



Full wwPDB EM Validation Report ⓘ

Sep 29, 2024 – 03:17 AM EDT

PDB ID : 7MBR
EMDB ID : EMD-23744
Title : Cryo-EM structure of zebrafish TRPM5 in the presence of 6 uM calcium (apo state)
Authors : Ruan, Z.; Lu, W.; Du, J.; Haley, E.
Deposited on : 2021-04-01
Resolution : Not provided

This is a Full wwPDB EM 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/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

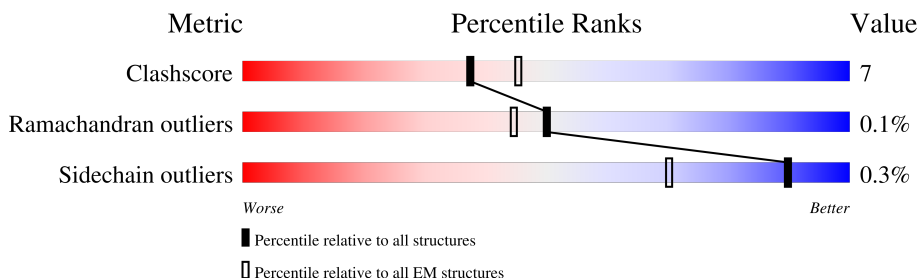
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is unknown.

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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	1165	
1	B	1165	
1	C	1165	
1	D	1165	

2 Entry composition [i](#)

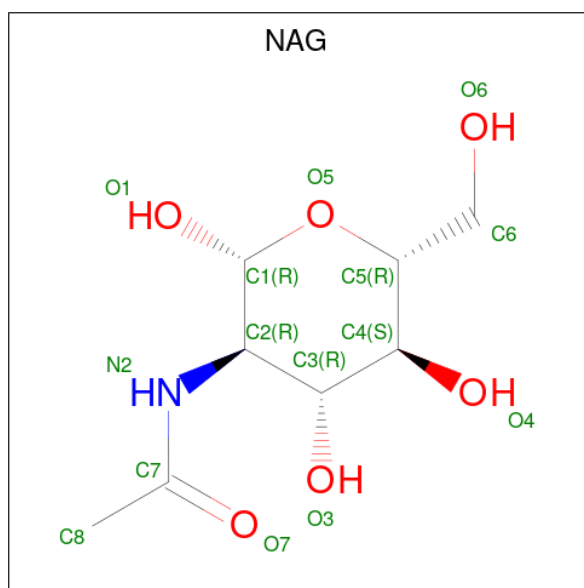
There are 4 unique types of molecules in this entry. The entry contains 30708 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Transient receptor potential melastatin 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	996	Total	C	N	O	S	0	0
			7574	4963	1296	1271	44		
1	B	996	Total	C	N	O	S	0	0
			7574	4963	1296	1271	44		
1	C	996	Total	C	N	O	S	0	0
			7574	4963	1296	1271	44		
1	D	996	Total	C	N	O	S	0	0
			7574	4963	1296	1271	44		

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$) (labeled as "Ligand of Interest" by depositor).



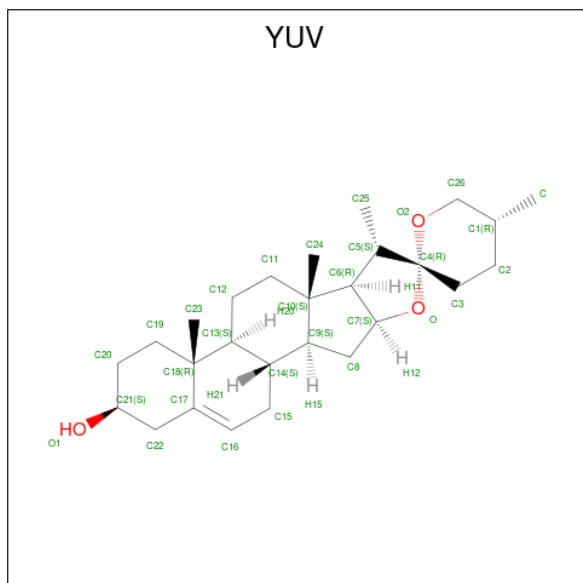
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	

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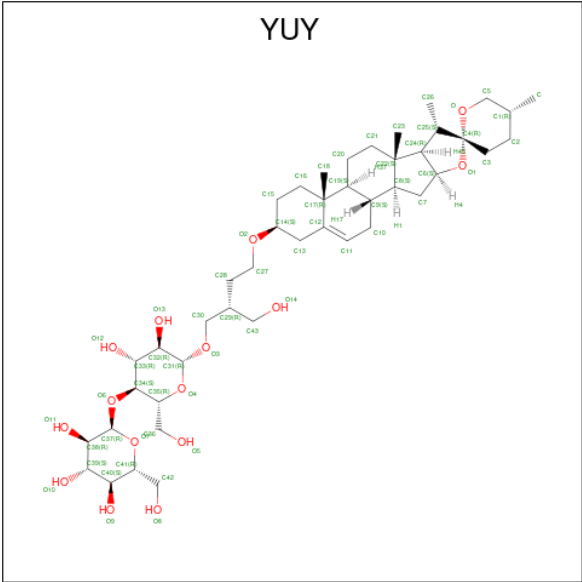
Mol	Chain	Residues	Atoms				AltConf
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (three-letter code: YUV) (formula: $C_{27}H_{42}O_3$) (labeled as "Ligand of Interest" by depositor).

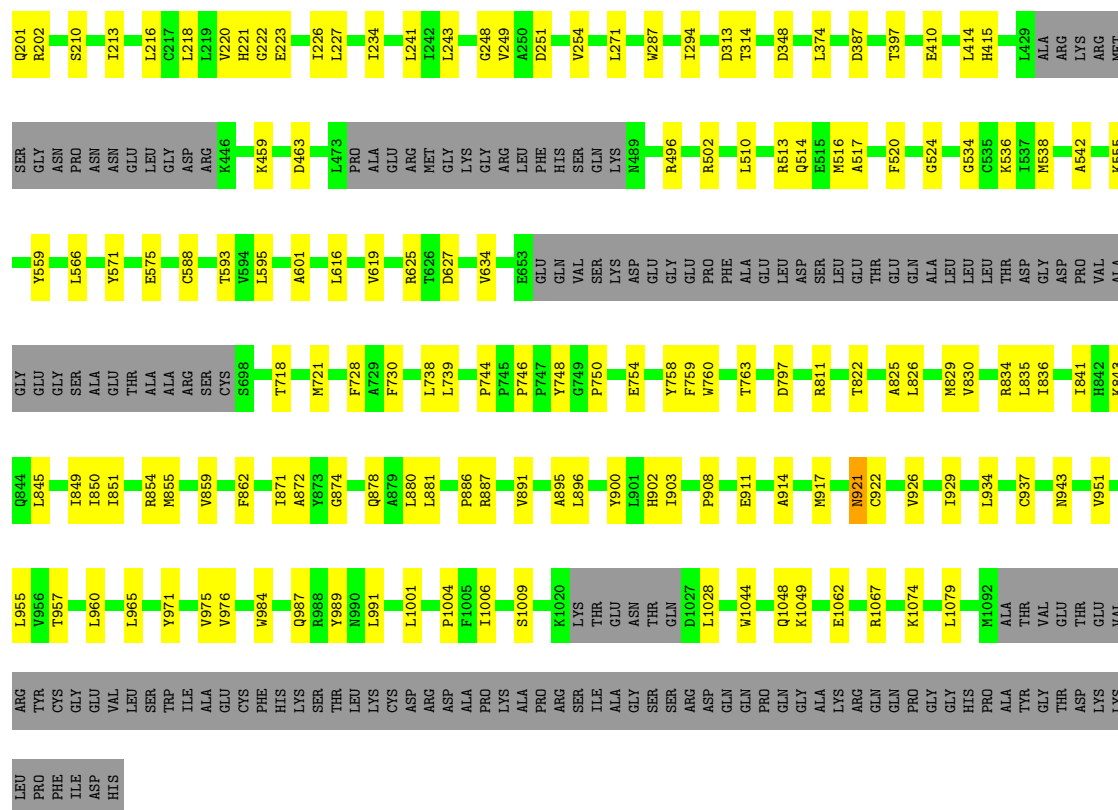


Mol	Chain	Residues	Atoms			AltConf
3	A	1	Total	C	O	0
			30	27	3	
3	B	1	Total	C	O	0
			30	27	3	
3	C	1	Total	C	O	0
			30	27	3	
3	D	1	Total	C	O	0
			30	27	3	

- Molecule 4 is (2R)-2-(hydroxymethyl)-4-{[(25R)-10alpha,14beta,17beta-spirost-5-en-3beta-yl]oxy}butyl 4-O-alpha-D-glucopyranosyl-beta-D-glucopyranoside (three-letter code: YUY) (formula: $C_{44}H_{72}O_{15}$) (labeled as "Ligand of Interest" by depositor).

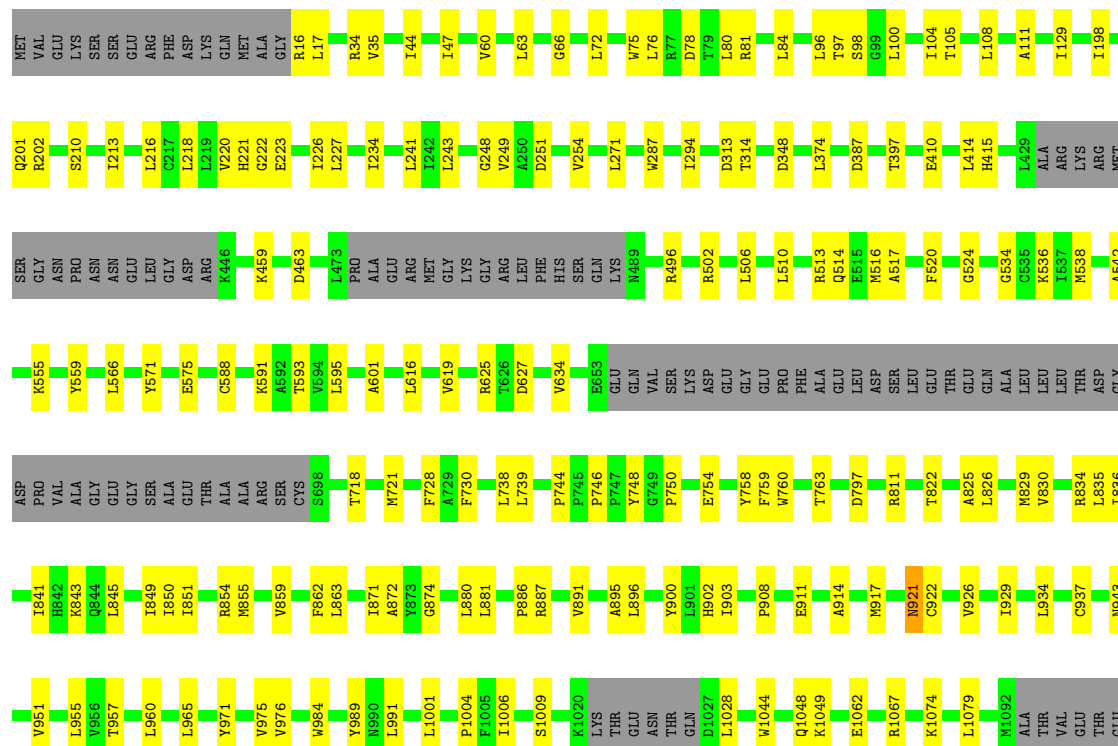


Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	C	O	0
			59	44	15	
4	B	1	Total	C	O	0
			59	44	15	
4	C	1	Total	C	O	0
			59	44	15	
4	D	1	Total	C	O	0
			59	44	15	



