



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 7MBU / pdb_00007mbu
EMDB ID : EMD-23747
Title : Cryo-EM structure of zebrafish TRPM5 E337A mutant in the presence of 5 mM calcium (high calcium occupancy in the transmembrane domain)
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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

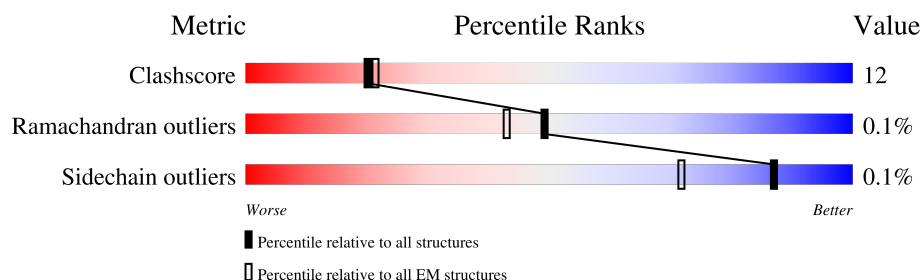
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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	67% 18% 15%
1	B	1165	67% 19% 15%
1	C	1165	67% 19% 15%
1	D	1165	67% 19% 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 30780 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.

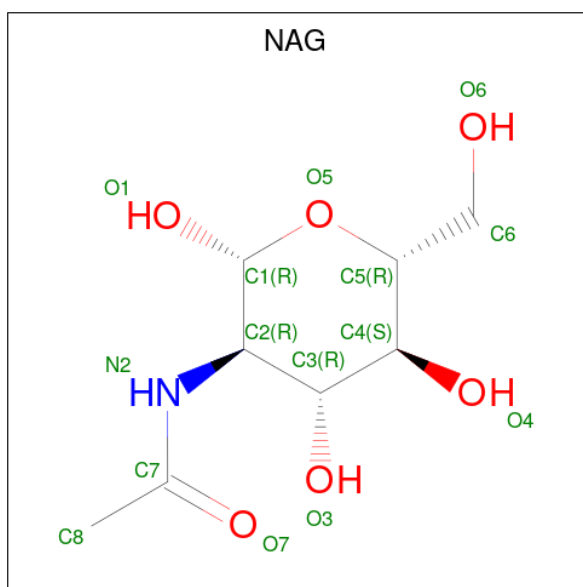
- Molecule 1 is a protein called Transient receptor potential melastatin 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	B	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	C	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		
1	D	996	Total	C	N	O	S	1	0
			7591	4976	1299	1272	44		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	337	ALA	GLU	engineered mutation	UNP S5UH55
B	337	ALA	GLU	engineered mutation	UNP S5UH55
C	337	ALA	GLU	engineered mutation	UNP S5UH55
D	337	ALA	GLU	engineered mutation	UNP S5UH55

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

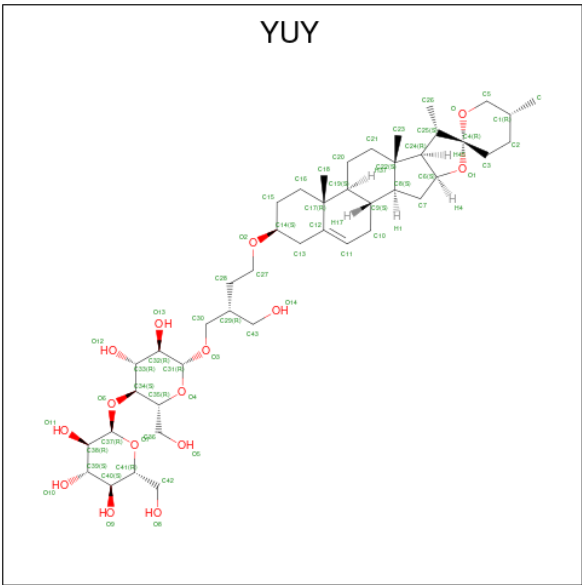


Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	B	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2	D	1	Total	C	N	O	0
			14	8	1	5	

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

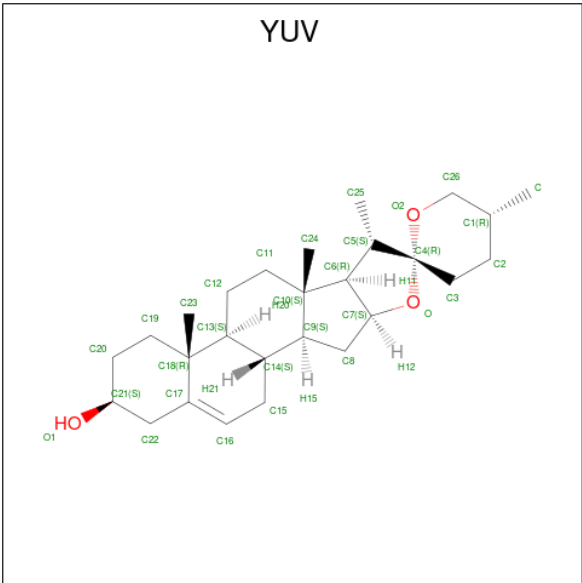
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	Ca	0
			1	1	
3	B	1	Total	Ca	0
			1	1	
3	C	1	Total	Ca	0
			1	1	
3	D	1	Total	Ca	0
			1	1	

- Molecule 4 is (2R)-2-(hydroxymethyl)-4-{[(25R)-10 α ,14 β ,17 β -spirost-5-en-3 β -yl]oxy}butyl 4-O- α -D-glucopyranosyl- β -D-glucopyranoside (CCD ID: YUY) (formula: C₄₄H₇₂O₁₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is (25R)-14beta,17beta-spirost-5-en-3beta-ol (CCD ID: YUV) (formula: C₂₇H₄₂O₃) (labeled as "Ligand of Interest" by depositor).

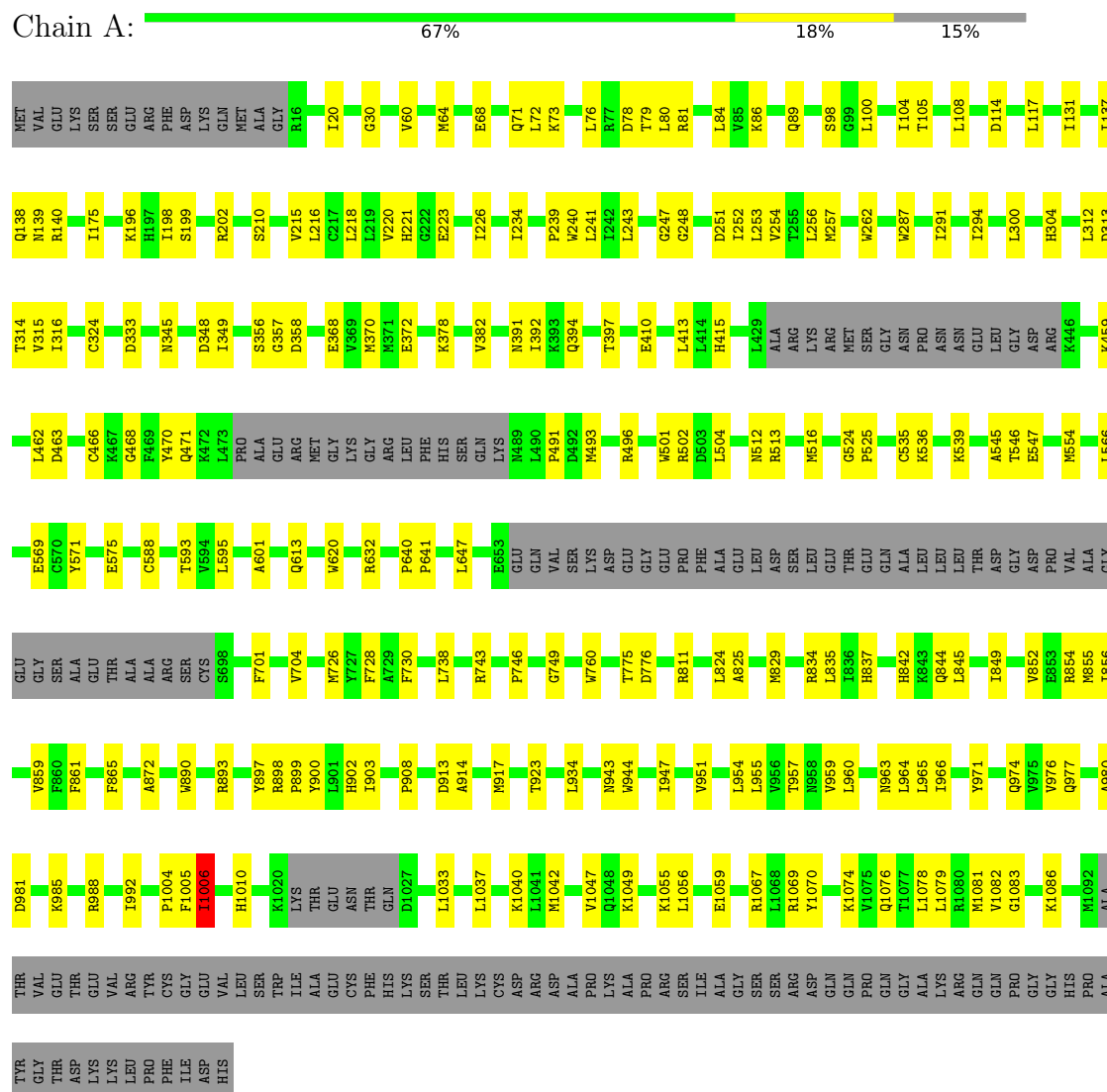


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total 30	C 27	O 3	0
5	B	1	Total 30	C 27	O 3	0
5	C	1	Total 30	C 27	O 3	0
5	D	1	Total 30	C 27	O 3	0

3 Residue-property plots

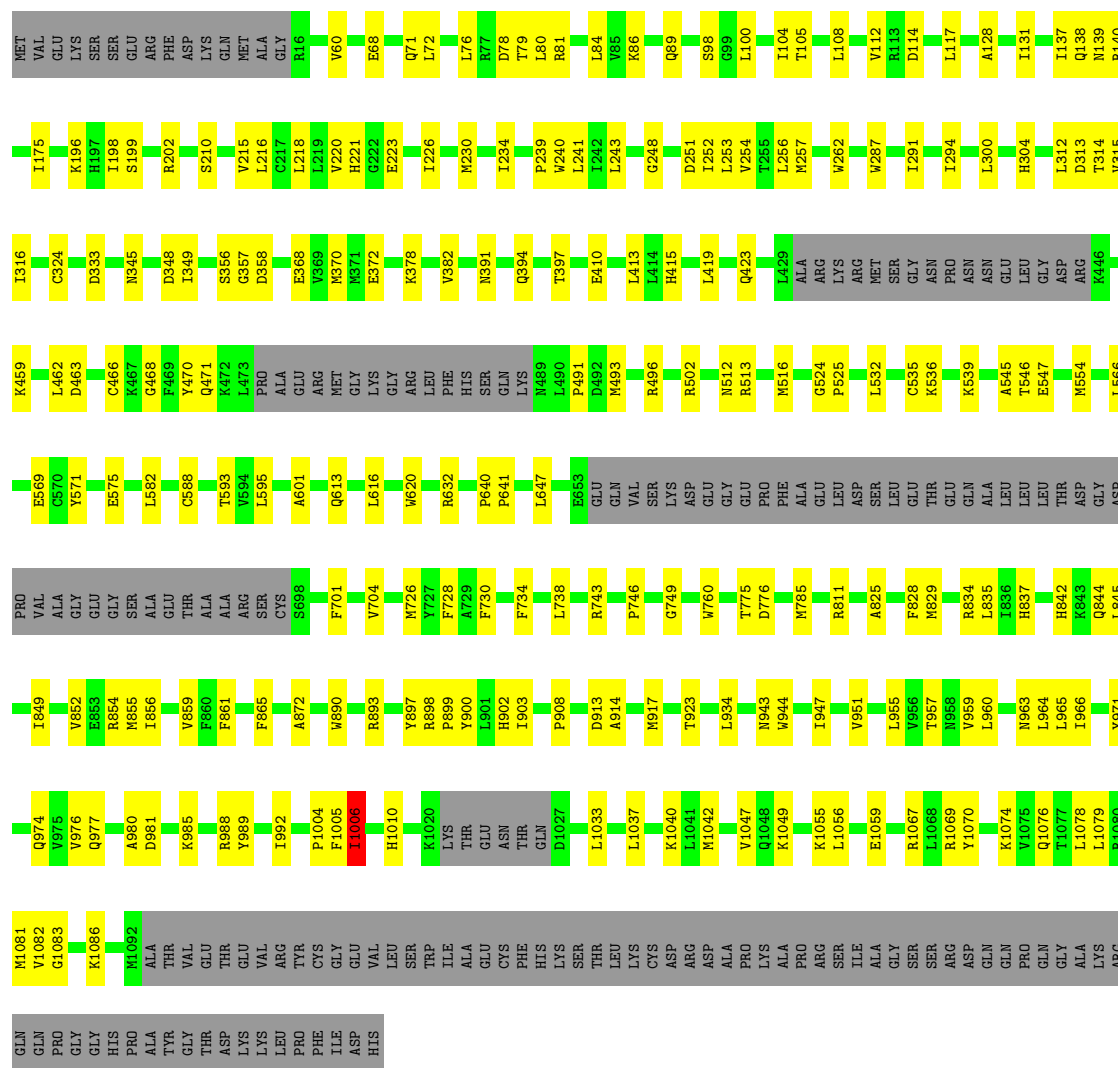
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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: Transient receptor potential melastatin 5



