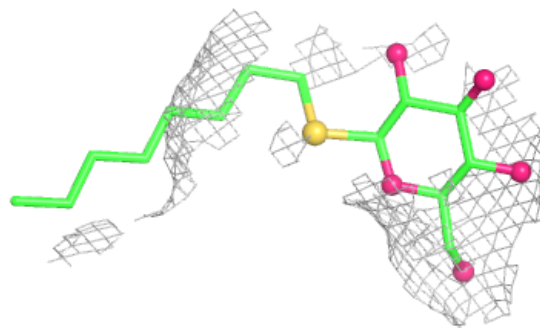
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SOG 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)

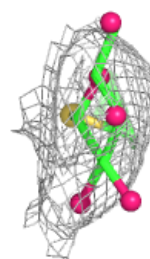
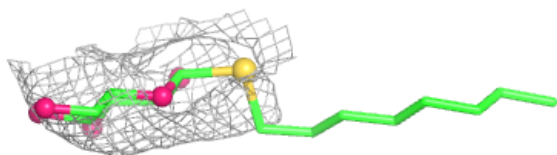
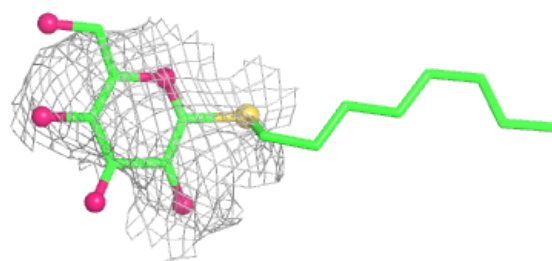
**Electron density around SOG A 406:**

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

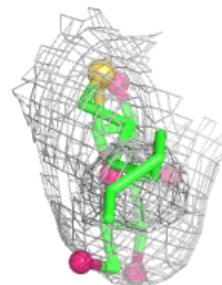
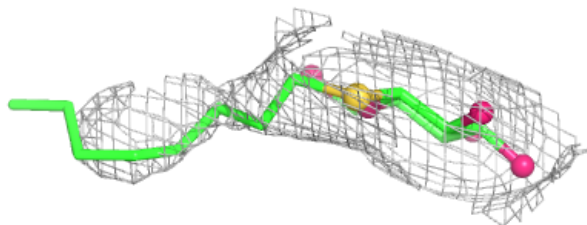
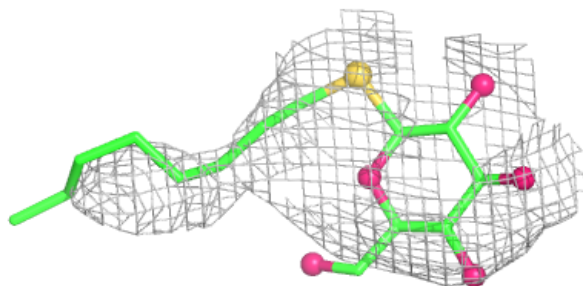


Electron density around SOG B 403:

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

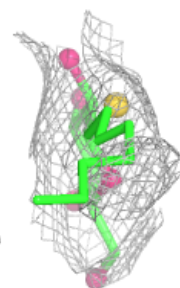
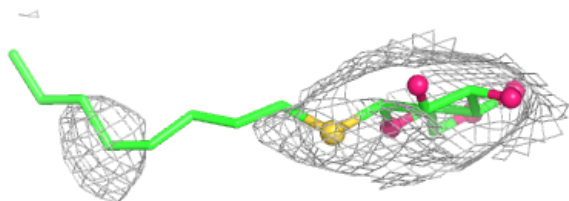
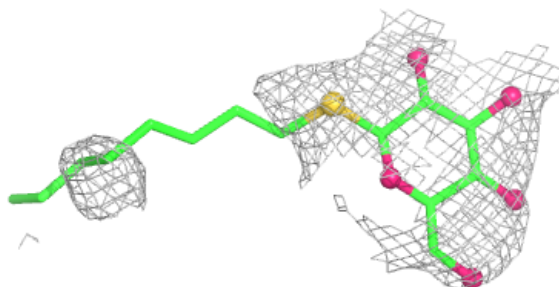
**Electron density around SOG A 407:**