• Molecule 1: Transient receptor potential melastatin 5

Chain C: 71% 15% 15%



VAL	ARG	LYS
TYR	CYS	LEU
GLY	PHE	PRO
ILE	ASP	HIS
VAL		
LEU		
SER		
TRP		
ILE		
ALA		
GLU		
CYS		
PHE		
HIS		
SER		
THR		
LEU		
LYS		
CYS		
ASP		
ARG		
ALA		
PRO		
LYS		
ALA		
PRO		
ARG		
SER		
ILE		
GLY		
SER		
ARG		
ASP		
GLN		
PRO		
GLY		
ALA		
LYS		
ARG		
GLN		
PRO		
GLY		
HIS		
PRO		
ALA		
TYR		
GLY		
THR		
ASP		
LYS		

- Molecule 1: Transient receptor potential melastatin 5



MET	VAL	GLY	LYS	SER	PRO	GLU	ARG	THR	LEU	LYS	ASP	ALA	PRO	LYS	ALA	PRO	GLY	HIS	PRO	ALA	TYR	GLY	THR	ASP	LYS																							
Q201	R202	S210	I213	L216	C217	L218	L219	V220	H221	G222	E223	R16	L17	R34	V35	I44	I47	V60	L63	G66	L72	W75	L76	D77	D78	D79	L80	R81	L84	L96	T97	S98	G99	L100	I104	T105	L108	A111	I129	A129	ALA	ARG	LYS					
ARG	MET	SER	GLY	ASN	PRO	ASN	ASN	GLU	LEU	GLY	ASP	ARG	K446	K459	D463	L473	PRO	ALA	GLU	ARG	MET	GLY	LYS	GLY	ARG	LEU	PHE	HIS	SER	GLN	L489	R496	R502	L510	R513	Q514	E515	M516	A517	F520	G524	H415	G534	C535	X536	K537	M538	A542
K555	Y559	L566	Y571	E575	C588	T593	V594	L595	A601	L616	V619	R625	T626	D627	V634	E663	GLU	GLN	VAL	SER	LYS	ASP	GLY	GLU	PRO	PHE	ALA	GLU	LEU	ASP	SER	L516	GLU	THR	GLU	GLN	ALA	LEU	LEU	LEU	THR	ASP	GLY	ASP	PRO			
VAL	ALA	GLY	GLY	SER	ALA	GLU	THR	ALA	ALA	ARG	CYS	S698	T718	M721	F728	A729	F730	L738	P744	P745	P746	P747	Y748	G749	P750	F759	W760	T763	D797	R811	T822	A825	L826	M829	V830	R834	L835	V951	I841	H842	K843	Q844	L845					
I849	I850	I851	R854	M855	V859	F862	I874	N890	A872	V873	G874	L880	L881	P886	R887	V891	A895	L896	Y900	L901	H902	D1027	L1028	W1044	Q1048	K1049	A914	M917	N921	C922	V926	T929	L934	C937	N943	V951	L955	V956	T957	L960								
L965	Y971	V975	V976	W984	Y989	N990	L991	L1001	P1004	F1005	I1006	S1009	K1020	THR	LYS	THR	GLU	ASN	THR	GLN	D1027	L1028	W1044	Q1048	K1049	E1062	R1067	K1074	L1079	M1092	ALA	THR	VAL	GLU	THR	GLY	THR	ASP	LYS	VAL	ARG	TYR	CYS	GLY	GLU	VAL	LEU	
SER	TRP	ILE	ALA	GLU	CYS	PHE	HIS	LYS	SER	THR	LEU	LYS	CYS	ASP	ARG	ASP	ALA	PRO	LYS	ALA	PRO	ARG	ILE	ALA	GLY	SER	THR	GLN	PRO	GLN	GLY	GLY	HIS	PRO	ALA	TYR	GLY	THR	ASP	LYS	VAL	ARG	TYR	CYS	GLY	GLU	VAL	LEU

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32000	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	49.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: YUY, NAG, YUV

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	0/7763	0.44	0/10588
1	B	0.25	0/7763	0.44	0/10588
1	C	0.25	0/7763	0.44	0/10588
1	D	0.25	0/7763	0.44	0/10588
All	All	0.25	0/31052	0.44	0/42352

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 [i](#)

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	7574	0	7394	119	0
1	B	7574	0	7394	116	0
1	C	7574	0	7394	118	0
1	D	7574	0	7394	114	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	0	0
3	C	30	0	0	0	0
3	D	30	0	0	0	0
4	A	59	0	0	1	0
4	B	59	0	0	1	0
4	C	59	0	0	1	0
4	D	59	0	0	1	0
All	All	30708	0	29628	438	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 7.