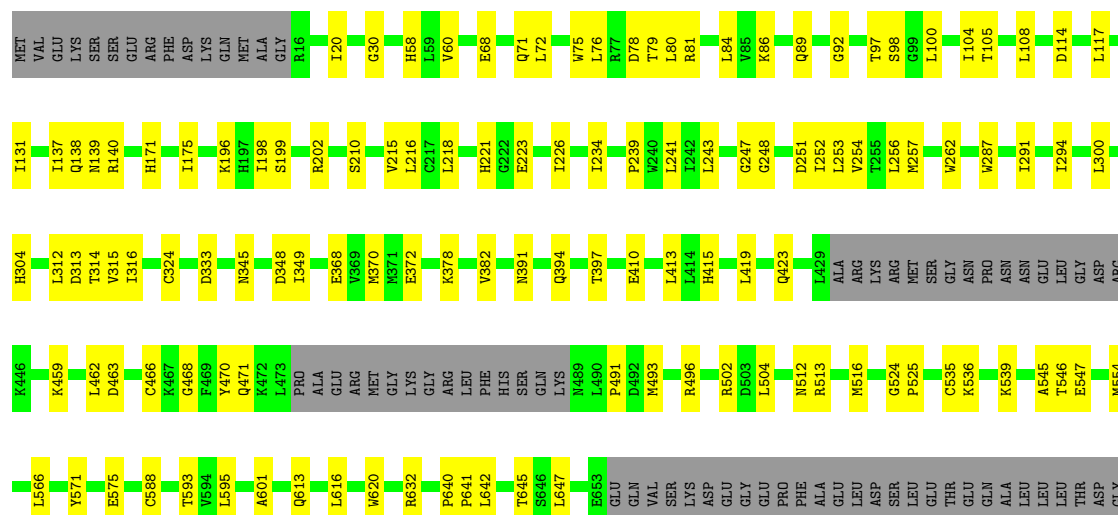
- Molecule 1: Transient receptor potential melastatin 5





• Molecule 1: Transient receptor potential melastatin 5

Chain C: 67% 19% 15%



ASP	PRO	VAL	ALA	GLY	GLY	SER	ALA	GLU	THR	ALA	ALA	ARG	SER	CYS	S698	F701	V704	M726	Y727	F728	A729	F730	F734	L738	R743	P746	G749	W760	T763	T775	D776	M785	R811	A825	F828	M829	R834	L835	I836	H837	L964	H842					
K843	Q844	L845	I849	V852	E853	R854	M855	I856	V859	F860	F861	F865	A872	W890	R893	Y897	R898	P899	Y900	L901	H902	I903	P908	D913	A914	M917	T923	L934	N943	W944	I947	V951	L955	V956	N958	V959	L960	N963	L964	L965							
I966	Y971	Q974	V975	Q976	Q977	A980	D981	K985	R988	Y989	I992	F1004	F1005	I1006	H1010	K1020	LYS	THR	GLU	ASN	THR	GLN	D1027	L1033	L1037	K1040	L1041	M1042	V1047	Q1048	K1049	L1056	E1059	R1067	L1068	R1069	Y1070	K1074	V1075	Q1076	T1077	L1078					
L1079	R1080	M1081	V1082	G1083	K1086	M1092	ALA	THR	VAL	GLU	THR	ASP	GLU	VAL	ARG	TYR	CYS	GLY	VAL	LEU	SER	TRP	ILE	ALA	GLU	CYS	ASP	ARG	ALA	PRO	LYS	ALA	PRO	ARG	ILE	ALA	GLY	SER	SER	ARG	ASP	GLN	PRO	GLN	GLY	ALA	
LYS	ARG	GLN	GLN	PRO	GLY	GLY	HIS	PRO	ALA	THR	GLY	ASP	LYS	VAL	LEU	PRO	PHE	ILE	HIS																												

• Molecule 1: Transient receptor potential melastatin 5

Chain D:  67% 19% 15%

LYS	L1079	Y971	Q844	GLY	M554	GLY	L300	L117	MET
ARG	R1080	Y971	L845	ASP	M554	ASP	L300	L117	GLU
GLN	M1081	Q974	L845	PRO	L566	ARG	H304	I131	LYS
PRO	G1083	V975	I849	VAL	L566	K446	L312	I137	SER
GLY	K1086	V976	V852	ALA	E569	K459	D313	Q138	SER
LYS		Q977	E853	GLY	C570	K459	D313	Q138	GLU
GLY			R854	GLU	Y571	L462	T314	N139	ARG
PRO	M1092	A980	M855	SER	E575	D463	V315	R140	PHE
ALA		D981	I856	ALA			I316	I175	ASP
THR				GLU		C466	C324	I175	LYS
VAL		K985	V859	THR	C588	K467	D333	K196	GLN
GLY			F860	ALA		G468	D333	H197	MET
THR		R988	F861	ALA	T593	F469	N345	I198	ALA
ASP		Y989	F865	ARG	V594	Y470	N345	S199	GLY
LYS				SER	L595	Q471			GLY
VAL		I992		CYS		K472		R202	R16
ARG			A872		A601	L473	D348		
LEU						PRO	I349		I20
PRO								S210	
PHE		P1004	W890		Q613	ALA	E368		G30
ILE		F1005		F701		GLU	V369	V215	
ASP		I1006			L616	ARG	M370	L216	H58
HIS			R893	V704		MET	M371	C217	L59
		H1010				GLY	E372	L218	V60
			Y897	M726	W820	LYS		L219	
		K1020	R898	Y727		GLY			M64
TRP			P899	F728	R632	GLY	K378	H221	
ILE		LYS	Y900	A729		ARG	V220		E68
ALA		ALA				ARG	V382	E223	LEU
GLU		GLU	L901	F730	P640	LEU			Q71
GLU		ASN	H902		P641	PHE	N391	I226	L72
CYS		THR	I903	F734		HIS	I392	L227	K73
PHE		GLN			L647	SER	K393		P74
HIS			P908	L738		GLN	Q394		W75
LYS		D1027			E653	LYS		L234	L76
SER			D913	R743	GLU	N489			R77
THR		L1033	A914		GLN	L490	T397	P239	D78
LEU				P746	VAL	P491		W240	T79
LYS		L1037	M917		SER	D492	E410	L241	L80
CYS				G749	LYS	M493	L413	L242	R81
ASP		K1040	T923		ASP		L413	L243	
ARG		L1041		W760	GLY	R496	H415		
ASP		M1042	L934		GLY			G247	L84
ALA					GLU	W501	L419	G248	V85
PRO		V1047	N943	T763	PRO	R502			K86
LYS		Q1048	W944	T775	PHE		Q423	D251	Q89
ALA		K1049		D776	ALA	N512		L252	
PRO			I947		GLU	R513		L253	G92
ARG		K1055		R811	LEU		L429	V254	S98
SER		L1056	V951		ASP	M516	ALA	T255	
ILE					SER		ARG		
ALA		E1059		A825	SER		LYS	M257	L100
GLY			L955		LEU	G524	ARG		
SER		R1067	V956	F828	GLU	P525	ARG		
SER				M829	THR		MET		
ARG		L1068	N957		GLY	C535	SER	W262	I104
ASP		R1069	N958		GLU	K536	GLY		T105
ASP		Y1070	V959	R834	GLN		ASN	W287	L108
GLN			L960	L835	ALA		ASN		
		K1074		H837	LEU	K539	PRO	I291	
PRO		V1075	N963		LEU		ASN		
GLN		Q1076	L964		LEU	A545	ASN		
GLN				H837	LEU	T546	GLU	I294	D114
GLY		T1077	L965	H842	THR		LEU		
ALA		L1078	T966	K843	ASP	E547	LEU		

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	139000	Depositor
Resolution determination method	Not provided	
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k 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: CA, NAG, YUV, YUY

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	0/7784	0.37	0/10616
1	B	0.25	0/7784	0.37	0/10616
1	C	0.25	0/7784	0.37	0/10616
1	D	0.25	0/7784	0.37	0/10616
All	All	0.25	0/31136	0.37	0/42464

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	7591	0	7422	249	0
1	B	7591	0	7422	251	0
1	C	7591	0	7422	250	0
1	D	7591	0	7422	252	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	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	118	0	0	9	0
4	B	59	0	0	4	0
4	C	59	0	0	4	0
5	A	30	0	0	0	0
5	B	30	0	0	0	0
5	C	30	0	0	0	0
5	D	30	0	0	0	0
All	All	30780	0	29740	742	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 12.