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

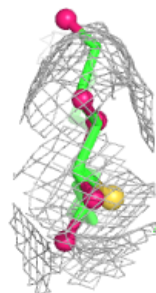
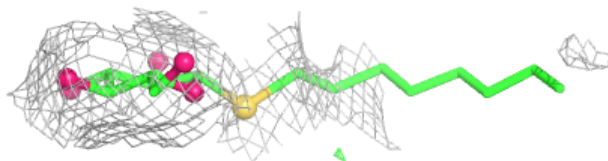
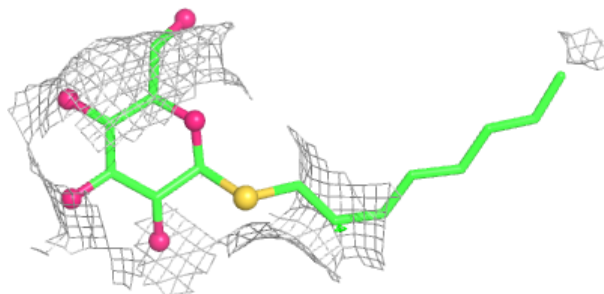


Electron density around SOG B 405:

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

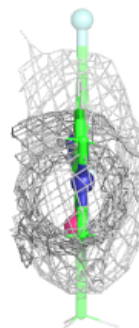
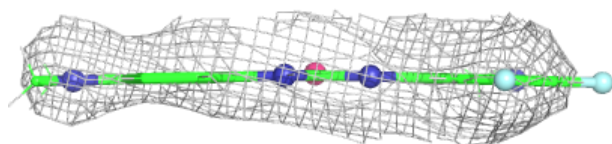
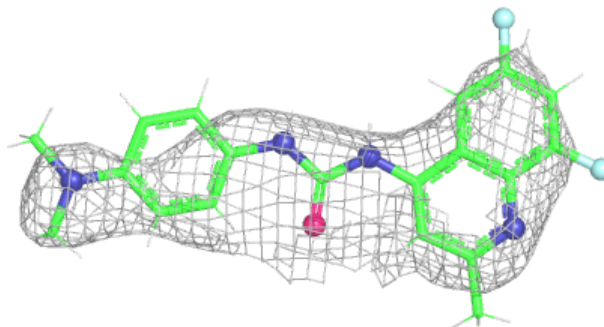
**Electron density around SOG B 406:**

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

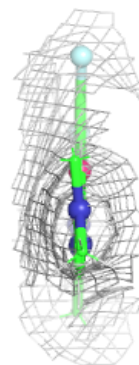
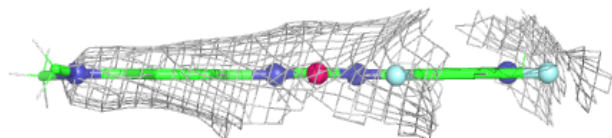
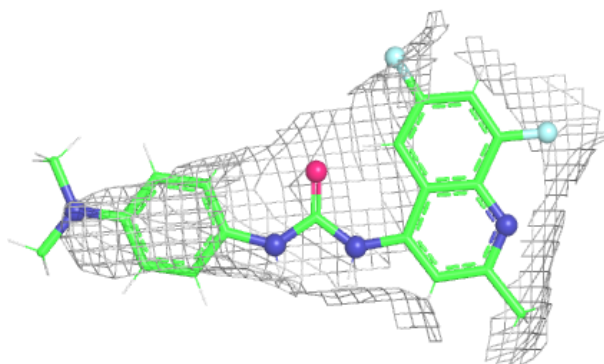


Electron density around NVN B 401:

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

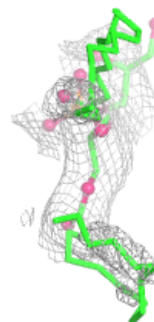
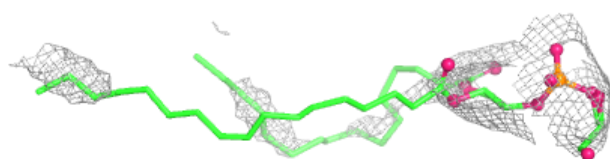
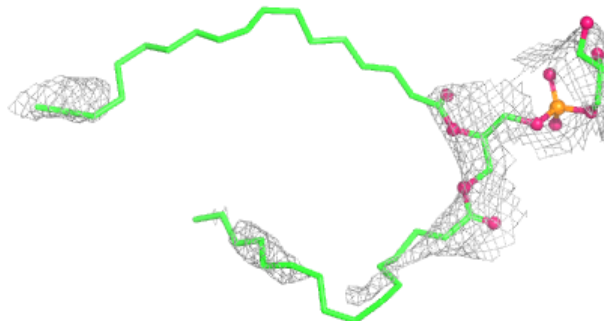
**Electron density around NVN A 402:**

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

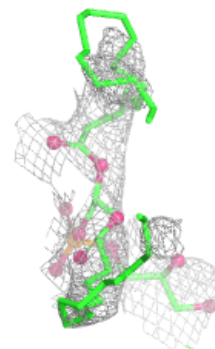
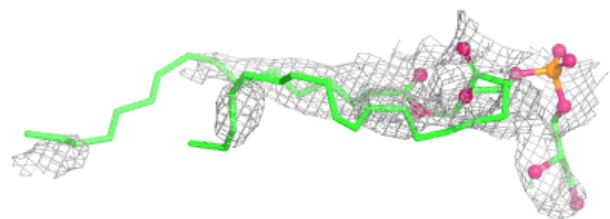
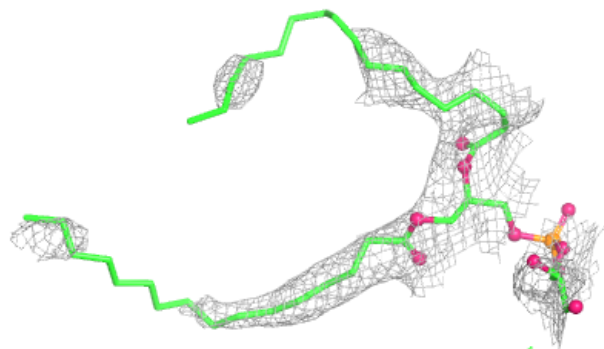


Electron density around PGW A 411:

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

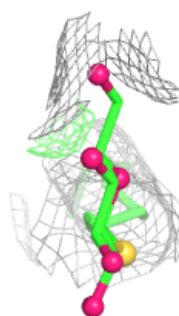
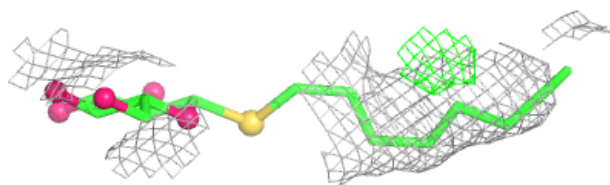
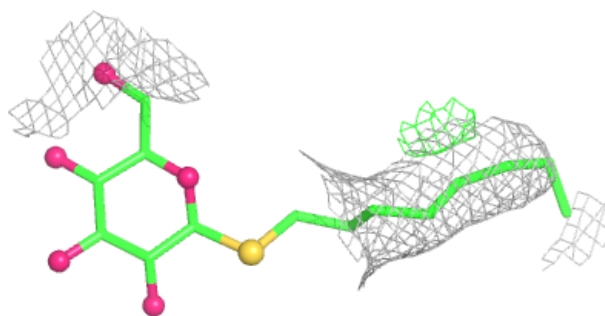
**Electron density around PGW A 410:**