All (438) 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:760:TRP:CZ3	1:B:1004:PRO:HD3	1.77	1.19
1:D:760:TRP:CZ3	1:D:1004:PRO:HD3	1.77	1.19
1:A:760:TRP:CZ3	1:A:1004:PRO:HD3	1.77	1.18
1:C:760:TRP:CZ3	1:C:1004:PRO:HD3	1.77	1.16
1:A:760:TRP:CZ3	1:A:1004:PRO:CD	2.58	0.86
1:C:760:TRP:CZ3	1:C:1004:PRO:CD	2.58	0.86
1:D:760:TRP:CZ3	1:D:1004:PRO:CD	2.58	0.86
1:B:760:TRP:CZ3	1:B:1004:PRO:CD	2.58	0.85
1:B:760:TRP:CH2	1:B:1004:PRO:HD3	2.16	0.80
1:C:760:TRP:CH2	1:C:1004:PRO:HD3	2.16	0.80
1:D:760:TRP:CH2	1:D:1004:PRO:HD3	2.16	0.80
1:A:760:TRP:CH2	1:A:1004:PRO:HD3	2.16	0.80
1:B:917:MET:O	4:B:1503:YUY:O8	2.03	0.77
1:C:917:MET:O	4:C:1503:YUY:O8	2.04	0.75
1:D:917:MET:O	4:D:3001:YUY:O8	2.04	0.74
1:A:917:MET:O	4:A:1503:YUY:O8	2.06	0.73
1:D:16:ARG:HE	1:D:34:ARG:HB2	1.54	0.73
1:A:16:ARG:HE	1:A:34:ARG:HB2	1.53	0.72
1:C:16:ARG:HE	1:C:34:ARG:HB2	1.53	0.72
1:B:16:ARG:HE	1:B:34:ARG:HB2	1.53	0.71
1:A:81:ARG:HE	1:A:111:ALA:HB2	1.57	0.70
1:B:81:ARG:HE	1:B:111:ALA:HB2	1.57	0.70
1:C:81:ARG:HE	1:C:111:ALA:HB2	1.57	0.69
1:D:81:ARG:HE	1:D:111:ALA:HB2	1.57	0.68
1:B:872:ALA:HB1	1:C:829:MET:HG3	1.76	0.68
1:A:859:VAL:HG21	1:D:960:LEU:HD12	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:960:LEU:HD12	1:C:859:VAL:HG21	1.76	0.66
1:C:960:LEU:HD12	1:D:859:VAL:HG21	1.78	0.66
1:A:502:ARG:NH1	1:A:588:CYS:O	2.29	0.65
1:B:502:ARG:NH1	1:B:588:CYS:O	2.29	0.65
1:D:502:ARG:NH1	1:D:588:CYS:O	2.29	0.65
1:A:829:MET:HG3	1:D:872:ALA:HB1	1.77	0.65
1:A:738:LEU:HD21	1:A:825:ALA:HA	1.79	0.65
1:C:738:LEU:HD21	1:C:825:ALA:HA	1.79	0.65
1:D:738:LEU:HD21	1:D:825:ALA:HA	1.79	0.65
1:A:872:ALA:HB1	1:B:829:MET:HG3	1.79	0.64
1:C:872:ALA:HB1	1:D:829:MET:HG3	1.78	0.64
1:A:524:GLY:O	1:A:1049:LYS:NZ	2.31	0.64
1:B:738:LEU:HD21	1:B:825:ALA:HA	1.79	0.64
1:C:502:ARG:NH1	1:C:588:CYS:O	2.29	0.64
1:B:524:GLY:O	1:B:1049:LYS:NZ	2.31	0.63
1:A:960:LEU:HD12	1:B:859:VAL:HG21	1.79	0.63
1:C:524:GLY:O	1:C:1049:LYS:NZ	2.31	0.63
1:D:524:GLY:O	1:D:1049:LYS:NZ	2.31	0.63
1:A:902:HIS:HE1	1:A:908:PRO:HD2	1.64	0.63
1:A:459:LYS:HD3	1:A:463:ASP:HA	1.81	0.63
1:B:902:HIS:HE1	1:B:908:PRO:HD2	1.64	0.62
1:D:459:LYS:HD3	1:D:463:ASP:HA	1.81	0.62
1:B:459:LYS:HD3	1:B:463:ASP:HA	1.81	0.62
1:A:1062:GLU:OE1	1:A:1067:ARG:NH2	2.33	0.62
1:B:1062:GLU:OE1	1:B:1067:ARG:NH2	2.33	0.62
1:C:902:HIS:HE1	1:C:908:PRO:HD2	1.64	0.62
1:D:902:HIS:HE1	1:D:908:PRO:HD2	1.64	0.62
1:C:459:LYS:HD3	1:C:463:ASP:HA	1.81	0.62
1:C:1062:GLU:OE1	1:C:1067:ARG:NH2	2.33	0.61
1:C:619:VAL:HG22	1:C:1028:LEU:HD22	1.83	0.61
1:D:1062:GLU:OE1	1:D:1067:ARG:NH2	2.33	0.60
1:D:619:VAL:HG22	1:D:1028:LEU:HD22	1.83	0.60
1:A:619:VAL:HG22	1:A:1028:LEU:HD22	1.83	0.60
1:B:619:VAL:HG22	1:B:1028:LEU:HD22	1.83	0.60
1:B:514:GLN:NE2	1:B:538:MET:HE2	2.17	0.60
1:B:271:LEU:HD21	1:B:287:TRP:HE3	1.67	0.59
1:B:17:LEU:HD11	1:B:47:ILE:HD11	1.85	0.59
1:C:17:LEU:HD11	1:C:47:ILE:HD11	1.85	0.59
1:A:271:LEU:HD21	1:A:287:TRP:HE3	1.67	0.59
1:D:730:PHE:HB2	1:D:760:TRP:CE2	2.38	0.59
1:A:202:ARG:NH2	1:A:210:SER:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:LEU:HD21	1:C:287:TRP:HE3	1.67	0.59
1:D:271:LEU:HD21	1:D:287:TRP:HE3	1.67	0.59
1:A:216:LEU:HD21	1:A:241:LEU:HD23	1.85	0.59
1:A:730:PHE:HB2	1:A:760:TRP:CE2	2.38	0.59
1:D:202:ARG:NH2	1:D:210:SER:O	2.36	0.59
1:C:202:ARG:NH2	1:C:210:SER:O	2.36	0.58
1:B:202:ARG:NH2	1:B:210:SER:O	2.36	0.58
1:C:760:TRP:CZ3	1:C:1004:PRO:HG3	2.38	0.58
1:D:760:TRP:CZ3	1:D:1004:PRO:HG3	2.38	0.58
1:A:760:TRP:CZ3	1:A:1004:PRO:HG3	2.38	0.58
1:B:760:TRP:CZ3	1:B:1004:PRO:HG3	2.38	0.58
1:C:730:PHE:HB2	1:C:760:TRP:CE2	2.38	0.58
1:A:17:LEU:HD11	1:A:47:ILE:HD11	1.85	0.58
1:D:17:LEU:HD11	1:D:47:ILE:HD11	1.85	0.58
1:B:730:PHE:HB2	1:B:760:TRP:CE2	2.38	0.58
1:D:216:LEU:HD21	1:D:241:LEU:HD23	1.85	0.58
1:C:216:LEU:HD21	1:C:241:LEU:HD23	1.85	0.57
1:A:760:TRP:CZ3	1:A:1004:PRO:CG	2.88	0.57
1:B:216:LEU:HD21	1:B:241:LEU:HD23	1.85	0.57
1:B:760:TRP:CZ3	1:B:1004:PRO:CG	2.88	0.57
1:C:514:GLN:NE2	1:C:538:MET:HE2	2.19	0.56
1:A:760:TRP:CE3	1:A:1004:PRO:HG3	2.41	0.56
1:C:760:TRP:CZ3	1:C:1004:PRO:CG	2.88	0.56
1:B:760:TRP:CE3	1:B:1004:PRO:HG3	2.41	0.56
1:D:760:TRP:CE3	1:D:1004:PRO:HG3	2.41	0.56
1:D:760:TRP:CZ3	1:D:1004:PRO:CG	2.88	0.56
1:C:760:TRP:CE3	1:C:1004:PRO:HG3	2.41	0.55
1:A:80:LEU:HD11	1:A:218:LEU:HD21	1.88	0.55
1:B:536:LYS:HD3	1:B:601:ALA:HA	1.89	0.54
1:C:80:LEU:HD11	1:C:218:LEU:HD21	1.89	0.54
1:D:35:VAL:HG21	1:D:44:ILE:HD11	1.89	0.54
1:A:634:VAL:HA	1:A:721:MET:HE1	1.89	0.54
1:D:514:GLN:NE2	1:D:538:MET:HE2	2.22	0.54
1:D:536:LYS:HD3	1:D:601:ALA:HA	1.90	0.54
1:A:35:VAL:HG21	1:A:44:ILE:HD11	1.89	0.54
1:C:536:LYS:HD3	1:C:601:ALA:HA	1.89	0.54
1:A:536:LYS:HD3	1:A:601:ALA:HA	1.90	0.54
1:D:80:LEU:HD11	1:D:218:LEU:HD21	1.88	0.54
1:B:80:LEU:HD11	1:B:218:LEU:HD21	1.88	0.54
1:B:616:LEU:HD21	1:B:989:TYR:HD1	1.73	0.54
1:A:84:LEU:HD23	1:A:108:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ASP:HB3	1:D:75:TRP:HB3	1.90	0.53
1:C:84:LEU:HD23	1:C:108:LEU:HD11	1.90	0.53
1:D:84:LEU:HD23	1:D:108:LEU:HD11	1.90	0.53
1:B:84:LEU:HD23	1:B:108:LEU:HD11	1.90	0.53
1:C:35:VAL:HG21	1:C:44:ILE:HD11	1.89	0.53
1:C:746:PRO:HA	1:C:750:PRO:HD3	1.90	0.53
1:A:616:LEU:HD21	1:A:989:TYR:HD1	1.73	0.53
1:C:616:LEU:HD21	1:C:989:TYR:HD1	1.73	0.53
1:A:746:PRO:HA	1:A:750:PRO:HD3	1.90	0.53
1:A:410:GLU:HA	1:A:415:HIS:CG	2.44	0.53
1:B:1079:LEU:HD22	1:C:1074:LYS:HD2	1.91	0.53
1:B:35:VAL:HG21	1:B:44:ILE:HD11	1.89	0.52
1:B:410:GLU:HA	1:B:415:HIS:CG	2.44	0.52
1:D:746:PRO:HA	1:D:750:PRO:HD3	1.90	0.52
1:B:75:TRP:HB3	1:C:387:ASP:HB3	1.90	0.52
1:C:63:LEU:HB2	1:C:97:THR:HG22	1.91	0.52
1:C:410:GLU:HA	1:C:415:HIS:CG	2.44	0.52
1:D:63:LEU:HB2	1:D:97:THR:HG22	1.92	0.52
1:D:410:GLU:HA	1:D:415:HIS:CG	2.44	0.52
1:A:514:GLN:NE2	1:A:538:MET:HE2	2.24	0.52
1:A:730:PHE:HB2	1:A:760:TRP:NE1	2.24	0.52
1:B:746:PRO:HA	1:B:750:PRO:HD3	1.90	0.52
1:D:397:THR:HA	1:D:496:ARG:HA	1.91	0.52
1:A:514:GLN:NE2	1:A:538:MET:CE	2.73	0.52
1:B:72:LEU:HD22	1:B:76:LEU:HD23	1.92	0.52
1:D:616:LEU:HD21	1:D:989:TYR:HD1	1.73	0.52
1:C:72:LEU:HD22	1:C:76:LEU:HD23	1.92	0.52
1:A:1074:LYS:HD2	1:D:1079:LEU:HD22	1.91	0.52
1:B:397:THR:HA	1:B:496:ARG:HA	1.91	0.52
1:A:397:THR:HA	1:A:496:ARG:HA	1.91	0.51
1:A:517:ALA:HB3	1:A:559:TYR:OH	2.10	0.51
1:C:514:GLN:NE2	1:C:538:MET:CE	2.73	0.51
1:D:517:ALA:HB3	1:D:559:TYR:OH	2.10	0.51
1:A:201:GLN:HB2	1:A:213:ILE:HD12	1.93	0.51
1:C:730:PHE:HB2	1:C:760:TRP:NE1	2.24	0.51
1:D:514:GLN:NE2	1:D:538:MET:CE	2.73	0.51
1:B:730:PHE:HB2	1:B:760:TRP:NE1	2.24	0.51
1:B:514:GLN:NE2	1:B:538:MET:CE	2.73	0.51
1:B:634:VAL:HA	1:B:721:MET:HE1	1.91	0.51
1:B:63:LEU:HB2	1:B:97:THR:HG22	1.92	0.51
1:C:397:THR:HA	1:C:496:ARG:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:ALA:HB3	1:B:559:TYR:OH	2.10	0.51
1:D:730:PHE:HB2	1:D:760:TRP:NE1	2.24	0.51
1:A:63:LEU:HB2	1:A:97:THR:HG22	1.92	0.51
1:C:517:ALA:HB3	1:C:559:TYR:OH	2.10	0.51
1:C:634:VAL:HA	1:C:721:MET:HE1	1.93	0.51
1:C:75:TRP:HB3	1:D:387:ASP:HB3	1.92	0.51
1:C:862:PHE:CG	1:C:965:LEU:HD22	2.46	0.51
1:B:571:TYR:CE1	1:B:575:GLU:HG3	2.47	0.50
1:A:72:LEU:HD22	1:A:76:LEU:HD23	1.92	0.50
1:A:571:TYR:CE1	1:A:575:GLU:HG3	2.47	0.50
1:C:201:GLN:HB2	1:C:213:ILE:HD12	1.93	0.50
1:D:201:GLN:HB2	1:D:213:ILE:HD12	1.92	0.50
1:A:227:LEU:HD21	1:A:249:VAL:HG11	1.94	0.50
1:B:862:PHE:CG	1:B:965:LEU:HD22	2.46	0.50
1:C:571:TYR:CE1	1:C:575:GLU:HG3	2.47	0.50
1:D:571:TYR:CE1	1:D:575:GLU:HG3	2.47	0.50
1:D:72:LEU:HD22	1:D:76:LEU:HD23	1.92	0.50
1:C:227:LEU:HD21	1:C:249:VAL:HG11	1.94	0.49
1:D:634:VAL:HA	1:D:721:MET:HE1	1.93	0.49
1:A:862:PHE:CG	1:A:965:LEU:HD22	2.46	0.49
1:B:201:GLN:HB2	1:B:213:ILE:HD12	1.93	0.49
1:B:841:ILE:HD13	1:B:991:LEU:HB2	1.94	0.49
1:B:903:ILE:HG12	1:B:957:THR:HG21	1.94	0.49
1:A:75:TRP:HB3	1:B:387:ASP:HB3	1.94	0.49
1:C:1079:LEU:HD22	1:D:1074:LYS:HD2	1.93	0.49
1:D:862:PHE:CG	1:D:965:LEU:HD22	2.46	0.49
1:A:841:ILE:HD13	1:A:991:LEU:HB2	1.94	0.49
1:D:854:ARG:HG3	1:D:976:VAL:HG11	1.95	0.49
1:A:1079:LEU:HD22	1:B:1074:LYS:HD2	1.94	0.49
1:C:854:ARG:HG3	1:C:976:VAL:HG11	1.95	0.49
1:A:903:ILE:HG12	1:A:957:THR:HG21	1.94	0.49
1:B:227:LEU:HD21	1:B:249:VAL:HG11	1.94	0.49
1:B:854:ARG:HG3	1:B:976:VAL:HG11	1.95	0.49
1:C:903:ILE:HG12	1:C:957:THR:HG21	1.94	0.49
1:A:414:LEU:HD13	1:A:510:LEU:HB3	1.94	0.48
1:D:227:LEU:HD21	1:D:249:VAL:HG11	1.94	0.48
1:C:593:THR:HG22	1:C:595:LEU:H	1.78	0.48
1:D:593:THR:HG22	1:D:595:LEU:H	1.78	0.48
1:D:841:ILE:HD13	1:D:991:LEU:HB2	1.94	0.48
1:A:854:ARG:HG3	1:A:976:VAL:HG11	1.95	0.48
1:C:921:ASN:O	1:C:934:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:921:ASN:O	1:D:934:LEU:HD22	2.13	0.48
1:A:348:ASP:OD1	1:A:348:ASP:N	2.46	0.48
1:C:841:ILE:HD13	1:C:991:LEU:HB2	1.94	0.48
1:D:414:LEU:HD13	1:D:510:LEU:HB3	1.94	0.48
1:B:921:ASN:O	1:B:934:LEU:HD22	2.13	0.48
1:C:44:ILE:O	1:C:47:ILE:HG22	2.13	0.48
1:D:903:ILE:HG12	1:D:957:THR:HG21	1.94	0.48
1:A:921:ASN:O	1:A:934:LEU:HD22	2.13	0.48
1:B:850:ILE:O	1:B:854:ARG:HG2	2.14	0.48
1:C:414:LEU:HD13	1:C:510:LEU:HB3	1.94	0.48
1:D:44:ILE:O	1:D:47:ILE:HG22	2.13	0.48
1:D:66:GLY:HA3	1:D:104:ILE:HG22	1.96	0.48
1:A:44:ILE:O	1:A:47:ILE:HG22	2.13	0.48
1:B:44:ILE:O	1:B:47:ILE:HG22	2.13	0.48
1:B:593:THR:HG22	1:B:595:LEU:H	1.78	0.48
1:A:850:ILE:O	1:A:854:ARG:HG2	2.14	0.48
1:B:414:LEU:HD13	1:B:510:LEU:HB3	1.94	0.48
1:A:98:SER:O	1:A:105:THR:HG21	2.13	0.48
1:D:850:ILE:O	1:D:854:ARG:HG2	2.14	0.48
1:A:971:TYR:O	1:A:975:VAL:HG23	2.14	0.48
1:B:98:SER:O	1:B:105:THR:HG21	2.14	0.48
1:C:98:SER:O	1:C:105:THR:HG21	2.14	0.48
1:C:971:TYR:O	1:C:975:VAL:HG23	2.14	0.48
1:A:593:THR:HG22	1:A:595:LEU:H	1.78	0.47
1:D:760:TRP:HZ3	1:D:1004:PRO:HD3	1.65	0.47
1:B:234:ILE:HD12	1:B:294:ILE:HG12	1.97	0.47
1:A:871:ILE:HD13	1:A:896:LEU:HD21	1.96	0.47
1:B:542:ALA:HB1	1:B:555:LYS:HZ3	1.79	0.47
1:C:850:ILE:O	1:C:854:ARG:HG2	2.14	0.47