All (742) 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:1083:GLY:CA	1:C:1081:MET:HE1	1.43	1.47
1:A:1083:GLY:CA	1:B:1081:MET:HE1	1.41	1.45
1:C:1083:GLY:CA	1:D:1081:MET:HE1	1.43	1.45
1:A:1081:MET:HE1	1:D:1083:GLY:CA	1.43	1.44
1:A:1078:LEU:HD11	1:D:1078:LEU:CD2	1.58	1.34
1:C:1078:LEU:CD2	1:D:1078:LEU:HD11	1.58	1.34
1:A:1078:LEU:CD2	1:B:1078:LEU:HD11	1.58	1.32
1:B:1078:LEU:CD2	1:C:1078:LEU:HD11	1.60	1.29
1:A:1083:GLY:HA2	1:B:1081:MET:CE	1.63	1.28
1:B:1083:GLY:HA2	1:C:1081:MET:CE	1.65	1.27
1:A:1081:MET:CE	1:D:1083:GLY:HA2	1.65	1.26
1:C:861:PHE:CE1	1:D:845:LEU:HA	1.70	1.25
1:C:1083:GLY:HA2	1:D:1081:MET:CE	1.66	1.24
1:C:861:PHE:HE1	1:D:845:LEU:CA	1.46	1.24
1:A:861:PHE:CE1	1:B:845:LEU:HA	1.71	1.23
1:B:861:PHE:HE1	1:C:845:LEU:CA	1.47	1.22
1:B:861:PHE:CE1	1:C:845:LEU:HA	1.71	1.21
1:A:845:LEU:CA	1:D:861:PHE:HE1	1.47	1.20
1:A:845:LEU:HA	1:D:861:PHE:CE1	1.71	1.19
1:A:861:PHE:HE1	1:B:845:LEU:CA	1.47	1.16
1:A:1081:MET:CE	1:D:1082:VAL:O	1.94	1.16
1:A:1082:VAL:O	1:B:1081:MET:CE	1.94	1.14
1:A:726:MET:HE2	1:A:1005:PHE:HE2	1.10	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:PHE:HZ	1:B:849:ILE:HD13	1.11	1.13
1:A:1078:LEU:HD11	1:D:1078:LEU:HD23	1.30	1.13
1:C:1082:VAL:O	1:D:1081:MET:CE	1.95	1.13
1:C:1078:LEU:HD23	1:D:1078:LEU:HD11	1.32	1.12
1:B:726:MET:HE2	1:B:1005:PHE:HE2	1.10	1.12
1:B:1082:VAL:O	1:C:1081:MET:CE	1.96	1.12
1:D:726:MET:HE2	1:D:1005:PHE:HE2	1.10	1.11
1:B:865:PHE:HZ	1:C:849:ILE:HD13	1.10	1.11
1:C:865:PHE:CZ	1:D:849:ILE:HD13	1.86	1.10
1:B:861:PHE:HE1	1:C:845:LEU:HA	1.02	1.09
1:B:865:PHE:CZ	1:C:849:ILE:HD13	1.88	1.09
1:C:726:MET:HE2	1:C:1005:PHE:HE2	1.10	1.09
1:B:1078:LEU:HD23	1:C:1078:LEU:HD11	1.32	1.09
1:C:861:PHE:HE1	1:D:845:LEU:HA	1.00	1.08
1:A:1078:LEU:HD23	1:B:1078:LEU:HD11	1.30	1.08
1:A:849:ILE:HD13	1:D:865:PHE:HZ	1.11	1.07
1:C:865:PHE:HZ	1:D:849:ILE:HD13	1.10	1.07
1:C:117:LEU:HD22	1:D:1040:LYS:HD3	1.34	1.07
1:A:865:PHE:CZ	1:B:849:ILE:HD13	1.88	1.07
1:A:849:ILE:HD13	1:D:865:PHE:CZ	1.88	1.06
1:A:845:LEU:HA	1:D:861:PHE:HE1	1.01	1.06
1:A:1082:VAL:C	1:B:1081:MET:HE2	1.81	1.06
1:B:117:LEU:HD22	1:C:1040:LYS:HD3	1.32	1.05
1:A:1081:MET:HE2	1:D:1082:VAL:C	1.81	1.05
1:C:1082:VAL:C	1:D:1081:MET:HE2	1.82	1.04
1:A:1040:LYS:HD3	1:D:117:LEU:HD22	1.32	1.04
1:A:861:PHE:CE1	1:B:845:LEU:CA	2.35	1.04
1:A:117:LEU:HD22	1:B:1040:LYS:HD3	1.33	1.04
1:C:861:PHE:CE1	1:D:845:LEU:CA	2.34	1.03
1:B:1082:VAL:C	1:C:1081:MET:HE2	1.84	1.03
1:A:971:TYR:HD1	1:B:974:GLN:OE1	1.41	1.01
1:C:971:TYR:HD1	1:D:974:GLN:OE1	1.42	1.01
1:C:1078:LEU:HD22	1:D:1078:LEU:HD11	1.42	1.01
1:A:974:GLN:OE1	1:D:971:TYR:HD1	1.41	1.01
1:A:1081:MET:CE	1:D:1082:VAL:C	2.35	1.00
1:A:1082:VAL:C	1:B:1081:MET:CE	2.34	1.00
1:B:971:TYR:HD1	1:C:974:GLN:OE1	1.43	1.00
1:A:1078:LEU:HD22	1:B:1078:LEU:HD11	1.43	0.99
1:A:861:PHE:HE1	1:B:845:LEU:HA	1.00	0.98
1:B:726:MET:HE2	1:B:1005:PHE:CE2	1.99	0.98
1:C:1082:VAL:C	1:D:1081:MET:CE	2.35	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:LEU:HD11	1:D:1078:LEU:HD22	1.43	0.97
1:C:726:MET:HE2	1:C:1005:PHE:CE2	1.99	0.97
1:D:726:MET:HE2	1:D:1005:PHE:CE2	1.99	0.97
1:B:1078:LEU:HD22	1:C:1078:LEU:HD11	1.45	0.96
1:A:726:MET:HE2	1:A:1005:PHE:CE2	1.99	0.96
1:B:1082:VAL:C	1:C:1081:MET:CE	2.37	0.96
1:C:861:PHE:CD1	1:D:845:LEU:HD23	2.00	0.96
1:A:845:LEU:HD23	1:D:861:PHE:CD1	2.01	0.95
1:B:861:PHE:CD1	1:C:845:LEU:HD23	2.01	0.95
1:A:861:PHE:CD1	1:B:845:LEU:HD23	2.01	0.94
1:A:861:PHE:HD1	1:B:845:LEU:HD23	1.32	0.94
1:B:1086:LYS:CB	1:C:1081:MET:HE3	1.97	0.94
1:A:951:VAL:HG13	1:B:900:TYR:CE2	2.02	0.93
1:C:951:VAL:HG13	1:D:900:TYR:CE2	2.03	0.93
1:A:845:LEU:HD23	1:D:861:PHE:HD1	1.32	0.93
1:B:951:VAL:HG13	1:C:900:TYR:CE2	2.03	0.93
1:C:861:PHE:HD1	1:D:845:LEU:HD23	1.31	0.93
1:B:861:PHE:CE2	1:C:844:GLN:HB3	1.98	0.93
1:A:1081:MET:HE3	1:D:1086:LYS:CB	1.98	0.92
1:A:900:TYR:CE2	1:D:951:VAL:HG13	2.03	0.92
1:D:726:MET:CE	1:D:1005:PHE:HE2	1.83	0.92
1:A:1086:LYS:CB	1:B:1081:MET:HE3	1.99	0.92
1:C:1086:LYS:CB	1:D:1081:MET:HE3	2.00	0.92
1:C:726:MET:CE	1:C:1005:PHE:HE2	1.83	0.92
1:C:861:PHE:CE2	1:D:844:GLN:HB3	1.98	0.92
1:A:1081:MET:CE	1:D:1083:GLY:CA	2.36	0.91
1:A:726:MET:CE	1:A:1005:PHE:HE2	1.83	0.91
1:D:726:MET:CE	1:D:1005:PHE:CE2	2.54	0.91
1:C:726:MET:CE	1:C:1005:PHE:CE2	2.54	0.91
1:B:726:MET:CE	1:B:1005:PHE:HE2	1.83	0.91
1:C:964:LEU:HD13	1:D:855:MET:HG3	1.52	0.91
1:B:726:MET:CE	1:B:1005:PHE:CE2	2.54	0.91
1:A:855:MET:HG3	1:D:964:LEU:HD13	1.53	0.90
1:A:726:MET:CE	1:A:1005:PHE:CE2	2.54	0.90
1:A:849:ILE:CD1	1:D:865:PHE:CZ	2.55	0.90
1:A:974:GLN:OE1	1:D:971:TYR:CD1	2.25	0.90
1:A:971:TYR:CD1	1:B:974:GLN:OE1	2.25	0.90
1:C:865:PHE:CZ	1:D:849:ILE:CD1	2.53	0.90
1:A:964:LEU:HD13	1:B:855:MET:HG3	1.53	0.89
1:B:861:PHE:HD1	1:C:845:LEU:HD23	1.32	0.89
1:B:865:PHE:CZ	1:C:849:ILE:CD1	2.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:PHE:CZ	1:B:849:ILE:CD1	2.55	0.89
1:A:1083:GLY:CA	1:B:1081:MET:CE	2.34	0.89
1:C:971:TYR:CD1	1:D:974:GLN:OE1	2.26	0.88
1:A:1078:LEU:CD2	1:B:1078:LEU:CD1	2.51	0.87
1:A:900:TYR:OH	1:D:955:LEU:HB2	1.74	0.87
1:B:971:TYR:CD1	1:C:974:GLN:OE1	2.27	0.87
1:C:1078:LEU:CD2	1:D:1078:LEU:CD1	2.51	0.87
1:A:844:GLN:HB3	1:D:861:PHE:CE2	1.99	0.87
1:C:955:LEU:HB2	1:D:900:TYR:OH	1.75	0.87
1:B:964:LEU:HD13	1:C:855:MET:HG3	1.54	0.86
1:A:955:LEU:HB2	1:B:900:TYR:OH	1.74	0.86
1:A:845:LEU:CA	1:D:861:PHE:CE1	2.35	0.86
1:B:861:PHE:CE1	1:C:845:LEU:CA	2.35	0.86
1:A:1078:LEU:CD1	1:D:1078:LEU:CD2	2.50	0.85
1:B:955:LEU:HB2	1:C:900:TYR:OH	1.75	0.85
1:C:1082:VAL:O	1:D:1081:MET:HE2	1.71	0.85
1:B:1083:GLY:CA	1:C:1081:MET:CE	2.36	0.84
1:C:1083:GLY:CA	1:D:1081:MET:CE	2.36	0.84
1:B:1078:LEU:CD2	1:C:1078:LEU:CD1	2.53	0.84
1:A:861:PHE:CE2	1:B:844:GLN:HB3	1.99	0.83
1:A:1083:GLY:N	1:B:1081:MET:HE1	1.93	0.83
1:C:1069:ARG:HG3	1:D:1067:ARG:NH2	1.94	0.83
1:A:1081:MET:HE1	1:D:1083:GLY:N	1.94	0.82
1:C:1078:LEU:HD22	1:D:1078:LEU:CD1	2.10	0.82
1:B:1069:ARG:HG3	1:C:1067:ARG:NH2	1.94	0.82
1:A:1069:ARG:HG3	1:B:1067:ARG:NH2	1.94	0.82
1:C:1083:GLY:N	1:D:1081:MET:HE1	1.94	0.82
1:A:1081:MET:HE2	1:D:1082:VAL:O	1.69	0.82
1:A:1078:LEU:CD1	1:D:1078:LEU:HD22	2.10	0.81
1:A:1067:ARG:NH2	1:D:1069:ARG:HG3	1.93	0.81
1:A:1078:LEU:HD22	1:B:1078:LEU:CD1	2.10	0.81
1:B:1083:GLY:N	1:C:1081:MET:HE1	1.96	0.80
1:A:117:LEU:HD22	1:B:1040:LYS:CD	2.12	0.80
1:A:1081:MET:HE1	1:D:1083:GLY:HA2	0.78	0.78
1:C:1083:GLY:HA2	1:D:1081:MET:HE1	0.78	0.78
1:B:1078:LEU:HD22	1:C:1078:LEU:CD1	2.12	0.77
1:A:1083:GLY:N	1:B:1081:MET:CE	2.48	0.76
1:A:1083:GLY:HA2	1:B:1081:MET:HE1	0.76	0.76
1:B:117:LEU:HD22	1:C:1040:LYS:CD	2.13	0.76
1:B:1083:GLY:HA2	1:C:1081:MET:HE1	0.77	0.76
1:C:117:LEU:HD22	1:D:1040:LYS:CD	2.14	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:LEU:CD2	1:B:1074:LYS:HD2	2.17	0.75
1:A:1074:LYS:HD2	1:D:1079:LEU:CD2	2.17	0.74
1:B:1079:LEU:CD2	1:C:1074:LYS:HD2	2.18	0.73
1:A:1040:LYS:CD	1:D:117:LEU:HD22	2.12	0.73
1:A:1081:MET:CE	1:D:1083:GLY:N	2.50	0.73
1:C:865:PHE:HZ	1:D:849:ILE:CD1	1.93	0.73
1:B:1082:VAL:O	1:C:1081:MET:HE2	1.71	0.73
1:C:1079:LEU:CD2	1:D:1074:LYS:HD2	2.19	0.73
1:C:1083:GLY:N	1:D:1081:MET:CE	2.50	0.72
1:A:1082:VAL:O	1:B:1081:MET:HE2	1.69	0.72
1:A:1074:LYS:HD2	1:D:1079:LEU:HD22	1.71	0.72
1:D:512:ASN:HB2	1:D:554:MET:HE2	1.71	0.72
1:A:1079:LEU:HD22	1:B:1074:LYS:HD2	1.72	0.72
1:B:512:ASN:HB2	1:B:554:MET:HE2	1.71	0.71
1:B:865:PHE:HZ	1:C:849:ILE:CD1	1.93	0.71
1:C:512:ASN:HB2	1:C:554:MET:HE2	1.71	0.70
1:C:1079:LEU:HD22	1:D:1074:LYS:HD2	1.72	0.70
1:D:632:ARG:NH2	1:D:647:LEU:O	2.25	0.70
1:B:632:ARG:NH2	1:B:647:LEU:O	2.25	0.70
1:B:1083:GLY:N	1:C:1081:MET:CE	2.51	0.70
1:C:944:TRP:HB3	4:C:1504:YUY:C15	2.22	0.70
1:C:1082:VAL:O	1:D:1081:MET:HE3	1.91	0.70
1:A:1082:VAL:O	1:B:1081:MET:HE3	1.90	0.70
1:A:512:ASN:HB2	1:A:554:MET:HE2	1.71	0.70
4:A:1503:YUY:C15	1:D:944:TRP:HB3	2.21	0.70
1:A:512:ASN:HB2	1:A:554:MET:CE	2.22	0.70
1:B:944:TRP:HB3	4:B:1504:YUY:C15	2.22	0.70
1:A:859:VAL:HG21	1:D:960:LEU:HD12	1.74	0.69
1:A:944:TRP:HB3	4:A:1505:YUY:C15	2.21	0.69
1:B:512:ASN:HB2	1:B:554:MET:CE	2.22	0.69
1:C:960:LEU:HD12	1:D:859:VAL:HG21	1.75	0.69
1:A:960:LEU:HD12	1:B:859:VAL:HG21	1.74	0.69
1:B:1079:LEU:HD22	1:C:1074:LYS:HD2	1.73	0.69
1:B:1082:VAL:O	1:C:1081:MET:HE3	1.93	0.69
1:C:632:ARG:NH2	1:C:647:LEU:O	2.25	0.69
1:D:512:ASN:HB2	1:D:554:MET:CE	2.22	0.69
1:A:632:ARG:NH2	1:A:647:LEU:O	2.25	0.68
1:C:512:ASN:HB2	1:C:554:MET:CE	2.22	0.68
1:B:960:LEU:HD12	1:C:859:VAL:HG21	1.76	0.68
1:C:971:TYR:CZ	1:D:977:GLN:HG2	2.29	0.68
1:B:834:ARG:HD2	1:B:834:ARG:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:977:GLN:HG2	1:D:971:TYR:CZ	2.29	0.67
1:C:834:ARG:HD2	1:C:834:ARG:O	1.94	0.67
1:D:391:ASN:HD22	1:D:394:GLN:HG2	1.60	0.67
1:C:391:ASN:HD22	1:C:394:GLN:HG2	1.60	0.67
1:D:834:ARG:HD2	1:D:834:ARG:O	1.94	0.67
1:B:391:ASN:HD22	1:B:394:GLN:HG2	1.60	0.67
1:B:971:TYR:CZ	1:C:977:GLN:HG2	2.30	0.67
1:A:971:TYR:CZ	1:B:977:GLN:HG2	2.30	0.67
1:B:760:TRP:CH2	1:B:1004:PRO:HD3	2.30	0.66
1:A:834:ARG:HD2	1:A:834:ARG:O	1.94	0.66
1:A:760:TRP:CH2	1:A:1004:PRO:HD3	2.30	0.66
1:C:68:GLU:O	1:C:71:GLN:NE2	2.29	0.66
1:C:760:TRP:CH2	1:C:1004:PRO:HD3	2.30	0.66
1:D:68:GLU:O	1:D:71:GLN:NE2	2.29	0.66
1:D:760:TRP:CH2	1:D:1004:PRO:HD3	2.30	0.66
1:A:391:ASN:HD22	1:A:394:GLN:HG2	1.60	0.66
1:A:959:VAL:CG1	1:B:965:LEU:HD23	2.27	0.65
1:A:1081:MET:HE3	1:D:1082:VAL:O	1.90	0.65
1:B:68:GLU:O	1:B:71:GLN:NE2	2.29	0.65
1:A:68:GLU:O	1:A:71:GLN:NE2	2.29	0.65
1:A:845:LEU:CD2	1:D:861:PHE:CD1	2.80	0.64
1:C:959:VAL:CG1	1:D:965:LEU:HD23	2.26	0.64
1:A:865:PHE:HZ	1:B:849:ILE:CD1	1.95	0.64
1:B:959:VAL:CG1	1:C:965:LEU:HD23	2.27	0.64
1:A:738:LEU:HD21	1:A:825:ALA:HA	1.80	0.64
1:A:965:LEU:HD23	1:D:959:VAL:CG1	2.27	0.64
1:B:738:LEU:HD21	1:B:825:ALA:HA	1.80	0.64
1:D:738:LEU:HD21	1:D:825:ALA:HA	1.80	0.64
1:C:738:LEU:HD21	1:C:825:ALA:HA	1.80	0.64
1:A:861:PHE:CD1	1:B:845:LEU:CD2	2.81	0.64
1:B:861:PHE:CD1	1:C:845:LEU:CD2	2.80	0.63
1:C:959:VAL:CG1	1:D:965:LEU:CD2	2.76	0.63
1:B:861:PHE:HD1	1:C:845:LEU:CD2	2.09	0.63
1:A:959:VAL:CG1	1:B:965:LEU:CD2	2.77	0.63
1:A:965:LEU:CD2	1:D:959:VAL:CG1	2.77	0.62
1:B:410:GLU:HA	1:B:415:HIS:CG	2.34	0.62
1:B:959:VAL:CG1	1:C:965:LEU:CD2	2.78	0.62
1:D:410:GLU:HA	1:D:415:HIS:CG	2.35	0.62
1:A:410:GLU:HA	1:A:415:HIS:CG	2.35	0.62
1:A:861:PHE:HD1	1:B:845:LEU:CD2	2.09	0.62
1:A:524:GLY:O	1:A:1049:LYS:NZ	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:964:LEU:HD13	1:C:855:MET:CG	2.29	0.62
1:A:845:LEU:CD2	1:D:861:PHE:HD1	2.09	0.62
1:B:524:GLY:O	1:B:1049:LYS:NZ	2.33	0.62
1:C:861:PHE:CD1	1:D:845:LEU:CD2	2.80	0.62
1:D:914:ALA:H	1:D:943:ASN:ND2	1.98	0.62
1:A:914:ALA:H	1:A:943:ASN:ND2	1.98	0.61
1:C:861:PHE:HD1	1:D:845:LEU:CD2	2.09	0.61
1:C:410:GLU:HA	1:C:415:HIS:CG	2.34	0.61
1:D:524:GLY:O	1:D:1049:LYS:NZ	2.33	0.61
1:C:914:ALA:H	1:C:943:ASN:ND2	1.98	0.61
1:C:524:GLY:O	1:C:1049:LYS:NZ	2.33	0.61
1:B:413:LEU:HD21	1:B:545:ALA:HA	1.83	0.61
1:A:413:LEU:HD21	1:A:545:ALA:HA	1.83	0.61
1:A:890:TRP:NE1	4:A:1503:YUY:O13	2.34	0.60
1:B:914:ALA:H	1:B:943:ASN:ND2	1.98	0.60
4:A:1505:YUY:O13	1:B:890:TRP:NE1	2.34	0.60
1:B:1006:ILE:CG2	1:B:1010:HIS:CE1	2.85	0.60
1:C:1006:ILE:CG2	1:C:1010:HIS:CE1	2.85	0.60
1:C:413:LEU:HD21	1:C:545:ALA:HA	1.83	0.59
1:D:1006:ILE:CG2	1:D:1010:HIS:CE1	2.85	0.59
1:C:964:LEU:HD13	1:D:855:MET:CG	2.27	0.59
1:D:202:ARG:NH2	1:D:210:SER:O	2.35	0.59
4:B:1504:YUY:O13	1:C:890:TRP:NE1	2.34	0.59
1:A:855:MET:CG	1:D:964:LEU:HD13	2.28	0.59
1:C:202:ARG:NH2	1:C:210:SER:O	2.35	0.59
4:C:1504:YUY:O13	1:D:890:TRP:NE1	2.34	0.59
1:A:202:ARG:NH2	1:A:210:SER:O	2.35	0.59
1:B:202:ARG:NH2	1:B:210:SER:O	2.35	0.59
1:D:413:LEU:HD21	1:D:545:ALA:HA	1.83	0.59
1:A:849:ILE:CD1	1:D:865:PHE:HZ	1.94	0.59
1:A:1006:ILE:CG2	1:A:1010:HIS:CE1	2.85	0.59
1:A:728:PHE:HE1	1:A:835:LEU:HD21	1.68	0.59
1:A:845:LEU:HD23	1:D:861:PHE:CE1	2.38	0.59
1:A:1081:MET:HE1	1:D:1082:VAL:C	2.18	0.59
1:A:964:LEU:HD13	1:B:855:MET:CG	2.28	0.58
1:D:78:ASP:OD1	1:D:79:THR:N	2.36	0.58
1:A:861:PHE:CE1	1:B:845:LEU:HD23	2.39	0.58
1:A:78:ASP:OD1	1:A:79:THR:N	2.36	0.58
1:D:728:PHE:HE1	1:D:835:LEU:HD21	1.68	0.58
1:C:78:ASP:OD1	1:C:79:THR:N	2.36	0.58
1:C:861:PHE:CE1	1:D:845:LEU:HD23	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASP:OD1	1:B:79:THR:N	2.36	0.58
1:B:902:HIS:HE1	1:B:908:PRO:HD2	1.69	0.58
1:A:902:HIS:HE1	1:A:908:PRO:HD2	1.69	0.57
1:C:728:PHE:HE1	1:C:835:LEU:HD21	1.68	0.57
1:C:902:HIS:HE1	1:C:908:PRO:HD2	1.69	0.57
1:A:760:TRP:CZ3	1:A:1004:PRO:HD3	2.39	0.57
1:B:728:PHE:HE1	1:B:835:LEU:HD21	1.68	0.57
1:B:760:TRP:CZ3	1:B:1004:PRO:HD3	2.39	0.57
1:D:138:GLN:NE2	1:D:139:ASN:OD1	2.35	0.57
1:D:902:HIS:HE1	1:D:908:PRO:HD2	1.69	0.57
1:A:138:GLN:NE2	1:A:139:ASN:OD1	2.35	0.57
1:D:775:THR:HG23	1:D:776:ASP:H	1.70	0.57
1:C:640:PRO:HG2	1:C:641:PRO:HD3	1.87	0.56
1:C:775:THR:HG23	1:C:776:ASP:H	1.70	0.56
1:D:760:TRP:CZ3	1:D:1004:PRO:HD3	2.39	0.56
1:B:502:ARG:NH1	1:B:588:CYS:O	2.39	0.56
1:B:640:PRO:HG2	1:B:641:PRO:HD3	1.86	0.56
1:C:760:TRP:CZ3	1:C:1004:PRO:HD3	2.39	0.56
1:A:502:ARG:NH1	1:A:588:CYS:O	2.39	0.56
1:D:502:ARG:NH1	1:D:588:CYS:O	2.39	0.56
1:B:861:PHE:CE1	1:C:845:LEU:HD23	2.38	0.56
1:D:640:PRO:HG2	1:D:641:PRO:HD3	1.87	0.56
1:C:1082:VAL:C	1:D:1081:MET:HE1	2.18	0.55
1:A:775:THR:HG23	1:A:776:ASP:H	1.70	0.55
1:B:775:THR:HG23	1:B:776:ASP:H	1.70	0.55
1:B:114:ASP:OD1	1:C:1047:VAL:CG2	2.54	0.55
1:A:1083:GLY:HA2	1:B:1081:MET:SD	2.47	0.55
1:A:1047:VAL:CG2	1:D:114:ASP:OD1	2.54	0.55
1:C:959:VAL:HG13	1:D:965:LEU:HD23	1.88	0.55
1:A:640:PRO:HG2	1:A:641:PRO:HD3	1.87	0.55
1:A:114:ASP:OD1	1:B:1047:VAL:CG2	2.54	0.55
1:B:251:ASP:HA	1:B:254:VAL:HG12	1.89	0.55
1:C:502:ARG:NH1	1:C:588:CYS:O	2.39	0.55
1:A:394:GLN:OE1	1:A:496:ARG:NH2	2.40	0.55
1:C:394:GLN:OE1	1:C:496:ARG:NH2	2.40	0.55
1:C:251:ASP:HA	1:C:254:VAL:HG12	1.89	0.54
1:A:251:ASP:HA	1:A:254:VAL:HG12	1.89	0.54
1:C:114:ASP:OD1	1:D:1047:VAL:CG2	2.55	0.54
1:D:394:GLN:OE1	1:D:496:ARG:NH2	2.40	0.54
1:A:104:ILE:HG13	1:A:108:LEU:HD23	1.89	0.54
1:A:397:THR:HA	1:A:496:ARG:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:HG13	1:B:108:LEU:HD23	1.89	0.54
1:C:397:THR:HA	1:C:496:ARG:HA	1.90	0.54
1:C:613:GLN:OE1	1:C:988:ARG:NH1	2.40	0.54
1:A:959:VAL:HG13	1:B:965:LEU:HD23	1.89	0.54
1:B:394:GLN:OE1	1:B:496:ARG:NH2	2.40	0.54
1:D:251:ASP:HA	1:D:254:VAL:HG12	1.89	0.54
1:A:1081:MET:SD	1:D:1083:GLY:HA2	2.48	0.54
1:B:138:GLN:NE2	1:B:139:ASN:OD1	2.35	0.54
1:D:513:ARG:HD3	1:D:516:MET:HE2	1.90	0.54
1:B:613:GLN:OE1	1:B:988:ARG:NH1	2.40	0.54
1:D:397:THR:HA	1:D:496:ARG:HA	1.90	0.53
1:B:98:SER:O	1:B:100:LEU:N	2.40	0.53
1:B:397:THR:HA	1:B:496:ARG:HA	1.90	0.53
1:A:513:ARG:HD3	1:A:516:MET:HE2	1.90	0.53
1:D:903:ILE:HG12	1:D:957:THR:HG21	1.91	0.53
1:A:613:GLN:OE1	1:A:988:ARG:NH1	2.40	0.53
1:A:462:LEU:HD12	1:A:466:CYS:SG	2.49	0.53
1:B:959:VAL:HG13	1:C:965:LEU:HD23	1.90	0.53
1:C:903:ILE:HG12	1:C:957:THR:HG21	1.91	0.53
1:A:903:ILE:HG12	1:A:957:THR:HG21	1.91	0.53
1:A:965:LEU:HD23	1:D:959:VAL:HG13	1.90	0.53
1:B:493:MET:HE3	1:B:493:MET:HA	1.91	0.53
1:C:104:ILE:HG13	1:C:108:LEU:HD23	1.89	0.53
1:B:1083:GLY:HA2	1:C:1081:MET:SD	2.50	0.52
1:C:256:LEU:HD12	1:C:262:TRP:HB3	1.91	0.52
1:C:1078:LEU:HD23	1:D:1078:LEU:CD1	2.23	0.52
1:D:104:ILE:HG13	1:D:108:LEU:HD23	1.89	0.52
1:C:462:LEU:HD12	1:C:466:CYS:SG	2.49	0.52
1:D:730:PHE:HB2	1:D:760:TRP:CE2	2.44	0.52
1:A:493:MET:HE3	1:A:493:MET:HA	1.91	0.52
1:B:468:GLY:HA2	1:B:471:GLN:HG3	1.92	0.52
1:D:256:LEU:HD12	1:D:262:TRP:HB3	1.91	0.52
1:A:1076:GLN:HG3	1:B:1070:TYR:OH	2.10	0.52
1:B:462:LEU:HD12	1:B:466:CYS:SG	2.49	0.52
1:B:513:ARG:HD3	1:B:516:MET:HE2	1.90	0.52
1:B:730:PHE:HB2	1:B:760:TRP:CE2	2.44	0.52
1:C:1083:GLY:HA2	1:D:1081:MET:SD	2.49	0.52
1:D:462:LEU:HD12	1:D:466:CYS:SG	2.49	0.52
1:D:613:GLN:OE1	1:D:988:ARG:NH1	2.40	0.52
1:A:1078:LEU:CD1	1:D:1078:LEU:HD23	2.22	0.52
1:C:468:GLY:HA2	1:C:471:GLN:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:493:MET:HE3	1:C:493:MET:HA	1.91	0.52
1:A:730:PHE:HB2	1:A:760:TRP:CE2	2.44	0.52
1:D:493:MET:HA	1:D:493:MET:HE3	1.91	0.52
1:B:345:ASN:OD1	1:B:378:LYS:HD2	2.09	0.51
1:C:513:ARG:HD3	1:C:516:MET:HE2	1.90	0.51
1:A:345:ASN:OD1	1:A:378:LYS:HD2	2.09	0.51
1:B:903:ILE:HG12	1:B:957:THR:HG21	1.91	0.51
1:A:256:LEU:HD12	1:A:262:TRP:HB3	1.91	0.51
1:A:914:ALA:HA	1:A:917:MET:HG3	1.93	0.51
1:C:914:ALA:HA	1:C:917:MET:HG3	1.93	0.51
1:D:468:GLY:HA2	1:D:471:GLN:HG3	1.92	0.51
1:A:1070:TYR:OH	1:D:1076:GLN:HG3	2.10	0.51
1:C:730:PHE:HB2	1:C:760:TRP:CE2	2.44	0.51
1:D:345:ASN:OD1	1:D:378:LYS:HD2	2.09	0.51
1:C:138:GLN:NE2	1:C:139:ASN:OD1	2.35	0.51
1:D:98:SER:O	1:D:100:LEU:N	2.40	0.51
1:B:256:LEU:HD12	1:B:262:TRP:HB3	1.91	0.51
1:C:345:ASN:OD1	1:C:378:LYS:HD2	2.09	0.51
1:A:468:GLY:HA2	1:A:471:GLN:HG3	1.92	0.51
1:B:914:ALA:HA	1:B:917:MET:HG3	1.93	0.50
1:B:1076:GLN:HG3	1:C:1070:TYR:OH	2.11	0.50