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

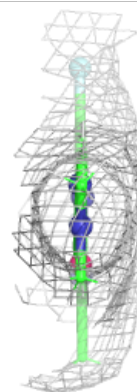
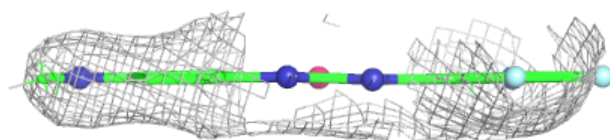
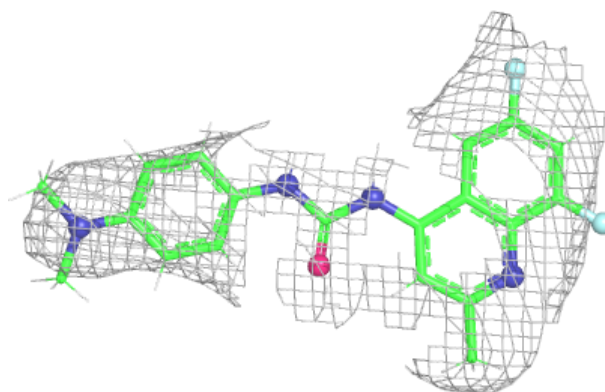


Electron density around SOG A 404:

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

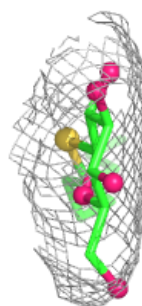
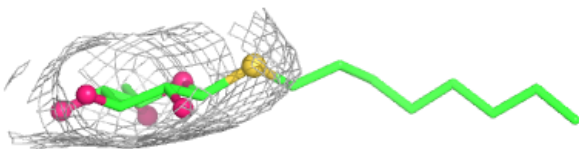
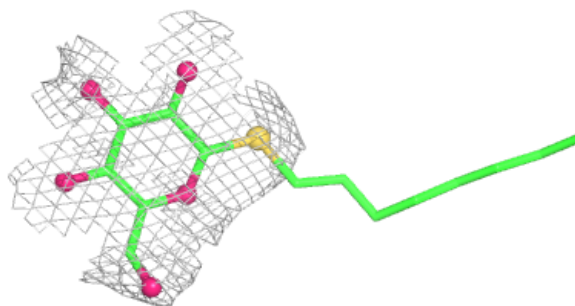
**Electron density around NVN A 401:**

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

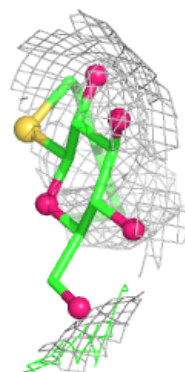
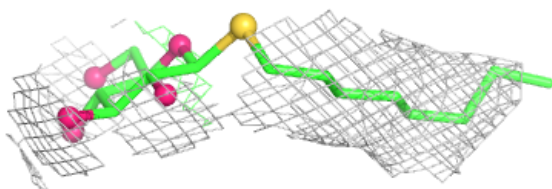
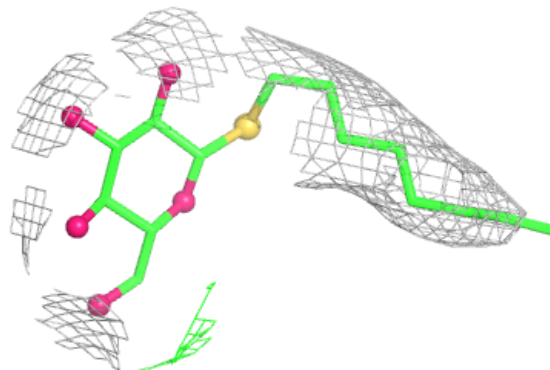


Electron density around SOG B 402:

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

**Electron density around SOG 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.