1:A:542:ALA:HB1	1:A:555:LYS:HZ3	1.79	0.47
1:C:66:GLY:HA3	1:C:104:ILE:HG22	1.96	0.47
1:C:542:ALA:HB1	1:C:555:LYS:HZ3	1.79	0.47
1:D:871:ILE:HD13	1:D:896:LEU:HD21	1.96	0.47
1:A:234:ILE:HD12	1:A:294:ILE:HG12	1.97	0.47
1:D:98:SER:O	1:D:105:THR:HG21	2.14	0.47
1:B:971:TYR:O	1:B:975:VAL:HG23	2.14	0.47
1:B:348:ASP:OD1	1:B:348:ASP:N	2.47	0.47
1:D:348:ASP:OD1	1:D:348:ASP:N	2.46	0.47
1:D:542:ALA:HB1	1:D:555:LYS:HZ3	1.79	0.47
1:D:730:PHE:CD1	1:D:760:TRP:CD1	3.03	0.47
1:C:234:ILE:HD12	1:C:294:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LEU:HD12	1:A:506:LEU:HA	1.78	0.46
1:B:797:ASP:OD1	1:B:834:ARG:NE	2.48	0.46
1:C:251:ASP:HA	1:C:254:VAL:HG12	1.98	0.46
1:C:730:PHE:CD1	1:C:760:TRP:CD1	3.03	0.46
1:C:797:ASP:OD1	1:C:834:ARG:NE	2.48	0.46
1:A:251:ASP:HA	1:A:254:VAL:HG12	1.98	0.46
1:A:514:GLN:HE21	1:A:538:MET:HE1	1.81	0.46
1:B:871:ILE:HD13	1:B:896:LEU:HD21	1.96	0.46
1:A:730:PHE:CD1	1:A:760:TRP:CD1	3.03	0.46
1:A:797:ASP:OD1	1:A:834:ARG:NE	2.48	0.46
1:B:251:ASP:HA	1:B:254:VAL:HG12	1.98	0.46
1:C:871:ILE:HD13	1:C:896:LEU:HD21	1.96	0.46
1:D:234:ILE:HD12	1:D:294:ILE:HG12	1.97	0.46
1:D:251:ASP:HA	1:D:254:VAL:HG12	1.97	0.46
1:D:971:TYR:O	1:D:975:VAL:HG23	2.14	0.46
1:A:66:GLY:HA3	1:A:104:ILE:HG22	1.96	0.46
1:B:66:GLY:HA3	1:B:104:ILE:HG22	1.96	0.46
1:D:797:ASP:OD1	1:D:834:ARG:NE	2.48	0.46
1:B:881:LEU:HD21	1:B:911:GLU:O	2.16	0.46
1:C:886:PRO:HG2	1:C:926:VAL:HG13	1.98	0.46
1:D:886:PRO:HG2	1:D:926:VAL:HG13	1.98	0.46
1:A:760:TRP:HZ3	1:A:1004:PRO:HD3	1.65	0.46
1:B:730:PHE:CD1	1:B:760:TRP:CD1	3.03	0.46
1:C:881:LEU:HD21	1:C:911:GLU:O	2.16	0.46
1:D:826:LEU:O	1:D:830:VAL:HG23	2.16	0.46
1:A:881:LEU:HD21	1:A:911:GLU:O	2.16	0.45
1:B:730:PHE:HB2	1:B:760:TRP:CZ2	2.51	0.45
1:B:922:CYS:HB3	1:B:937:CYS:HB2	1.99	0.45
1:C:730:PHE:HB2	1:C:760:TRP:CZ2	2.51	0.45
1:A:220:VAL:HG22	1:A:243:LEU:HD12	1.98	0.45
1:A:730:PHE:HB2	1:A:760:TRP:CZ2	2.51	0.45
1:A:902:HIS:CE1	1:A:908:PRO:HD2	2.49	0.45
1:B:534:GLY:O	1:B:538:MET:HG2	2.17	0.45
1:C:922:CYS:HB3	1:C:937:CYS:HB2	1.99	0.45
1:A:826:LEU:O	1:A:830:VAL:HG23	2.16	0.45
1:A:922:CYS:HB3	1:A:937:CYS:HB2	1.99	0.45
1:D:730:PHE:HB2	1:D:760:TRP:CZ2	2.51	0.45
1:C:826:LEU:O	1:C:830:VAL:HG23	2.16	0.45
1:D:220:VAL:HG22	1:D:243:LEU:HD12	1.98	0.45
1:C:98:SER:O	1:C:100:LEU:N	2.46	0.45
1:A:534:GLY:O	1:A:538:MET:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG22	1:B:243:LEU:HD12	1.98	0.45
1:C:220:VAL:HG22	1:C:243:LEU:HD12	1.98	0.45
1:C:887:ARG:O	1:C:891:VAL:HG23	2.17	0.45
1:A:625:ARG:NH1	1:A:627:ASP:OD2	2.50	0.45
1:B:886:PRO:HG2	1:B:926:VAL:HG13	1.98	0.45
1:B:887:ARG:O	1:B:891:VAL:HG23	2.17	0.45
1:C:534:GLY:O	1:C:538:MET:HG2	2.17	0.45
1:D:534:GLY:O	1:D:538:MET:HG2	2.17	0.45
1:D:625:ARG:NH1	1:D:627:ASP:OD2	2.50	0.45
1:D:914:ALA:HB2	1:D:943:ASN:HD22	1.83	0.45
1:A:886:PRO:HG2	1:A:926:VAL:HG13	1.98	0.44
1:D:881:LEU:HD21	1:D:911:GLU:O	2.16	0.44
1:D:902:HIS:CE1	1:D:908:PRO:HD2	2.49	0.44
1:D:1001:LEU:HD12	1:D:1009:SER:OG	2.18	0.44
1:C:625:ARG:NH1	1:C:627:ASP:OD2	2.50	0.44
1:B:566:LEU:HD11	1:B:1049:LYS:HB2	2.00	0.44
1:D:922:CYS:HB3	1:D:937:CYS:HB2	1.98	0.44
1:B:221:HIS:HA	1:B:248:GLY:H	1.82	0.44
1:D:728:PHE:HE1	1:D:835:LEU:HD21	1.82	0.44
1:A:1001:LEU:HD12	1:A:1009:SER:OG	2.18	0.44
1:B:826:LEU:O	1:B:830:VAL:HG23	2.16	0.44
1:B:851:ILE:O	1:B:855:MET:HG2	2.18	0.44
1:B:914:ALA:HB2	1:B:943:ASN:HD22	1.82	0.44
1:C:313:ASP:OD1	1:C:314:THR:N	2.51	0.44
1:D:887:ARG:O	1:D:891:VAL:HG23	2.17	0.44
1:B:1001:LEU:HD12	1:B:1009:SER:OG	2.18	0.44
1:C:221:HIS:HA	1:C:248:GLY:H	1.82	0.44
1:A:221:HIS:HA	1:A:248:GLY:H	1.82	0.44
1:A:887:ARG:O	1:A:891:VAL:HG23	2.17	0.44
1:B:98:SER:O	1:B:100:LEU:N	2.46	0.44
1:B:221:HIS:O	1:B:221:HIS:ND1	2.51	0.44
1:C:566:LEU:HD11	1:C:1049:LYS:HB2	2.00	0.44
1:D:221:HIS:HA	1:D:248:GLY:H	1.83	0.44
1:A:914:ALA:HB2	1:A:943:ASN:HD22	1.83	0.43
1:C:851:ILE:O	1:C:855:MET:HG2	2.18	0.43
1:D:313:ASP:OD1	1:D:314:THR:N	2.51	0.43
1:D:1044:TRP:O	1:D:1048:GLN:HG2	2.18	0.43
1:A:728:PHE:HE1	1:A:835:LEU:HD21	1.82	0.43
1:C:223:GLU:O	1:C:226:ILE:HG12	2.18	0.43
1:C:1001:LEU:HD12	1:C:1009:SER:OG	2.18	0.43
1:A:566:LEU:HD11	1:A:1049:LYS:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:O	1:A:849:ILE:HG12	2.18	0.43
1:B:728:PHE:HE1	1:B:835:LEU:HD21	1.82	0.43
1:D:845:LEU:O	1:D:849:ILE:HG12	2.18	0.43
1:A:760:TRP:CE3	1:A:1004:PRO:CG	3.02	0.43
1:A:851:ILE:O	1:A:855:MET:HG2	2.18	0.43
1:B:60:VAL:HG13	1:B:96:LEU:HD23	2.01	0.43
1:B:625:ARG:NH1	1:B:627:ASP:OD2	2.50	0.43
1:B:880:LEU:HD21	1:C:822:THR:HG23	2.00	0.43
1:D:851:ILE:O	1:D:855:MET:HG2	2.18	0.43
1:A:223:GLU:O	1:A:226:ILE:HG12	2.18	0.43
1:A:374:LEU:HD11	1:A:520:PHE:HZ	1.84	0.43
1:C:845:LEU:O	1:C:849:ILE:HG12	2.18	0.43
1:C:914:ALA:HB2	1:C:943:ASN:HD22	1.83	0.43
1:D:374:LEU:HD11	1:D:520:PHE:HZ	1.84	0.43
1:B:223:GLU:O	1:B:226:ILE:HG12	2.18	0.43
1:B:313:ASP:OD1	1:B:314:THR:N	2.51	0.43
1:C:60:VAL:HG13	1:C:96:LEU:HD23	2.01	0.43
1:C:1044:TRP:O	1:C:1048:GLN:HG2	2.18	0.43
1:D:874:GLY:HA3	1:D:895:ALA:O	2.19	0.43
1:B:1044:TRP:O	1:B:1048:GLN:HG2	2.18	0.43
1:C:728:PHE:HE1	1:C:835:LEU:HD21	1.83	0.43
1:C:874:GLY:HA3	1:C:895:ALA:O	2.19	0.43
1:D:223:GLU:O	1:D:226:ILE:HG12	2.18	0.43
1:D:421:LYS:HD3	1:D:421:LYS:HA	1.86	0.43
1:A:514:GLN:HE21	1:A:538:MET:CE	2.32	0.43
1:A:900:TYR:CE2	1:D:951:VAL:HG13	2.54	0.43
1:B:374:LEU:HD11	1:B:520:PHE:HZ	1.84	0.43
1:B:902:HIS:CE1	1:B:908:PRO:HD2	2.49	0.43
1:B:955:LEU:HB2	1:C:900:TYR:OH	2.19	0.43
1:D:514:GLN:HE21	1:D:538:MET:CE	2.32	0.43
1:D:566:LEU:HD11	1:D:1049:LYS:HB2	2.00	0.43
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.92	0.43
1:A:1044:TRP:O	1:A:1048:GLN:HG2	2.18	0.43
1:B:760:TRP:CE3	1:B:1004:PRO:CG	3.02	0.43
1:B:845:LEU:O	1:B:849:ILE:HG12	2.18	0.43
1:C:374:LEU:HD11	1:C:520:PHE:HZ	1.84	0.43
1:C:514:GLN:HE21	1:C:538:MET:CE	2.32	0.43
1:D:221:HIS:O	1:D:221:HIS:ND1	2.51	0.43
1:A:60:VAL:HG13	1:A:96:LEU:HD23	2.01	0.42
1:A:313:ASP:OD1	1:A:314:THR:N	2.51	0.42
1:C:60:VAL:HG21	1:C:198:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:760:TRP:CE3	1:C:1004:PRO:CG	3.02	0.42
1:D:60:VAL:HG21	1:D:198:ILE:HG21	2.01	0.42
1:D:514:GLN:HE21	1:D:538:MET:HE1	1.84	0.42
1:A:900:TYR:OH	1:D:955:LEU:HB2	2.19	0.42
1:B:514:GLN:HE21	1:B:538:MET:CE	2.32	0.42
1:C:348:ASP:N	1:C:348:ASP:OD1	2.46	0.42
1:B:96:LEU:HD13	1:B:129:ILE:HB	2.01	0.42
1:C:96:LEU:HD13	1:C:129:ILE:HB	2.02	0.42
1:C:591:LYS:HA	1:C:591:LYS:HD3	1.85	0.42
1:D:760:TRP:CE3	1:D:1004:PRO:CG	3.02	0.42
1:A:874:GLY:HA3	1:A:895:ALA:O	2.19	0.42
1:D:1049:LYS:HB3	1:D:1049:LYS:HE2	1.87	0.42
1:A:843:LYS:HA	1:A:984:TRP:CZ2	2.55	0.42
1:B:60:VAL:HG21	1:B:198:ILE:HG21	2.01	0.42
1:C:955:LEU:HB2	1:D:900:TYR:OH	2.20	0.42
1:D:513:ARG:HD3	1:D:516:MET:HE2	2.01	0.42
1:A:822:THR:HG23	1:D:880:LEU:HD21	2.01	0.42
1:B:874:GLY:HA3	1:B:895:ALA:O	2.19	0.42
1:A:914:ALA:H	1:A:943:ASN:ND2	2.18	0.42
1:A:1049:LYS:HB3	1:A:1049:LYS:HE2	1.88	0.42
1:C:718:THR:HA	1:C:721:MET:HG2	2.02	0.42
1:C:863:LEU:HD23	1:C:863:LEU:HA	1.94	0.42
1:C:902:HIS:CE1	1:C:908:PRO:HD2	2.49	0.42
1:A:98:SER:O	1:A:100:LEU:N	2.46	0.42
1:A:221:HIS:O	1:A:221:HIS:ND1	2.51	0.42
1:B:744:PRO:HB2	1:B:748:TYR:HB2	2.01	0.42
1:B:914:ALA:H	1:B:943:ASN:ND2	2.18	0.42
1:D:914:ALA:H	1:D:943:ASN:ND2	2.18	0.42
1:D:60:VAL:HG13	1:D:96:LEU:HD23	2.01	0.42
1:D:718:THR:HA	1:D:721:MET:HG2	2.02	0.42
1:D:744:PRO:HB2	1:D:748:TYR:HB2	2.01	0.42
1:A:60:VAL:HG21	1:A:198:ILE:HG21	2.01	0.41
1:A:375:VAL:O	1:A:513:ARG:NH2	2.49	0.41
1:A:954:LEU:HD23	1:A:954:LEU:HA	1.93	0.41
1:C:951:VAL:HG13	1:D:900:TYR:CE2	2.55	0.41
1:D:78:ASP:O	1:D:81:ARG:HG2	2.20	0.41
1:A:887:ARG:NH1	1:A:929:ILE:O	2.54	0.41
1:B:754:GLU:OE2	1:B:758:TYR:OH	2.35	0.41
1:C:880:LEU:HD21	1:D:822:THR:HG23	2.02	0.41
1:C:914:ALA:H	1:C:943:ASN:ND2	2.18	0.41
1:B:78:ASP:O	1:B:81:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ASP:O	1:C:81:ARG:HG2	2.20	0.41
1:D:887:ARG:NH1	1:D:929:ILE:O	2.54	0.41
1:A:880:LEU:HD21	1:B:822:THR:HG23	2.02	0.41
1:B:759:PHE:O	1:B:763:THR:HG23	2.20	0.41
1:C:843:LYS:HA	1:C:984:TRP:CZ2	2.55	0.41
1:A:744:PRO:HB2	1:A:748:TYR:HB2	2.01	0.41
1:A:759:PHE:O	1:A:763:THR:HG23	2.20	0.41
1:C:744:PRO:HB2	1:C:748:TYR:HB2	2.01	0.41
1:A:513:ARG:HD3	1:A:516:MET:HE2	2.01	0.41
1:A:718:THR:HA	1:A:721:MET:HG2	2.02	0.41
1:D:843:LYS:HA	1:D:984:TRP:CZ2	2.55	0.41
1:A:96:LEU:HD13	1:A:129:ILE:HB	2.02	0.41
1:B:718:THR:HA	1:B:721:MET:HG2	2.02	0.41
1:C:72:LEU:HD12	1:C:104:ILE:HD13	2.03	0.41
1:C:759:PHE:O	1:C:763:THR:HG23	2.20	0.41
1:A:138:GLN:O	1:A:154:TYR:OH	2.27	0.41
1:A:836:ILE:HG23	1:A:849:ILE:HD12	2.02	0.41
1:A:951:VAL:HG13	1:B:900:TYR:CE2	2.56	0.41
1:B:513:ARG:HD3	1:B:516:MET:HE2	2.02	0.41
1:C:221:HIS:O	1:C:221:HIS:ND1	2.51	0.41
1:C:513:ARG:HD3	1:C:516:MET:HE2	2.01	0.41
1:C:754:GLU:OE2	1:C:758:TYR:OH	2.36	0.41
1:A:78:ASP:O	1:A:81:ARG:HG2	2.20	0.41
1:B:72:LEU:HD12	1:B:104:ILE:HD13	2.03	0.41
1:B:843:LYS:HA	1:B:984:TRP:CZ2	2.55	0.41
1:C:222:GLY:O	1:C:249:VAL:HG23	2.21	0.41
1:D:222:GLY:O	1:D:249:VAL:HG23	2.21	0.41
1:B:836:ILE:HG23	1:B:849:ILE:HD12	2.02	0.40
1:B:887:ARG:NH1	1:B:929:ILE:O	2.53	0.40
1:B:1049:LYS:HB3	1:B:1049:LYS:HE2	1.87	0.40
1:C:887:ARG:NH1	1:C:929:ILE:O	2.54	0.40
1:B:878:GLN:HG3	1:C:739:LEU:HD22	2.04	0.40
1:D:96:LEU:HD13	1:D:129:ILE:HB	2.02	0.40
1:D:759:PHE:O	1:D:763:THR:HG23	2.20	0.40
1:A:878:GLN:HG3	1:B:739:LEU:HD22	2.02	0.40
1:B:987:GLN:O	1:B:991:LEU:HG	2.22	0.40
1:B:222:GLY:O	1:B:249:VAL:HG23	2.22	0.40
1:C:836:ILE:HG23	1:C:849:ILE:HD12	2.02	0.40
1:C:1049:LYS:HB3	1:C:1049:LYS:HE2	1.87	0.40
1:A:222:GLY:O	1:A:249:VAL:HG23	2.22	0.40
1:B:951:VAL:HG13	1:C:900:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LEU:HA	1:C:506:LEU:HD12	1.78	0.40
1:D:98:SER:O	1:D:100:LEU:N	2.46	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 PDB entries followed by that with respect to all EM entries.