1:C:1076:GLN:HG3	1:D:1070:TYR:OH	2.11	0.50
1:D:914:ALA:HA	1:D:917:MET:HG3	1.93	0.50
1:A:98:SER:O	1:A:100:LEU:N	2.40	0.50
1:C:913:ASP:OD1	1:D:893:ARG:NH2	2.36	0.50
1:C:842:HIS:CD2	1:C:844:GLN:HB2	2.46	0.50
1:D:842:HIS:CD2	1:D:844:GLN:HB2	2.46	0.50
1:A:842:HIS:CD2	1:A:844:GLN:HB2	2.46	0.50
1:A:947:ILE:HG23	1:B:897:TYR:CE1	2.46	0.50
1:B:842:HIS:CD2	1:B:844:GLN:HB2	2.46	0.50
1:B:593:THR:HG22	1:B:595:LEU:H	1.77	0.50
1:C:947:ILE:HG23	1:D:897:TYR:CE1	2.46	0.50
1:D:914:ALA:H	1:D:943:ASN:HD21	1.60	0.50
1:A:861:PHE:HE2	1:B:844:GLN:OE1	1.95	0.50
1:B:370:MET:HE1	1:B:382:VAL:HG13	1.94	0.50
1:B:861:PHE:CE2	1:C:844:GLN:CB	2.82	0.50
1:C:348:ASP:OD1	1:C:349:ILE:N	2.45	0.50
1:C:593:THR:HG22	1:C:595:LEU:H	1.77	0.50
1:C:861:PHE:HE2	1:D:844:GLN:OE1	1.95	0.50
1:A:897:TYR:CE1	1:D:947:ILE:HG23	2.46	0.49
1:A:370:MET:HE1	1:A:382:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:861:PHE:HE2	1:C:844:GLN:OE1	1.95	0.49
1:B:947:ILE:HG23	1:C:897:TYR:CE1	2.47	0.49
1:C:196:LYS:O	1:C:199:SER:OG	2.31	0.49
1:D:324:CYS:SG	1:D:333:ASP:O	2.71	0.49
1:A:844:GLN:OE1	1:D:861:PHE:HE2	1.96	0.49
1:C:324:CYS:SG	1:C:333:ASP:O	2.71	0.49
1:A:196:LYS:O	1:A:199:SER:OG	2.31	0.49
1:A:593:THR:HG22	1:A:595:LEU:H	1.77	0.49
1:B:72:LEU:HD12	1:B:104:ILE:HD13	1.95	0.49
1:D:348:ASP:OD1	1:D:349:ILE:N	2.45	0.49
1:A:324:CYS:SG	1:A:333:ASP:O	2.71	0.49
1:C:914:ALA:H	1:C:943:ASN:HD21	1.61	0.49
1:A:348:ASP:OD1	1:A:349:ILE:N	2.45	0.49
1:B:914:ALA:H	1:B:943:ASN:HD21	1.60	0.49
1:B:196:LYS:O	1:B:199:SER:OG	2.31	0.49
1:D:72:LEU:HD12	1:D:104:ILE:HD13	1.95	0.49
1:A:571:TYR:CE1	1:A:575:GLU:HG3	2.48	0.48
1:A:1078:LEU:HD23	1:B:1078:LEU:CD1	2.22	0.48
1:B:324:CYS:SG	1:B:333:ASP:O	2.71	0.48
1:B:348:ASP:OD1	1:B:349:ILE:N	2.45	0.48
1:B:117:LEU:HA	1:C:1040:LYS:HE2	1.42	0.48
1:C:760:TRP:O	1:C:763:THR:OG1	2.27	0.48
1:D:370:MET:HE1	1:D:382:VAL:HG13	1.94	0.48
1:A:137:ILE:O	1:A:140:ARG:NH2	2.47	0.48
1:A:80:LEU:HD11	1:A:218:LEU:HD21	1.96	0.48
1:D:593:THR:HG22	1:D:595:LEU:H	1.77	0.48
1:A:852:VAL:O	1:A:856:ILE:HG12	2.14	0.48
1:B:80:LEU:HD11	1:B:218:LEU:HD21	1.96	0.48
1:B:852:VAL:O	1:B:856:ILE:HG12	2.14	0.48
1:C:72:LEU:HD12	1:C:104:ILE:HD13	1.95	0.48
1:A:914:ALA:H	1:A:943:ASN:HD21	1.60	0.48
1:A:963:ASN:ND2	1:B:966:ILE:HG13	2.29	0.48
1:B:137:ILE:O	1:B:140:ARG:NH2	2.46	0.48
1:C:117:LEU:HB3	1:D:1040:LYS:HD2	1.72	0.48
1:D:80:LEU:HD22	1:D:243:LEU:HD11	1.95	0.48
1:D:72:LEU:HD22	1:D:76:LEU:HD23	1.96	0.48
1:D:368:GLU:O	1:D:372:GLU:HG2	2.14	0.48
1:C:137:ILE:O	1:C:140:ARG:NH2	2.46	0.48
1:D:459:LYS:HD3	1:D:463:ASP:HA	1.96	0.48
1:D:571:TYR:CE1	1:D:575:GLU:HG3	2.48	0.48
1:A:80:LEU:HD22	1:A:243:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HB3	1:C:1040:LYS:HD2	1.72	0.48
1:B:566:LEU:HD11	1:B:1049:LYS:HB2	1.96	0.48
1:A:72:LEU:HD22	1:A:76:LEU:HD23	1.96	0.48
1:C:963:ASN:ND2	1:D:966:ILE:HG13	2.29	0.48
1:D:80:LEU:HD11	1:D:218:LEU:HD21	1.96	0.48
1:C:370:MET:HE1	1:C:382:VAL:HG13	1.94	0.47
1:C:571:TYR:CE1	1:C:575:GLU:HG3	2.48	0.47
1:C:852:VAL:O	1:C:856:ILE:HG12	2.14	0.47
1:A:60:VAL:HG21	1:A:198:ILE:HG21	1.96	0.47
1:B:459:LYS:HD3	1:B:463:ASP:HA	1.96	0.47
1:C:368:GLU:O	1:C:372:GLU:HG2	2.14	0.47
1:C:872:ALA:HB1	1:D:829:MET:HG3	1.96	0.47
1:D:852:VAL:O	1:D:856:ILE:HG12	2.14	0.47
1:A:459:LYS:HD3	1:A:463:ASP:HA	1.96	0.47
1:A:1040:LYS:HE2	1:D:117:LEU:HA	1.42	0.47
1:D:137:ILE:O	1:D:140:ARG:NH2	2.46	0.47
1:D:253:LEU:O	1:D:257:MET:HG2	2.15	0.47
1:A:72:LEU:HD12	1:A:104:ILE:HD13	1.95	0.47
1:A:1040:LYS:CD	1:D:117:LEU:CD2	2.90	0.47
1:B:571:TYR:CE1	1:B:575:GLU:HG3	2.48	0.47
1:C:459:LYS:HD3	1:C:463:ASP:HA	1.96	0.47
1:D:234:ILE:HD12	1:D:294:ILE:HG12	1.97	0.47
1:D:1033:LEU:HD22	1:D:1037:LEU:HD23	1.96	0.47
1:A:1083:GLY:C	1:B:1081:MET:HE1	2.30	0.47
1:C:80:LEU:HD11	1:C:218:LEU:HD21	1.96	0.47
1:D:196:LYS:O	1:D:199:SER:OG	2.31	0.47
1:A:566:LEU:HD11	1:A:1049:LYS:HB2	1.96	0.47
1:A:981:ASP:O	1:A:985:LYS:HG2	2.15	0.47
1:B:72:LEU:HD22	1:B:76:LEU:HD23	1.96	0.47
1:B:80:LEU:HD22	1:B:243:LEU:HD11	1.96	0.47
1:B:368:GLU:O	1:B:372:GLU:HG2	2.14	0.47
1:C:234:ILE:HD12	1:C:294:ILE:HG12	1.97	0.47
1:C:253:LEU:O	1:C:257:MET:HG2	2.15	0.47
1:C:525:PRO:HB2	1:C:1042:MET:HE2	1.97	0.47
1:A:253:LEU:O	1:A:257:MET:HG2	2.14	0.47
1:A:368:GLU:O	1:A:372:GLU:HG2	2.14	0.47
1:A:1033:LEU:HD22	1:A:1037:LEU:HD23	1.97	0.47
1:B:854:ARG:HG3	1:B:976:VAL:HG21	1.97	0.47
1:A:525:PRO:HB2	1:A:1042:MET:HE2	1.97	0.47
1:A:872:ALA:HB1	1:B:829:MET:HG3	1.97	0.47
1:B:963:ASN:ND2	1:C:966:ILE:HG13	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LEU:HD22	1:C:243:LEU:HD11	1.96	0.47
1:C:730:PHE:HB2	1:C:760:TRP:CZ2	2.50	0.47
1:D:60:VAL:HG21	1:D:198:ILE:HG21	1.96	0.47
1:D:566:LEU:HD11	1:D:1049:LYS:HB2	1.96	0.47
1:D:834:ARG:NH2	1:D:837[B]:HIS:CG	2.83	0.47
1:D:981:ASP:O	1:D:985:LYS:HG2	2.15	0.47
1:A:844:GLN:CB	1:D:861:PHE:CE2	2.83	0.47
1:A:897:TYR:CZ	1:D:947:ILE:HG23	2.50	0.47
1:A:947:ILE:HG23	1:B:897:TYR:CZ	2.50	0.47
1:A:966:ILE:HG13	1:D:963:ASN:ND2	2.29	0.47
1:C:981:ASP:O	1:C:985:LYS:HG2	2.15	0.47
1:A:854:ARG:HG3	1:A:976:VAL:HG21	1.97	0.46
4:A:1503:YUY:C16	1:D:944:TRP:HB2	2.45	0.46
1:B:834:ARG:NH2	1:B:837[B]:HIS:CG	2.83	0.46
1:D:730:PHE:HB2	1:D:760:TRP:CZ2	2.50	0.46
1:D:854:ARG:HG3	1:D:976:VAL:HG21	1.97	0.46
1:B:981:ASP:O	1:B:985:LYS:HG2	2.15	0.46
1:A:234:ILE:HD12	1:A:294:ILE:HG12	1.97	0.46
1:A:834:ARG:NH2	1:A:837[B]:HIS:CG	2.83	0.46
1:A:944:TRP:HB2	4:A:1505:YUY:C16	2.45	0.46
1:B:60:VAL:HG21	1:B:198:ILE:HG21	1.96	0.46
1:C:834:ARG:NH2	1:C:837[B]:HIS:CG	2.83	0.46
1:C:1033:LEU:HD22	1:C:1037:LEU:HD23	1.97	0.46
1:B:1078:LEU:HD23	1:C:1078:LEU:CD1	2.24	0.46
1:C:72:LEU:HD22	1:C:76:LEU:HD23	1.96	0.46
1:C:98:SER:O	1:C:100:LEU:N	2.39	0.46
1:C:504:LEU:HD23	1:C:504:LEU:HA	1.78	0.46
1:D:976:VAL:HG12	1:D:980:ALA:HB2	1.98	0.46
1:A:357:GLY:HA2	1:D:73:LYS:HE2	1.67	0.46
1:A:536:LYS:HD3	1:A:601:ALA:HA	1.98	0.46
1:B:234:ILE:HD12	1:B:294:ILE:HG12	1.97	0.46
1:B:525:PRO:HB2	1:B:1042:MET:HE2	1.97	0.46
1:B:536:LYS:HD3	1:B:601:ALA:HA	1.98	0.46
1:C:60:VAL:HG21	1:C:198:ILE:HG21	1.96	0.46
1:C:221:HIS:O	1:C:221:HIS:ND1	2.49	0.46
1:C:536:LYS:HD3	1:C:601:ALA:HA	1.98	0.46
1:C:566:LEU:HD11	1:C:1049:LYS:HB2	1.96	0.46
1:C:854:ARG:HG3	1:C:976:VAL:HG21	1.97	0.46
1:D:413:LEU:H	1:D:413:LEU:HD12	1.81	0.46
1:A:413:LEU:HD12	1:A:413:LEU:H	1.80	0.46
1:B:872:ALA:HB1	1:C:829:MET:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:913:ASP:OD1	1:C:893:ARG:NH2	2.38	0.46
1:B:1033:LEU:HD22	1:B:1037:LEU:HD23	1.96	0.46
1:D:525:PRO:HB2	1:D:1042:MET:HE2	1.97	0.46
1:D:536:LYS:HD3	1:D:601:ALA:HA	1.98	0.46
1:A:829:MET:HG3	1:D:872:ALA:HB1	1.98	0.46
1:A:117:LEU:CD2	1:B:1040:LYS:CD	2.91	0.46
1:B:413:LEU:HD12	1:B:413:LEU:H	1.81	0.46
1:B:730:PHE:HB2	1:B:760:TRP:CZ2	2.50	0.46
1:B:944:TRP:HB2	4:B:1504:YUY:C16	2.46	0.46
1:A:221:HIS:O	1:A:221:HIS:ND1	2.49	0.45
1:A:976:VAL:HG12	1:A:980:ALA:HB2	1.98	0.45
1:C:413:LEU:HD12	1:C:413:LEU:H	1.80	0.45
1:D:701:PHE:HA	1:D:704:VAL:HG12	1.98	0.45
1:A:701:PHE:HA	1:A:704:VAL:HG12	1.98	0.45
1:A:730:PHE:HB2	1:A:760:TRP:CZ2	2.50	0.45
1:B:947:ILE:HG23	1:C:897:TYR:CZ	2.51	0.45
1:C:944:TRP:HB2	4:C:1504:YUY:C16	2.45	0.45
1:C:976:VAL:HG12	1:C:980:ALA:HB2	1.98	0.45
1:B:253:LEU:O	1:B:257:MET:HG2	2.15	0.45
1:B:775:THR:HG23	1:B:776:ASP:N	2.32	0.45
1:C:86:LYS:O	1:C:89:GLN:HG2	2.17	0.45
1:A:86:LYS:O	1:A:89:GLN:HG2	2.17	0.45
1:B:86:LYS:O	1:B:89:GLN:HG2	2.17	0.45
1:D:86:LYS:O	1:D:89:GLN:HG2	2.17	0.45
1:A:775:THR:HG23	1:A:776:ASP:N	2.32	0.45
1:C:947:ILE:HG23	1:D:897:TYR:CZ	2.52	0.45
1:C:546:THR:OG1	1:C:547:GLU:N	2.50	0.45
1:C:701:PHE:HA	1:C:704:VAL:HG12	1.98	0.45
1:A:546:THR:OG1	1:A:547:GLU:N	2.50	0.45
1:B:216:LEU:HD21	1:B:241:LEU:HD23	1.99	0.45
1:C:1040:LYS:HD2	1:C:1040:LYS:HA	1.70	0.45
1:C:775:THR:HG23	1:C:776:ASP:N	2.32	0.44
1:D:1040:LYS:HD2	1:D:1040:LYS:HA	1.70	0.44
1:C:216:LEU:HD21	1:C:241:LEU:HD23	1.99	0.44
1:C:971:TYR:CE2	1:D:977:GLN:HG2	2.53	0.44
1:D:546:THR:OG1	1:D:547:GLU:N	2.50	0.44
1:D:760:TRP:O	1:D:763:THR:OG1	2.27	0.44
1:B:701:PHE:HA	1:B:704:VAL:HG12	1.98	0.44
1:B:976:VAL:HG12	1:B:980:ALA:HB2	1.98	0.44
1:B:785:MET:HE2	1:B:785:MET:HB3	1.79	0.44
1:B:1040:LYS:HD2	1:B:1040:LYS:HA	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:THR:OG1	1:B:547:GLU:N	2.50	0.44
1:C:287:TRP:O	1:C:291:ILE:HG12	2.18	0.44
1:D:221:HIS:O	1:D:221:HIS:ND1	2.49	0.44
1:B:1056:LEU:O	1:B:1059:GLU:HG3	2.18	0.44
1:C:785:MET:HE2	1:C:785:MET:HB3	1.79	0.44
1:A:1081:MET:HE1	1:D:1083:GLY:C	2.31	0.44
1:C:861:PHE:CE2	1:D:844:GLN:CB	2.82	0.44
1:C:98:SER:O	1:C:105:THR:HG21	2.18	0.44
1:C:1056:LEU:O	1:C:1059:GLU:HG3	2.18	0.44
1:D:743:ARG:O	1:D:811:ARG:NH2	2.51	0.44
1:A:394:GLN:NE2	1:A:496:ARG:HH12	2.16	0.43
1:B:98:SER:O	1:B:105:THR:HG21	2.18	0.43
1:B:923:THR:HB	1:B:934:LEU:HD12	2.00	0.43
1:D:394:GLN:NE2	1:D:496:ARG:HH12	2.16	0.43
1:D:728:PHE:CE1	1:D:835:LEU:HD21	2.52	0.43
1:D:1056:LEU:O	1:D:1059:GLU:HG3	2.18	0.43
1:A:98:SER:O	1:A:105:THR:HG21	2.18	0.43
1:A:117:LEU:HA	1:B:1040:LYS:HE2	1.44	0.43
1:B:743:ARG:O	1:B:811:ARG:NH2	2.51	0.43
1:C:131:ILE:HG12	1:C:175:ILE:HB	2.00	0.43
1:A:20:ILE:N	1:A:30:GLY:O	2.44	0.43
1:A:216:LEU:HD21	1:A:241:LEU:HD23	1.99	0.43
1:A:743:ARG:O	1:A:811:ARG:NH2	2.51	0.43
1:A:898:ARG:HB3	1:A:899:PRO:HD3	2.00	0.43
1:B:287:TRP:O	1:B:291:ILE:HG12	2.18	0.43
1:B:394:GLN:NE2	1:B:496:ARG:HH12	2.16	0.43
1:C:394:GLN:NE2	1:C:496:ARG:HH12	2.16	0.43
1:D:131:ILE:HG12	1:D:175:ILE:HB	2.00	0.43
1:D:216:LEU:HD21	1:D:241:LEU:HD23	1.99	0.43
1:A:1067:ARG:CZ	1:D:1069:ARG:HG3	2.47	0.43
1:B:131:ILE:HG12	1:B:175:ILE:HB	2.00	0.43
1:C:728:PHE:CE1	1:C:835:LEU:HD21	2.52	0.43
1:D:730:PHE:CD1	1:D:760:TRP:CD1	3.07	0.43
1:A:287:TRP:O	1:A:291:ILE:HG12	2.18	0.43
1:D:20:ILE:N	1:D:30:GLY:O	2.44	0.43
1:B:216:LEU:HD13	1:B:316:ILE:HG23	2.00	0.43
1:B:221:HIS:O	1:B:221:HIS:ND1	2.49	0.43
1:A:73:LYS:HE2	1:B:357:GLY:HA2	1.66	0.43
1:A:131:ILE:HG12	1:A:175:ILE:HB	2.00	0.43
1:B:1082:VAL:C	1:C:1081:MET:HE1	2.21	0.43
1:A:72:LEU:HD23	1:A:72:LEU:HA	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ASP:OD1	1:A:314:THR:N	2.52	0.43
1:A:893:ARG:NH2	1:D:913:ASP:OD1	2.38	0.43
1:A:923:THR:HB	1:A:934:LEU:HD12	2.00	0.43
1:C:730:PHE:CD1	1:C:760:TRP:CD1	3.07	0.43
1:C:743:ARG:O	1:C:811:ARG:NH2	2.51	0.43
1:D:216:LEU:HD13	1:D:316:ILE:HG23	2.00	0.43
1:D:287:TRP:O	1:D:291:ILE:HG12	2.18	0.43
1:D:898:ARG:HB3	1:D:899:PRO:HD3	2.01	0.43
1:A:944:TRP:CB	4:A:1505:YUY:C16	2.97	0.43
1:A:971:TYR:CE2	1:B:977:GLN:HG2	2.54	0.43
1:B:1083:GLY:C	1:C:1081:MET:HE1	2.32	0.43
1:C:313:ASP:OD1	1:C:314:THR:N	2.52	0.43
1:C:923:THR:HB	1:C:934:LEU:HD12	2.00	0.43
1:D:98:SER:O	1:D:105:THR:HG21	2.18	0.43
1:D:221:HIS:HA	1:D:248:GLY:H	1.83	0.43
1:D:923:THR:HB	1:D:934:LEU:HD12	2.00	0.43
1:A:746:PRO:C	1:A:749:GLY:H	2.27	0.43
1:D:775:THR:HG23	1:D:776:ASP:N	2.32	0.43
1:A:221:HIS:HA	1:A:248:GLY:H	1.83	0.42
1:A:1056:LEU:O	1:A:1059:GLU:HG3	2.18	0.42
1:B:532:LEU:HD23	1:B:532:LEU:HA	1.85	0.42
1:B:730:PHE:CD1	1:B:760:TRP:CD1	3.07	0.42
1:D:313:ASP:OD1	1:D:314:THR:N	2.52	0.42
1:A:730:PHE:CD1	1:A:760:TRP:CD1	3.07	0.42
1:A:977:GLN:HG2	1:D:971:TYR:CE2	2.54	0.42
1:B:117:LEU:CD2	1:C:1040:LYS:CD	2.91	0.42
1:B:221:HIS:HA	1:B:248:GLY:H	1.83	0.42
1:B:898:ARG:HB3	1:B:899:PRO:HD3	2.00	0.42
1:C:944:TRP:CB	4:C:1504:YUY:C16	2.97	0.42
1:D:1049:LYS:HB3	1:D:1049:LYS:HE2	1.84	0.42
1:A:216:LEU:HD13	1:A:316:ILE:HG23	2.00	0.42
1:A:234:ILE:HG23	1:A:300:LEU:HD12	2.02	0.42
1:A:1069:ARG:HG3	1:B:1067:ARG:CZ	2.48	0.42
1:B:72:LEU:HD23	1:B:72:LEU:HA	1.90	0.42
1:C:223:GLU:O	1:C:226:ILE:HG12	2.19	0.42
1:C:234:ILE:HG23	1:C:300:LEU:HD12	2.02	0.42
1:B:582:LEU:HD23	1:B:582:LEU:HA	1.91	0.42
1:B:746:PRO:C	1:B:749:GLY:H	2.27	0.42
1:B:971:TYR:CE2	1:C:977:GLN:HG2	2.55	0.42
1:B:223:GLU:O	1:B:226:ILE:HG12	2.19	0.42
1:B:313:ASP:OD1	1:B:314:THR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:419:LEU:HD12	1:B:419:LEU:HA	1.88	0.42
1:C:221:HIS:HA	1:C:248:GLY:H	1.83	0.42
1:C:241:LEU:HD11	1:C:315:VAL:HG12	2.02	0.42
1:D:58:HIS:N	1:D:92:GLY:O	2.49	0.42
1:D:223:GLU:O	1:D:226:ILE:HG12	2.19	0.42
1:D:535:CYS:O	1:D:539:LYS:HG2	2.20	0.42
1:C:117:LEU:CD2	1:D:1040:LYS:CD	2.92	0.42
1:C:216:LEU:HD13	1:C:316:ILE:HG23	2.00	0.42
4:A:1503:YUY:C16	1:D:944:TRP:CB	2.97	0.42
1:C:642:LEU:O	1:C:645:THR:OG1	2.31	0.42
1:C:898:ARG:HB3	1:C:899:PRO:HD3	2.01	0.42
1:D:616:LEU:HD23	1:D:616:LEU:HA	1.91	0.42
1:B:728:PHE:CE1	1:B:835:LEU:HD21	2.52	0.42
1:C:746:PRO:C	1:C:749:GLY:H	2.27	0.42
1:D:234:ILE:HG23	1:D:300:LEU:HD12	2.02	0.42
1:A:223:GLU:O	1:A:226:ILE:HG12	2.19	0.42
1:A:304:HIS:CD2	1:A:312:LEU:HD13	2.55	0.42
1:B:234:ILE:HG23	1:B:300:LEU:HD12	2.02	0.42
1:B:241:LEU:HD11	1:B:315:VAL:HG12	2.02	0.42
1:C:58:HIS:N	1:C:92:GLY:O	2.49	0.42
1:A:252:ILE:O	1:A:256:LEU:HD23	2.20	0.41
1:A:913:ASP:OD1	1:B:893:ARG:NH2	2.38	0.41
1:A:944:TRP:CB	4:A:1505:YUY:C15	2.96	0.41
1:D:78:ASP:HA	1:D:81:ARG:HG2	2.02	0.41
1:D:215:VAL:O	1:D:239:PRO:HD2	2.20	0.41
1:D:252:ILE:O	1:D:256:LEU:HD23	2.20	0.41
1:D:746:PRO:C	1:D:749:GLY:H	2.27	0.41
1:A:215:VAL:O	1:A:239:PRO:HD2	2.20	0.41
1:B:356:SER:O	1:B:358:ASP:N	2.49	0.41
1:B:1069:ARG:HG3	1:C:1067:ARG:CZ	2.49	0.41
1:A:1040:LYS:HD3	1:D:117:LEU:CD2	2.24	0.41
1:B:215:VAL:O	1:B:239:PRO:HD2	2.20	0.41
1:C:620:TRP:CE3	1:C:992:ILE:HG12	2.55	0.41
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.92	0.41
1:D:620:TRP:CE3	1:D:992:ILE:HG12	2.55	0.41
1:A:84:LEU:HD23	1:A:108:LEU:HD11	2.03	0.41
1:B:84:LEU:HD23	1:B:108:LEU:HD11	2.03	0.41
1:B:304:HIS:CD2	1:B:312:LEU:HD13	2.55	0.41
1:B:513:ARG:HH11	1:B:516:MET:CE	2.33	0.41
1:C:513:ARG:HH11	1:C:516:MET:CE	2.33	0.41
1:A:117:LEU:CD2	1:B:1040:LYS:CE	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:535:CYS:O	1:C:539:LYS:HG2	2.20	0.41
1:A:392:ILE:HG13	1:A:501:TRP:CH2	2.56	0.41
1:A:504:LEU:HA	1:A:504:LEU:HD23	1.78	0.41
1:A:1049:LYS:HB3	1:A:1049:LYS:HE2	1.84	0.41
1:B:470:TYR:O	1:B:491:PRO:HD3	2.21	0.41
1:C:78:ASP:HA	1:C:81:ARG:HG2	2.03	0.41
1:D:304:HIS:CD2	1:D:312:LEU:HD13	2.55	0.41
1:A:241:LEU:HD11	1:A:315:VAL:HG12	2.01	0.41
1:A:535:CYS:O	1:A:539:LYS:HG2	2.20	0.41
1:A:620:TRP:CE3	1:A:992:ILE:HG12	2.55	0.41
1:B:78:ASP:HA	1:B:81:ARG:HG2	2.02	0.41
1:B:535:CYS:O	1:B:539:LYS:HG2	2.20	0.41
1:C:84:LEU:HD23	1:C:108:LEU:HD11	2.03	0.41
1:C:97:THR:OG1	1:C:171:HIS:NE2	2.49	0.41
1:C:304:HIS:CD2	1:C:312:LEU:HD13	2.55	0.41
1:D:84:LEU:HD23	1:D:108:LEU:HD11	2.03	0.41
1:A:513:ARG:HH11	1:A:516:MET:CE	2.33	0.41
1:B:117:LEU:CD2	1:C:1040:LYS:CE	2.98	0.41
1:C:470:TYR:O	1:C:491:PRO:HD3	2.21	0.41
1:D:221:HIS:HD2	1:D:247:GLY:HA3	1.86	0.41
1:A:221:HIS:HD2	1:A:247:GLY:HA3	1.86	0.41
1:A:356:SER:O	1:A:358:ASP:N	2.49	0.41
1:A:470:TYR:O	1:A:491:PRO:HD3	2.21	0.41
1:B:569:GLU:OE1	1:B:1055:LYS:NZ	2.54	0.41
1:B:616:LEU:HD11	1:B:989:TYR:HD1	1.86	0.41
1:B:944:TRP:CB	4:B:1504:YUY:C16	2.98	0.41
1:C:75:TRP:CG	1:C:76:LEU:N	2.89	0.41
1:C:616:LEU:HD11	1:C:989:TYR:HD1	1.86	0.41
1:C:1069:ARG:HG3	1:D:1067:ARG:CZ	2.49	0.41
1:D:241:LEU:HD11	1:D:315:VAL:HG12	2.01	0.41
1:D:470:TYR:O	1:D:491:PRO:HD3	2.21	0.41
1:A:78:ASP:HA	1:A:81:ARG:HG2	2.02	0.41
1:A:220:VAL:HG22	1:A:243:LEU:HD12	2.03	0.41
1:B:220:VAL:HG22	1:B:243:LEU:HD12	2.03	0.41
1:B:252:ILE:O	1:B:256:LEU:HD23	2.20	0.41
1:C:215:VAL:O	1:C:239:PRO:HD2	2.20	0.41
1:D:734:PHE:CE1	1:D:828:PHE:HB2	2.56	0.41
1:B:620:TRP:CE3	1:B:992:ILE:HG12	2.56	0.40
1:C:419:LEU:O	1:C:423:GLN:HG2	2.22	0.40
1:C:1049:LYS:HE2	1:C:1049:LYS:HB3	1.84	0.40
1:D:220:VAL:HG22	1:D:243:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:569:GLU:OE1	1:D:1055:LYS:NZ	2.54	0.40
1:D:616:LEU:HD11	1:D:989:TYR:HD1	1.86	0.40
1:A:569:GLU:OE1	1:A:1055:LYS:NZ	2.54	0.40
1:B:112:VAL:HG11	1:B:128:ALA:HB2	2.04	0.40
1:B:419:LEU:O	1:B:423:GLN:HG2	2.22	0.40
1:C:221:HIS:HD2	1:C:247:GLY:HA3	1.86	0.40
1:C:252:ILE:O	1:C:256:LEU:HD23	2.20	0.40
1:C:734:PHE:CE1	1:C:828:PHE:HB2	2.56	0.40
1:A:64:MET:HG3	1:A:240:TRP:CH2	2.57	0.40
1:A:954:LEU:HD23	1:A:954:LEU:HA	1.94	0.40
1:A:1040:LYS:CE	1:D:117:LEU:CD2	2.99	0.40
1:C:1006:ILE:HG21	1:C:1010:HIS:CE1	2.56	0.40
1:D:75:TRP:CG	1:D:76:LEU:N	2.89	0.40
1:A:824:LEU:HD23	1:A:824:LEU:HA	1.89	0.40
1:B:734:PHE:CE1	1:B:828:PHE:HB2	2.56	0.40
1:D:64:MET:HG3	1:D:240:TRP:CH2	2.57	0.40
1:B:230:MET:HG3	1:B:240:TRP:CZ2	2.57	0.40
1:B:1006:ILE:HG21	1:B:1010:HIS:CE1	2.56	0.40
1:C:20:ILE:N	1:C:30:GLY:O	2.44	0.40
1:D:392:ILE:HG13	1:D:501:TRP:CH2	2.56	0.40
1:D:419:LEU:O	1:D:423:GLN:HG2	2.22	0.40
1:D:513:ARG:HH11	1:D:516:MET:CE	2.33	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	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48
1	B	987/1165 (85%)	949 (96%)	37 (4%)	1 (0%)	48	48
1	C	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	987/1165 (85%)	948 (96%)	38 (4%)	1 (0%)	48	48
All	All	3948/4660 (85%)	3793 (96%)	151 (4%)	4 (0%)	49	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 ⓘ