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	986/1165 (85%)	958 (97%)	27 (3%)	1 (0%)	48	48
1	B	986/1165 (85%)	958 (97%)	27 (3%)	1 (0%)	48	48
1	C	986/1165 (85%)	958 (97%)	27 (3%)	1 (0%)	48	48
1	D	986/1165 (85%)	957 (97%)	28 (3%)	1 (0%)	48	48
All	All	3944/4660 (85%)	3831 (97%)	109 (3%)	4 (0%)	50	48

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1006	Ile
1	B	1006	Ile
1	C	1006	Ile
1	D	1006	Ile

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 PDB entries followed by that with respect to all EM entries.

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	743/1018 (73%)	741 (100%)	2 (0%)	91	91
1	B	743/1018 (73%)	741 (100%)	2 (0%)	91	91
1	C	743/1018 (73%)	741 (100%)	2 (0%)	91	91
1	D	743/1018 (73%)	741 (100%)	2 (0%)	91	91
All	All	2972/4072 (73%)	2964 (100%)	8 (0%)	90	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	811	ARG
1	A	921	ASN
1	B	811	ARG
1	B	921	ASN
1	C	811	ARG
1	C	921	ASN
1	D	811	ARG
1	D	921	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	514	GLN
1	A	794	ASN
1	A	1010	HIS
1	B	514	GLN
1	B	794	ASN
1	B	1010	HIS
1	C	304	HIS
1	C	514	GLN
1	C	794	ASN
1	C	1010	HIS
1	D	304	HIS
1	D	514	GLN
1	D	794	ASN
1	D	943	ASN
1	D	1010	HIS

5.3.3 RNA ⓘ

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](#)

12 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	NAG	D	3002	1	14,14,15	0.32	0	17,19,21	0.67	0
3	YUV	C	1502	-	35,35,35	0.12	0	58,58,58	0.19	0
3	YUV	B	1502	-	35,35,35	0.12	0	58,58,58	0.19	0
2	NAG	B	1501	1	14,14,15	0.31	0	17,19,21	0.68	0
4	YUY	D	3001	-	66,66,66	0.13	0	98,102,102	0.21	0
4	YUY	C	1503	-	66,66,66	0.13	0	98,102,102	0.21	0
4	YUY	B	1503	-	66,66,66	0.13	0	98,102,102	0.21	0
2	NAG	C	1501	1	14,14,15	0.32	0	17,19,21	0.68	0
3	YUV	D	3003	-	35,35,35	0.14	0	58,58,58	0.18	0
3	YUV	A	1502	-	35,35,35	0.13	0	58,58,58	0.18	0
2	NAG	A	1501	1	14,14,15	0.30	0	17,19,21	0.69	0
4	YUY	A	1503	-	66,66,66	0.13	0	98,102,102	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	3002	1	-	2/6/23/26	0/1/1/1
3	YUV	C	1502	-	-	-	0/6/6/6
3	YUV	B	1502	-	-	-	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1501	1	-	2/6/23/26	0/1/1/1
4	YUY	D	3001	-	-	16/21/149/149	0/8/8/8
4	YUY	C	1503	-	-	16/21/149/149	0/8/8/8
4	YUY	B	1503	-	-	16/21/149/149	0/8/8/8
2	NAG	C	1501	1	-	2/6/23/26	0/1/1/1
3	YUV	D	3003	-	-	-	0/6/6/6
3	YUV	A	1502	-	-	-	0/6/6/6
2	NAG	A	1501	1	-	2/6/23/26	0/1/1/1
4	YUY	A	1503	-	-	16/21/149/149	0/8/8/8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (72) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1503	YUY	C43-C29-C30-O3
4	A	1503	YUY	C28-C29-C43-O14
4	B	1503	YUY	C43-C29-C30-O3
4	B	1503	YUY	C28-C29-C43-O14
4	C	1503	YUY	C43-C29-C30-O3
4	C	1503	YUY	C28-C29-C43-O14
4	D	3001	YUY	C43-C29-C30-O3
4	D	3001	YUY	C28-C29-C43-O14
4	A	1503	YUY	O4-C35-C36-O5
4	B	1503	YUY	O4-C35-C36-O5
4	C	1503	YUY	O4-C35-C36-O5
4	D	3001	YUY	O4-C35-C36-O5
4	A	1503	YUY	C34-C35-C36-O5
4	B	1503	YUY	C34-C35-C36-O5
4	C	1503	YUY	C34-C35-C36-O5
4	D	3001	YUY	C34-C35-C36-O5
4	A	1503	YUY	O7-C37-O6-C34
4	B	1503	YUY	O7-C37-O6-C34
4	C	1503	YUY	O7-C37-O6-C34
4	D	3001	YUY	O7-C37-O6-C34
4	A	1503	YUY	O7-C41-C42-O8
4	B	1503	YUY	O7-C41-C42-O8
4	C	1503	YUY	O7-C41-C42-O8

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Mol	Chain	Res	Type	Atoms
4	D	3001	YUY	O7-C41-C42-O8
4	A	1503	YUY	C40-C41-C42-O8
4	B	1503	YUY	C40-C41-C42-O8
4	C	1503	YUY	C40-C41-C42-O8
4	D	3001	YUY	C40-C41-C42-O8
4	A	1503	YUY	C38-C37-O6-C34
4	B	1503	YUY	C38-C37-O6-C34
4	C	1503	YUY	C38-C37-O6-C34
4	D	3001	YUY	C38-C37-O6-C34
4	A	1503	YUY	C28-C29-C30-O3
4	B	1503	YUY	C28-C29-C30-O3
4	C	1503	YUY	C28-C29-C30-O3
4	D	3001	YUY	C28-C29-C30-O3
2	A	1501	NAG	O5-C5-C6-O6
2	B	1501	NAG	O5-C5-C6-O6
2	C	1501	NAG	O5-C5-C6-O6
2	D	3002	NAG	O5-C5-C6-O6
4	A	1503	YUY	C30-C29-C43-O14
4	B	1503	YUY	C30-C29-C43-O14
4	C	1503	YUY	C30-C29-C43-O14
4	D	3001	YUY	C30-C29-C43-O14
4	A	1503	YUY	C28-C27-O2-C14
4	B	1503	YUY	C28-C27-O2-C14
4	C	1503	YUY	C28-C27-O2-C14
4	D	3001	YUY	C28-C27-O2-C14
4	A	1503	YUY	C13-C14-O2-C27
4	A	1503	YUY	C15-C14-O2-C27
4	B	1503	YUY	C13-C14-O2-C27
4	B	1503	YUY	C15-C14-O2-C27
4	C	1503	YUY	C13-C14-O2-C27
4	C	1503	YUY	C15-C14-O2-C27
4	D	3001	YUY	C13-C14-O2-C27
4	D	3001	YUY	C15-C14-O2-C27
4	A	1503	YUY	O4-C31-O3-C30
4	C	1503	YUY	O4-C31-O3-C30
4	A	1503	YUY	C29-C30-O3-C31
4	B	1503	YUY	C29-C30-O3-C31
4	C	1503	YUY	C29-C30-O3-C31
4	D	3001	YUY	C29-C30-O3-C31
4	B	1503	YUY	O4-C31-O3-C30
4	D	3001	YUY	O4-C31-O3-C30
2	A	1501	NAG	C1-C2-N2-C7

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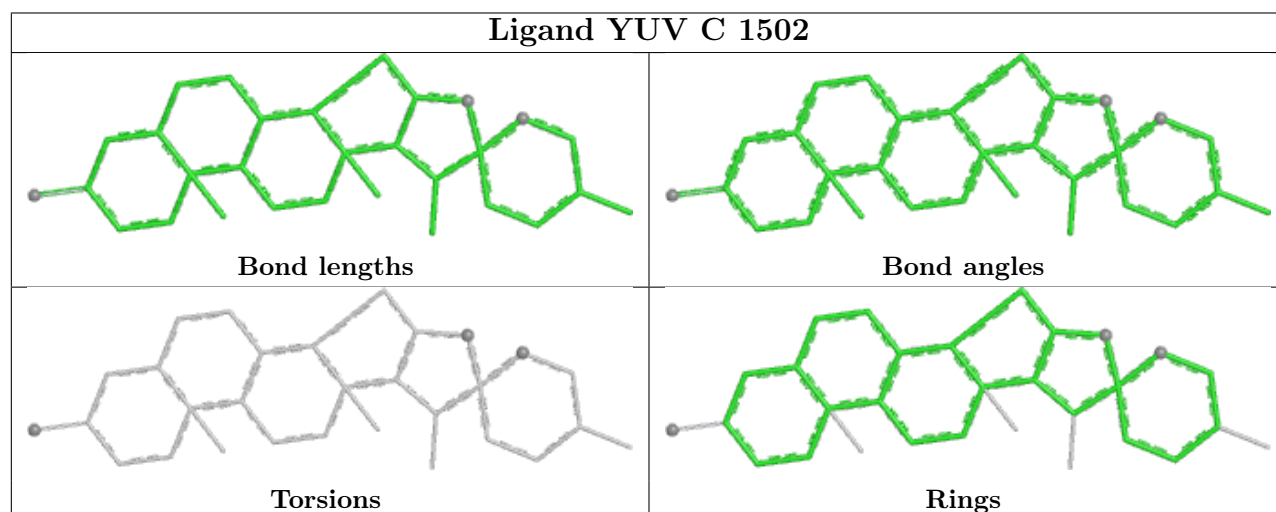
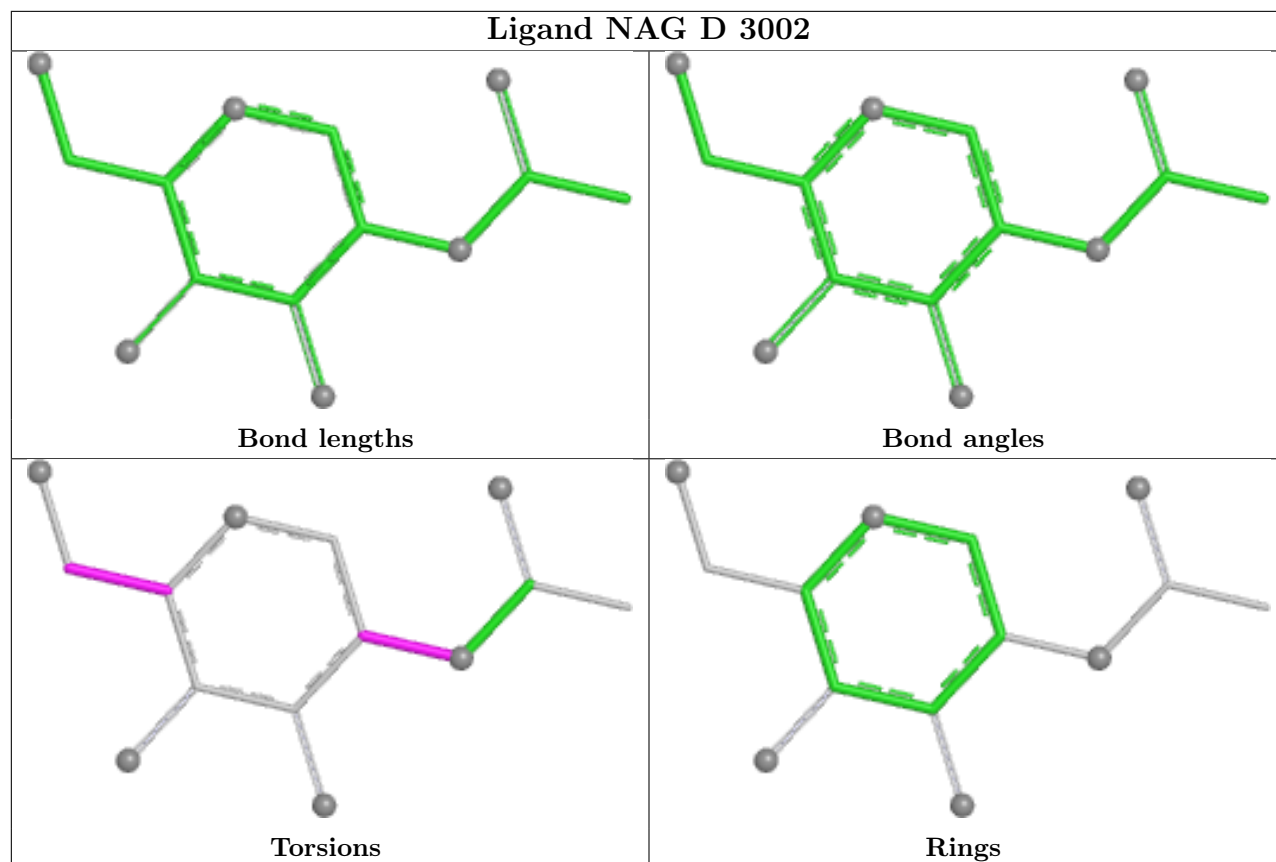
Mol	Chain	Res	Type	Atoms
2	B	1501	NAG	C1-C2-N2-C7
2	C	1501	NAG	C1-C2-N2-C7
2	D	3002	NAG	C1-C2-N2-C7
4	A	1503	YUY	O2-C27-C28-C29
4	B	1503	YUY	O2-C27-C28-C29
4	C	1503	YUY	O2-C27-C28-C29
4	D	3001	YUY	O2-C27-C28-C29