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	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	B	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	C	747/1017 (74%)	746 (100%)	1 (0%)	88	88
1	D	747/1017 (74%)	746 (100%)	1 (0%)	88	88
All	All	2988/4068 (74%)	2984 (100%)	4 (0%)	87	88

All (4) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	391	ASN
1	A	415	HIS
1	A	514	GLN
1	A	723	ASN
1	A	842	HIS
1	A	943	ASN
1	A	974	GLN
1	A	990	ASN
1	A	1010	HIS
1	A	1060	HIS
1	B	71	GLN
1	B	107	ASN
1	B	391	ASN
1	B	415	HIS
1	B	514	GLN
1	B	723	ASN
1	B	842	HIS
1	B	943	ASN
1	B	990	ASN
1	B	1010	HIS
1	B	1060	HIS
1	C	71	GLN
1	C	107	ASN
1	C	391	ASN
1	C	415	HIS
1	C	514	GLN
1	C	723	ASN
1	C	842	HIS
1	C	943	ASN
1	C	974	GLN
1	C	990	ASN
1	C	1010	HIS
1	C	1060	HIS
1	D	71	GLN
1	D	107	ASN
1	D	391	ASN
1	D	415	HIS
1	D	514	GLN
1	D	723	ASN
1	D	842	HIS
1	D	943	ASN

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Mol	Chain	Res	Type
1	D	974	GLN
1	D	990	ASN
1	D	1010	HIS
1	D	1060	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
4	YUY	A	1505	-	66,66,66	0.12	0	98,102,102	0.19	0
5	YUV	B	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
5	YUV	C	1503	-	35,35,35	0.12	0	58,58,58	0.18	0
4	YUY	A	1503	-	66,66,66	0.12	0	98,102,102	0.19	0
4	YUY	C	1504	-	66,66,66	0.12	0	98,102,102	0.19	0
2	NAG	A	1501	1	14,14,15	0.29	0	17,19,21	0.59	0
5	YUV	D	1503	-	35,35,35	0.11	0	58,58,58	0.18	0
2	NAG	B	1501	1	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	C	1501	1	14,14,15	0.28	0	17,19,21	0.59	0
4	YUY	B	1504	-	66,66,66	0.12	0	98,102,102	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	YUV	A	1504	-	35,35,35	0.11	0	58,58,58	0.18	0
2	NAG	D	1501	1	14,14,15	0.29	0	17,19,21	0.59	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
4	YUY	A	1505	-	-	11/21/149/149	0/8/8/8
5	YUV	B	1503	-	-	-	0/6/6/6
5	YUV	C	1503	-	-	-	0/6/6/6
4	YUY	A	1503	-	-	11/21/149/149	0/8/8/8
4	YUY	C	1504	-	-	11/21/149/149	0/8/8/8
2	NAG	A	1501	1	-	3/6/23/26	0/1/1/1
5	YUV	D	1503	-	-	-	0/6/6/6
2	NAG	B	1501	1	-	3/6/23/26	0/1/1/1
2	NAG	C	1501	1	-	3/6/23/26	0/1/1/1
4	YUY	B	1504	-	-	11/21/149/149	0/8/8/8
5	YUV	A	1504	-	-	-	0/6/6/6
2	NAG	D	1501	1	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (56) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1501	NAG	O7-C7-N2-C2
2	B	1501	NAG	O7-C7-N2-C2
2	C	1501	NAG	O7-C7-N2-C2
2	D	1501	NAG	O7-C7-N2-C2
4	A	1503	YUY	C43-C29-C30-O3
4	A	1503	YUY	C28-C29-C43-O14
4	A	1503	YUY	C30-C29-C43-O14
4	A	1505	YUY	C43-C29-C30-O3
4	A	1505	YUY	C28-C29-C43-O14
4	A	1505	YUY	C30-C29-C43-O14
4	B	1504	YUY	C43-C29-C30-O3