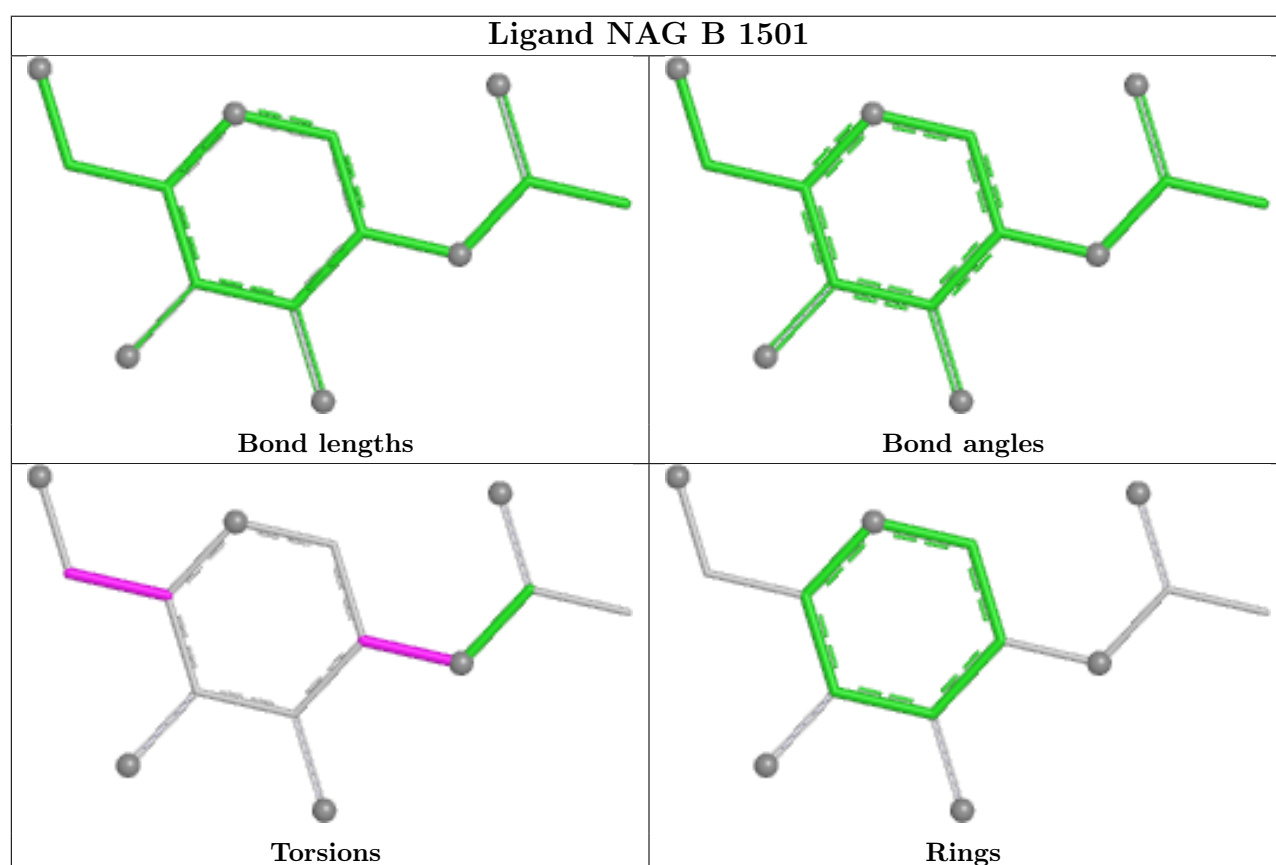
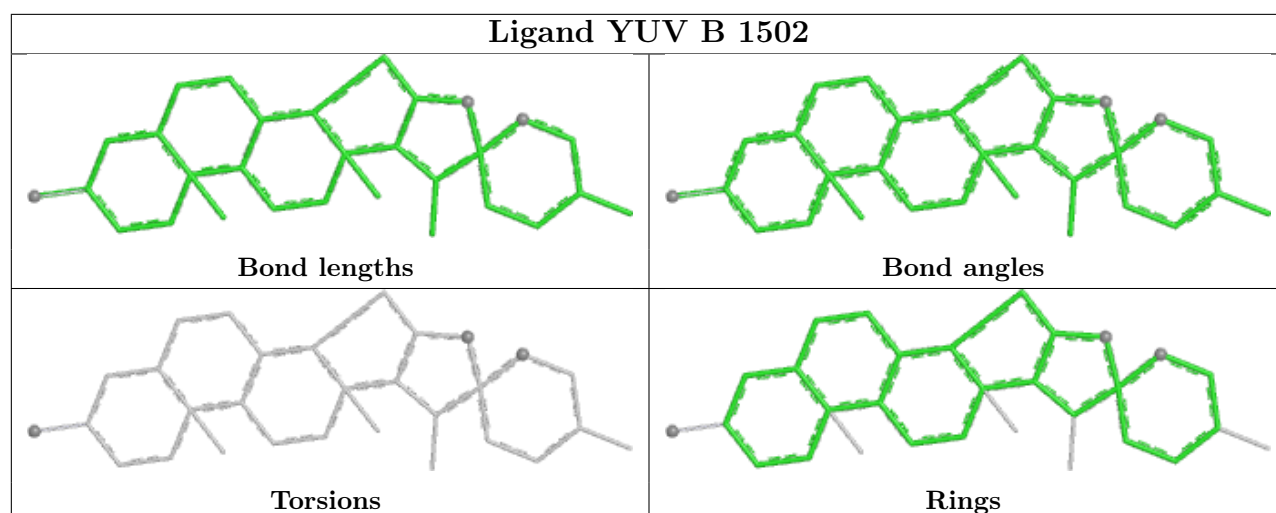
There are no ring outliers.

4 monomers are involved in 4 short contacts:

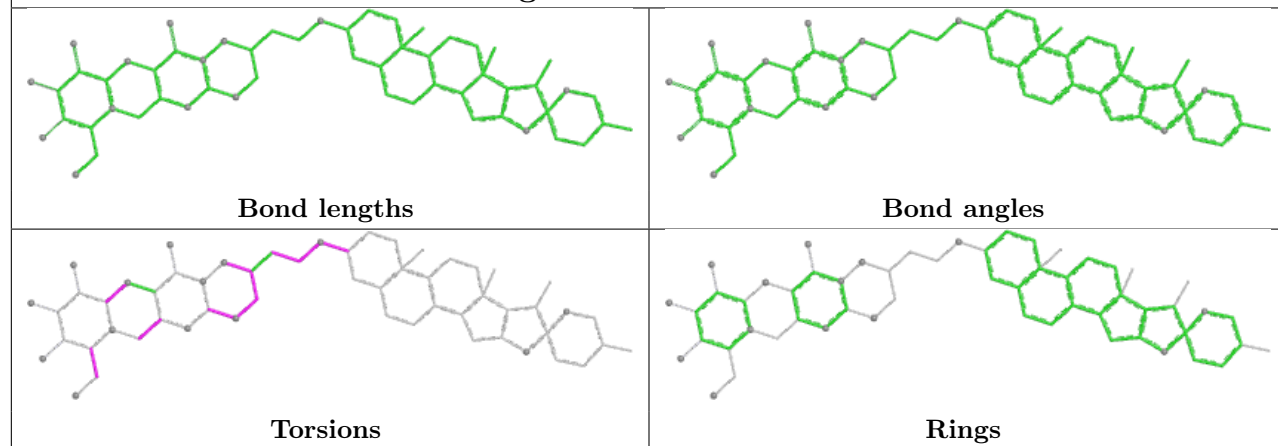
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	3001	YUY	1	0
4	C	1503	YUY	1	0
4	B	1503	YUY	1	0
4	A	1503	YUY	1	0

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.