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Mol	Chain	Res	Type	Atoms
4	B	1504	YUY	C28-C29-C43-O14
4	B	1504	YUY	C30-C29-C43-O14
4	C	1504	YUY	C43-C29-C30-O3
4	C	1504	YUY	C28-C29-C43-O14
4	C	1504	YUY	C30-C29-C43-O14
2	A	1501	NAG	C8-C7-N2-C2
2	B	1501	NAG	C8-C7-N2-C2
2	C	1501	NAG	C8-C7-N2-C2
2	D	1501	NAG	C8-C7-N2-C2
4	A	1503	YUY	O4-C35-C36-O5
4	A	1505	YUY	O4-C35-C36-O5
4	B	1504	YUY	O4-C35-C36-O5
4	C	1504	YUY	O4-C35-C36-O5
4	A	1503	YUY	C34-C35-C36-O5
4	A	1505	YUY	C34-C35-C36-O5
4	B	1504	YUY	C34-C35-C36-O5
4	C	1504	YUY	C34-C35-C36-O5
4	A	1503	YUY	O7-C41-C42-O8
4	A	1505	YUY	O7-C41-C42-O8
4	B	1504	YUY	O7-C41-C42-O8
4	C	1504	YUY	O7-C41-C42-O8
4	A	1503	YUY	C28-C29-C30-O3
4	A	1505	YUY	C28-C29-C30-O3
4	B	1504	YUY	C28-C29-C30-O3
4	C	1504	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	1501	NAG	O5-C5-C6-O6
4	A	1503	YUY	C13-C14-O2-C27
4	A	1503	YUY	C15-C14-O2-C27
4	A	1505	YUY	C13-C14-O2-C27
4	A	1505	YUY	C15-C14-O2-C27
4	B	1504	YUY	C13-C14-O2-C27
4	B	1504	YUY	C15-C14-O2-C27
4	C	1504	YUY	C13-C14-O2-C27
4	C	1504	YUY	C15-C14-O2-C27
4	C	1504	YUY	C40-C41-C42-O8
4	A	1503	YUY	C40-C41-C42-O8
4	A	1505	YUY	C40-C41-C42-O8
4	B	1504	YUY	C40-C41-C42-O8
4	A	1503	YUY	C29-C30-O3-C31

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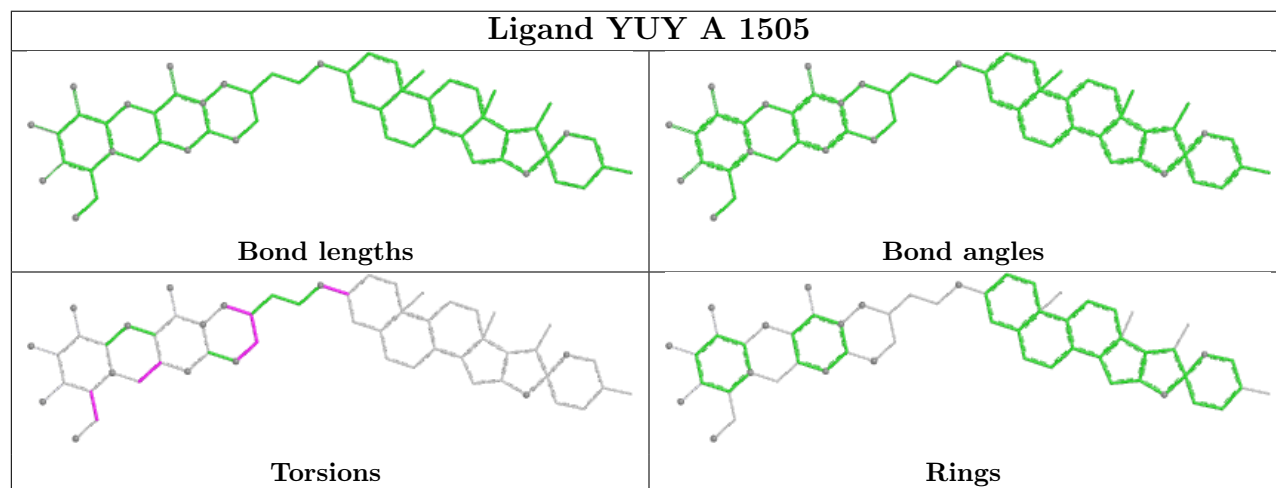
Mol	Chain	Res	Type	Atoms
4	A	1505	YUY	C29-C30-O3-C31
4	B	1504	YUY	C29-C30-O3-C31
4	C	1504	YUY	C29-C30-O3-C31

There are no ring outliers.

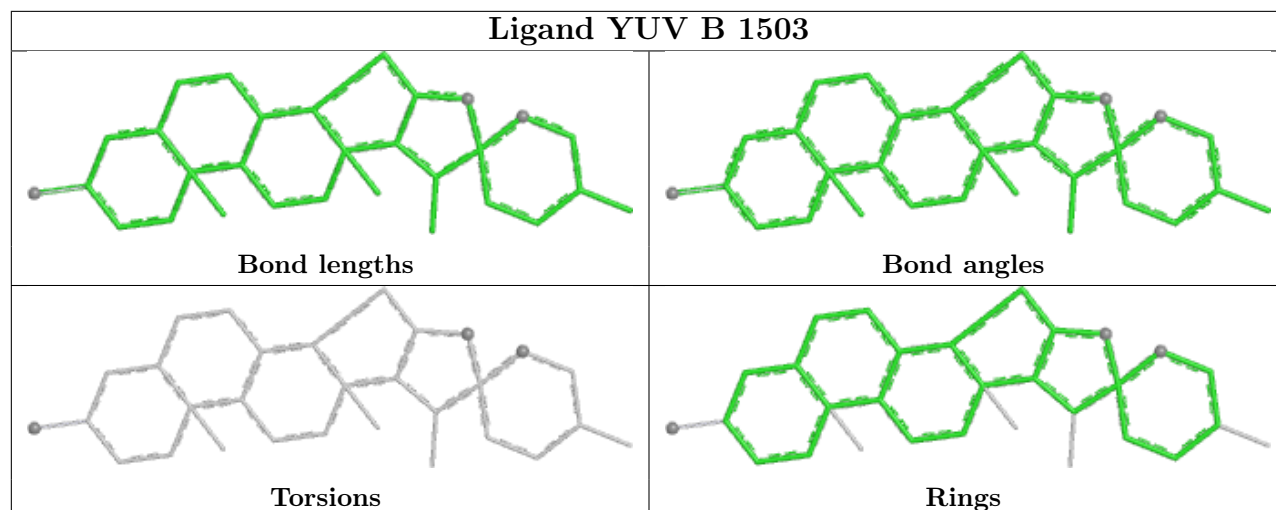
4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1505	YUY	5	0
4	A	1503	YUY	4	0
4	C	1504	YUY	4	0
4	B	1504	YUY	4	0

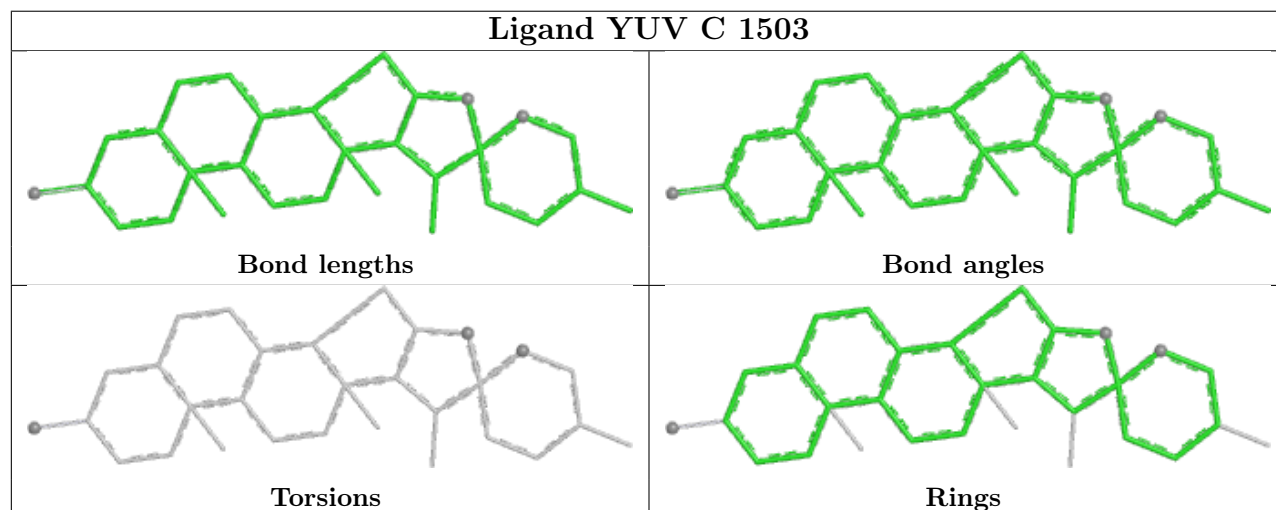
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