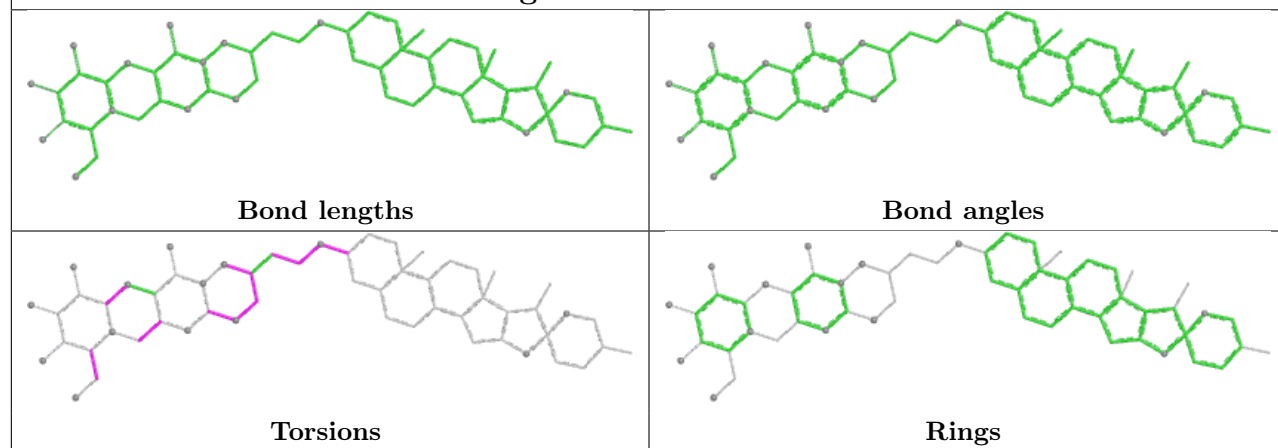




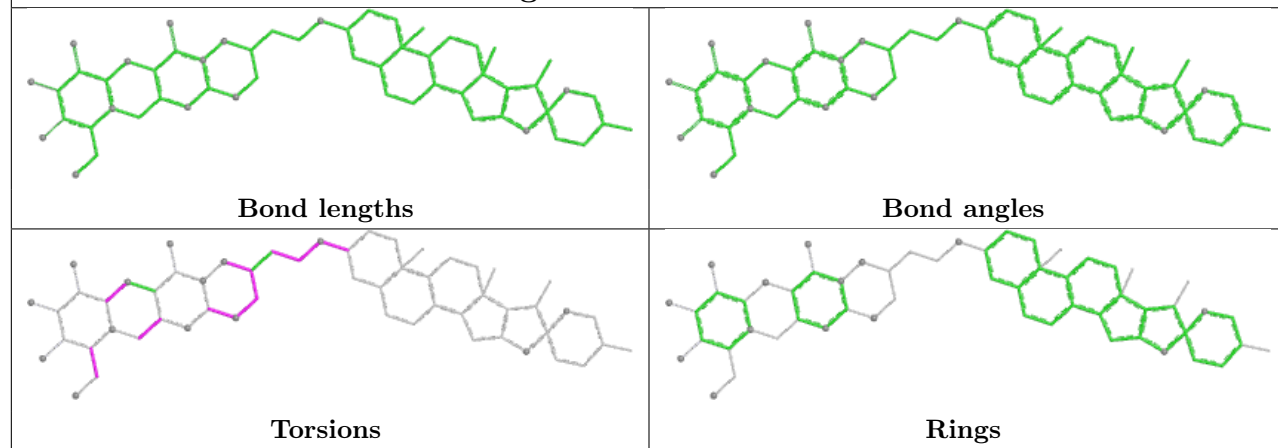
Ligand YUY D 3001

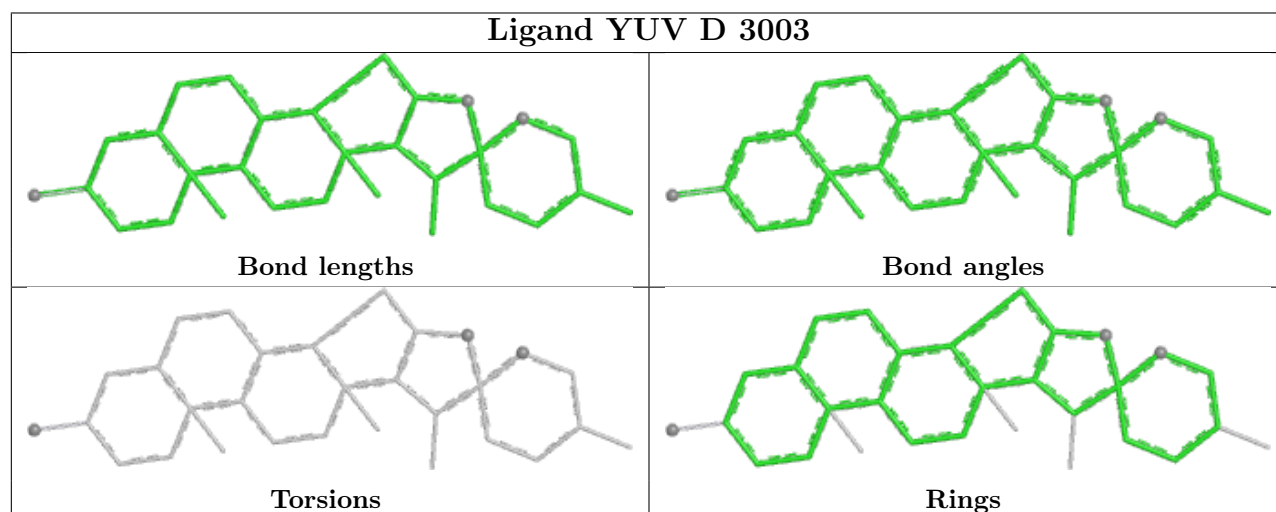
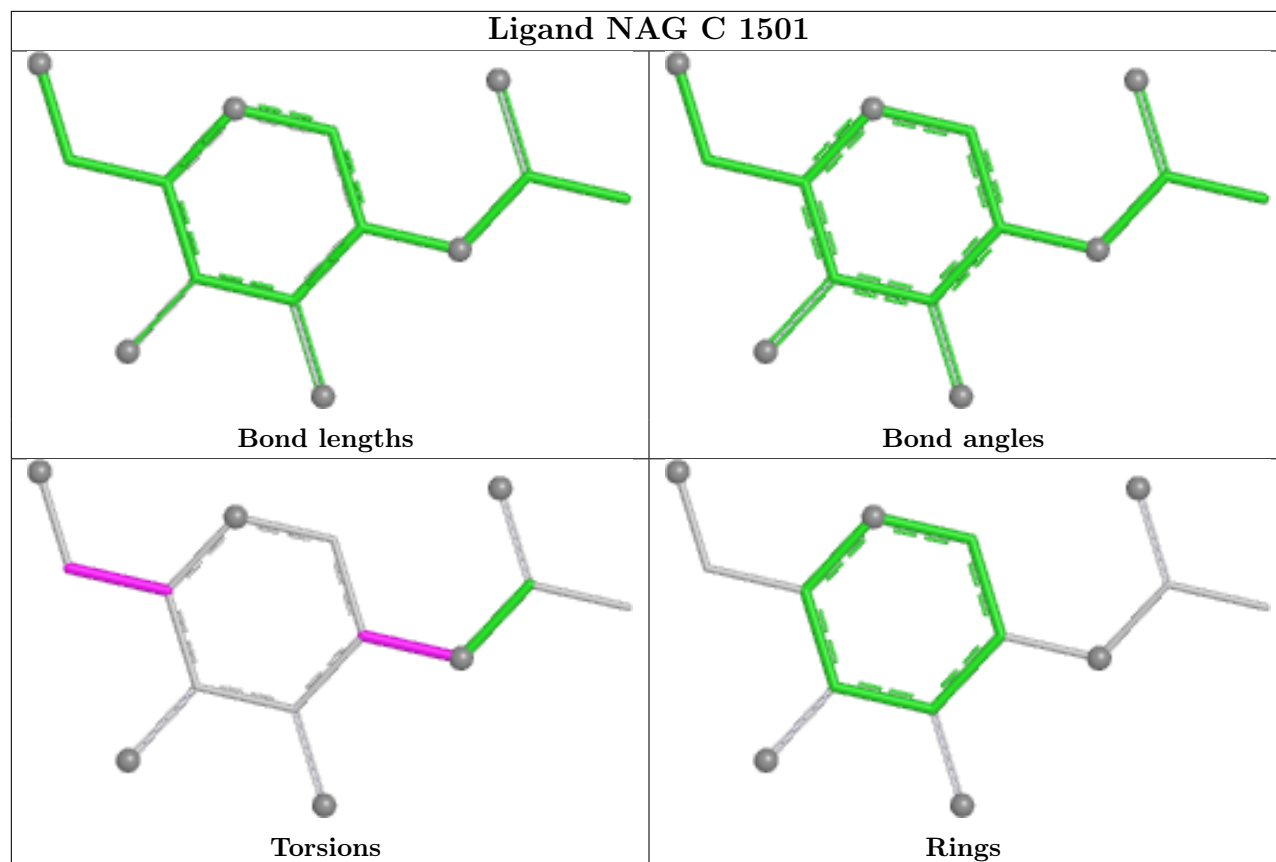


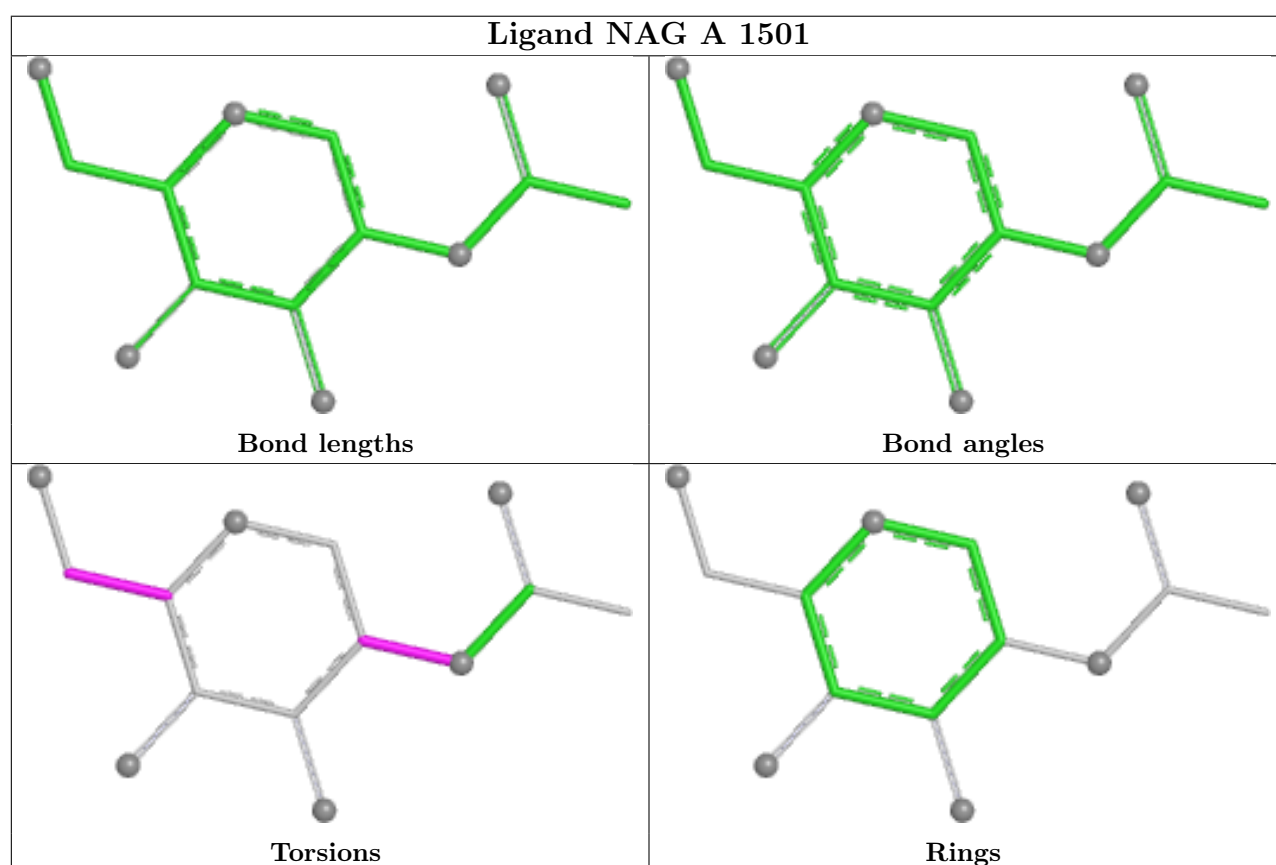
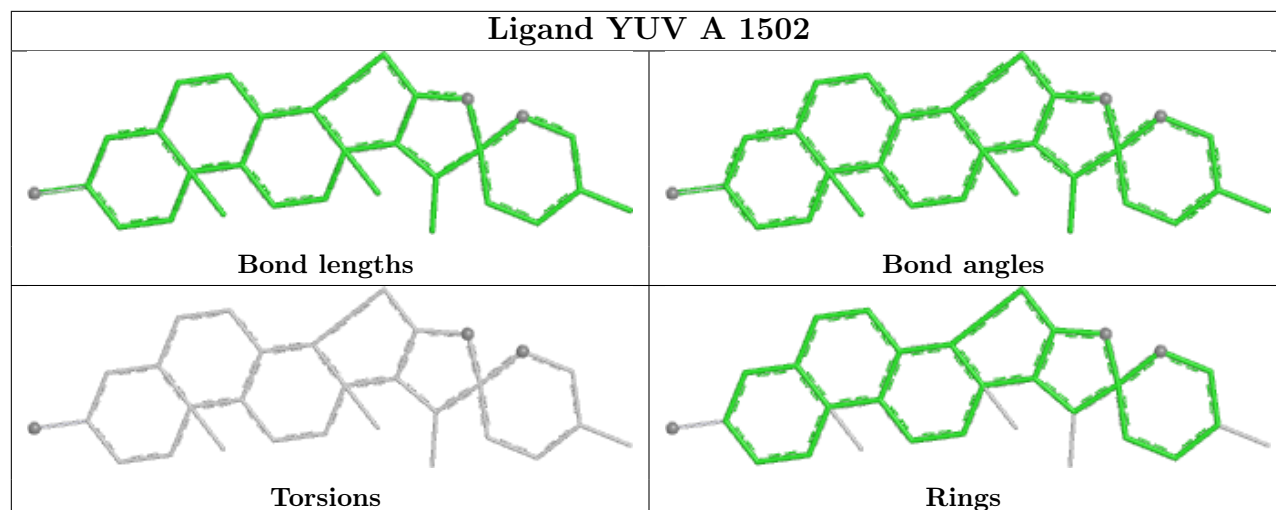
Ligand YUY C 1503

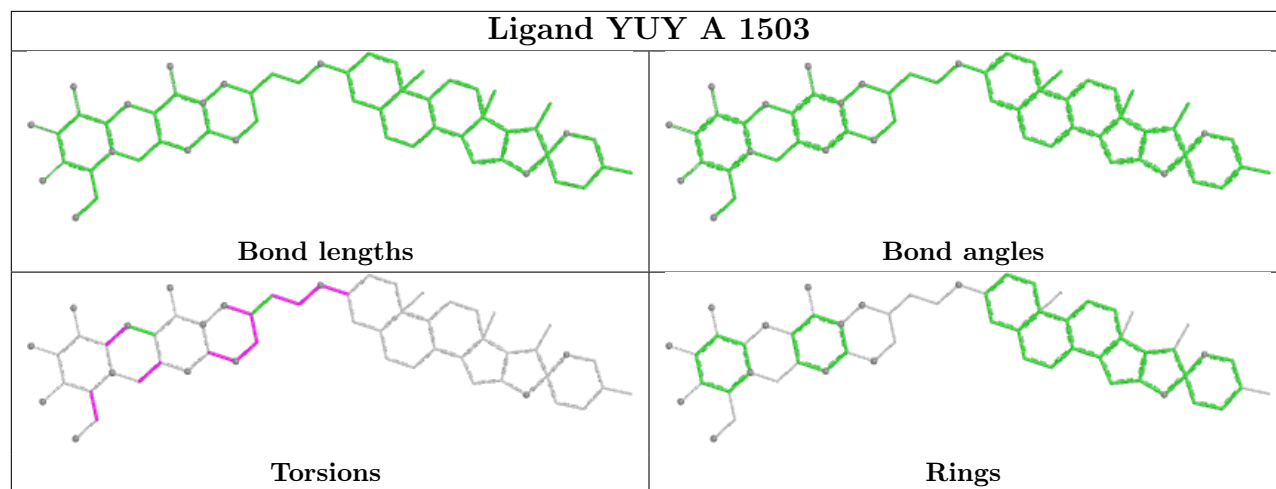


Ligand YUY B 1503









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 Map visualisation

This section contains visualisations of the EMDB entry EMD-23744. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.