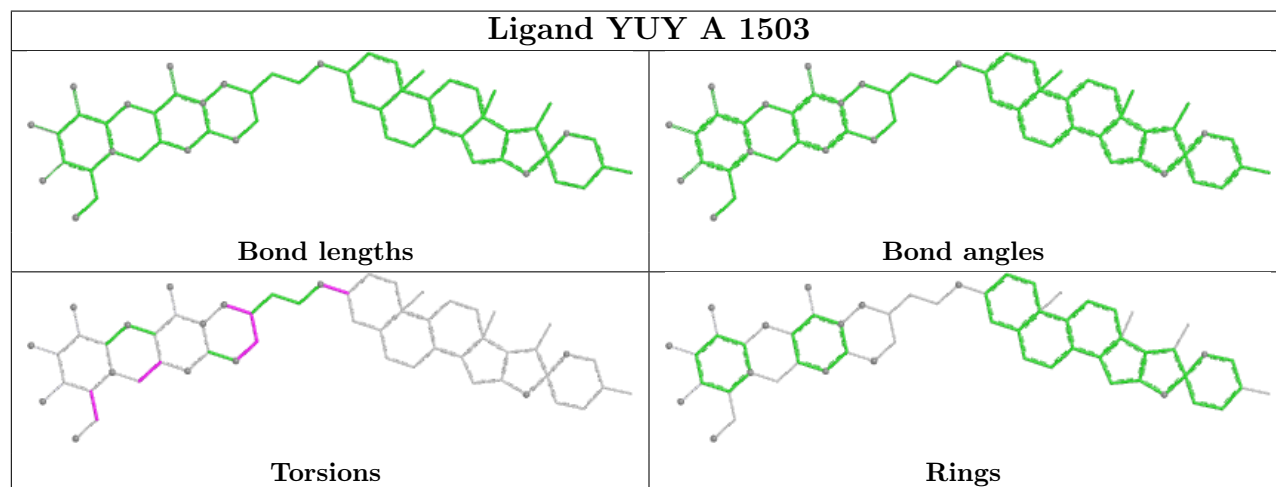
Ligand YUV B 1503

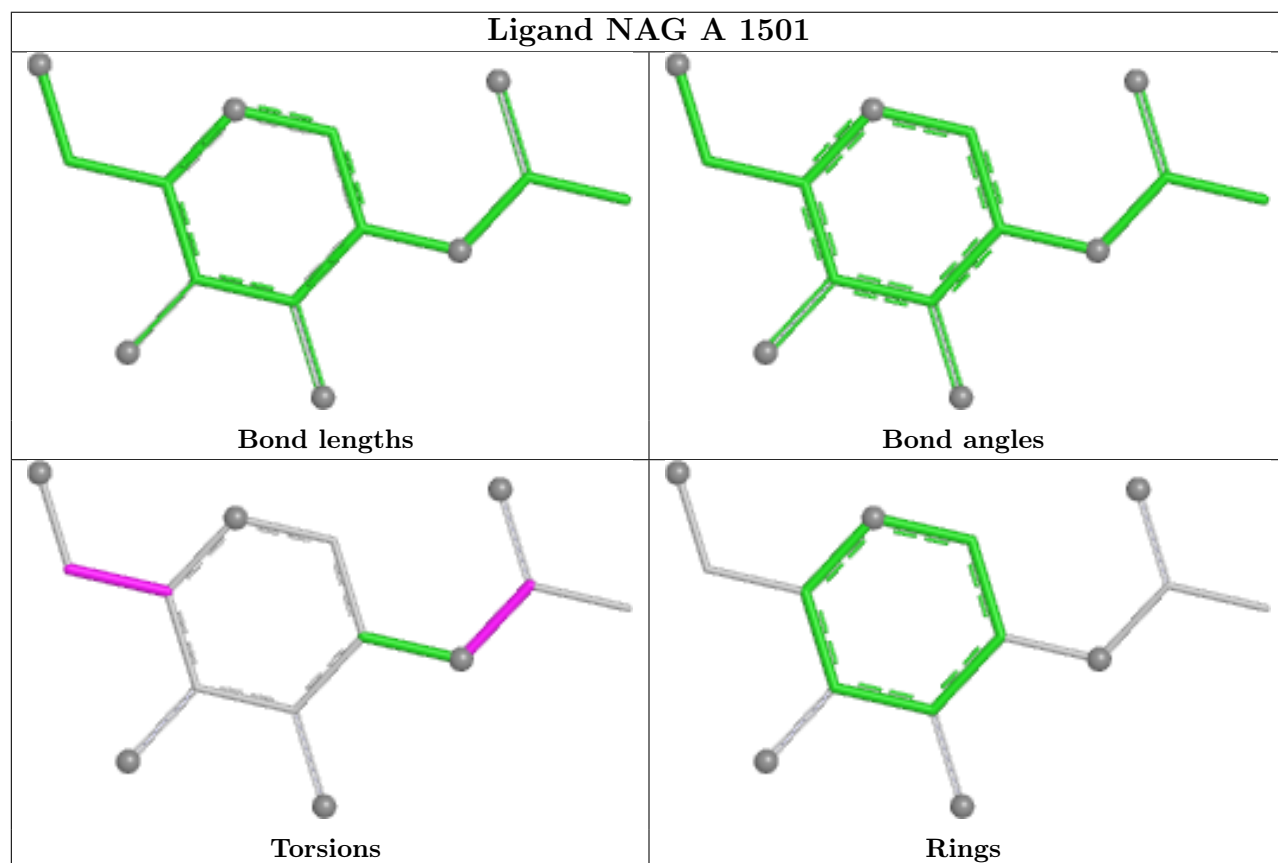
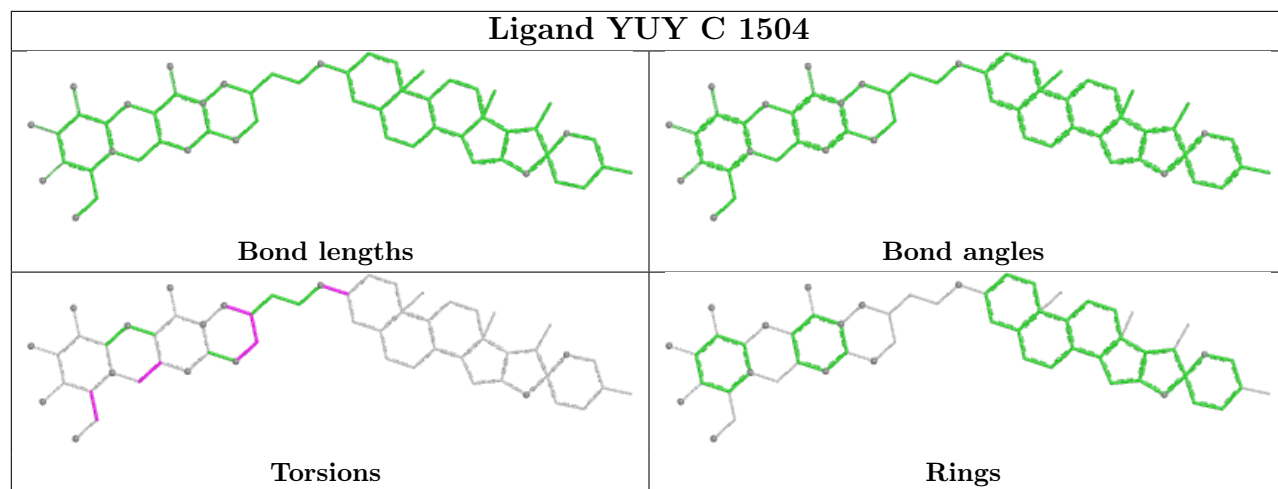


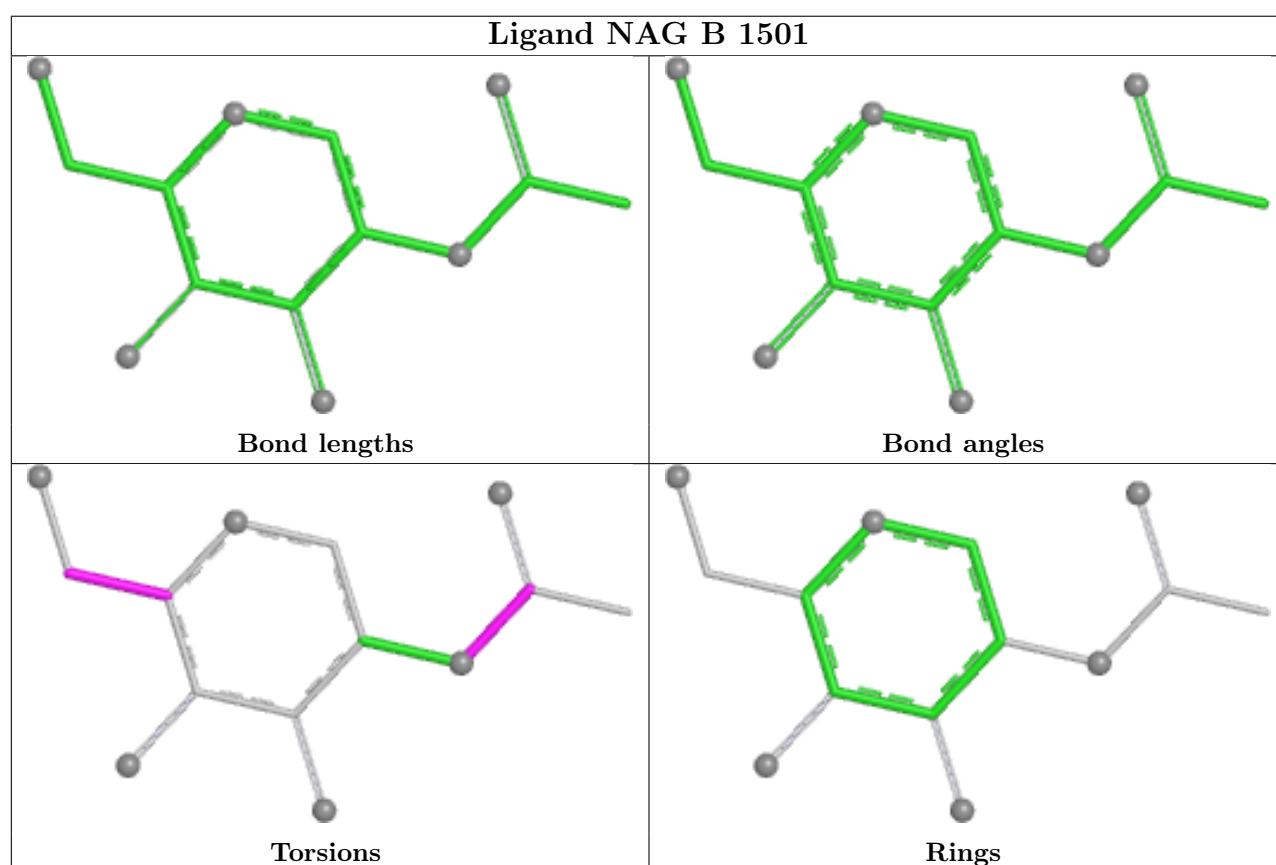
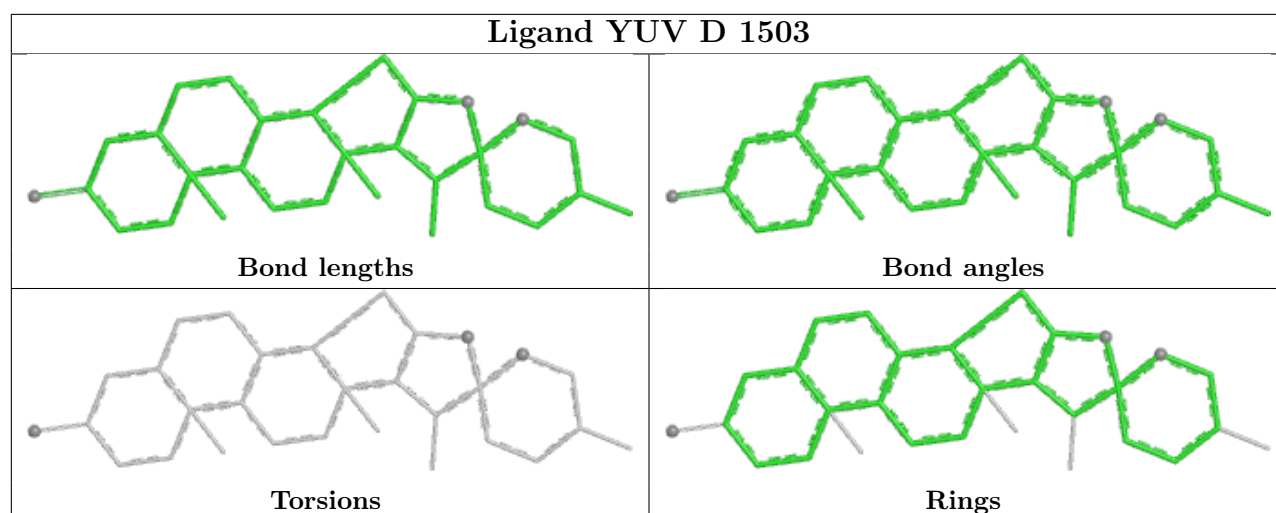
Ligand YUV C 1503

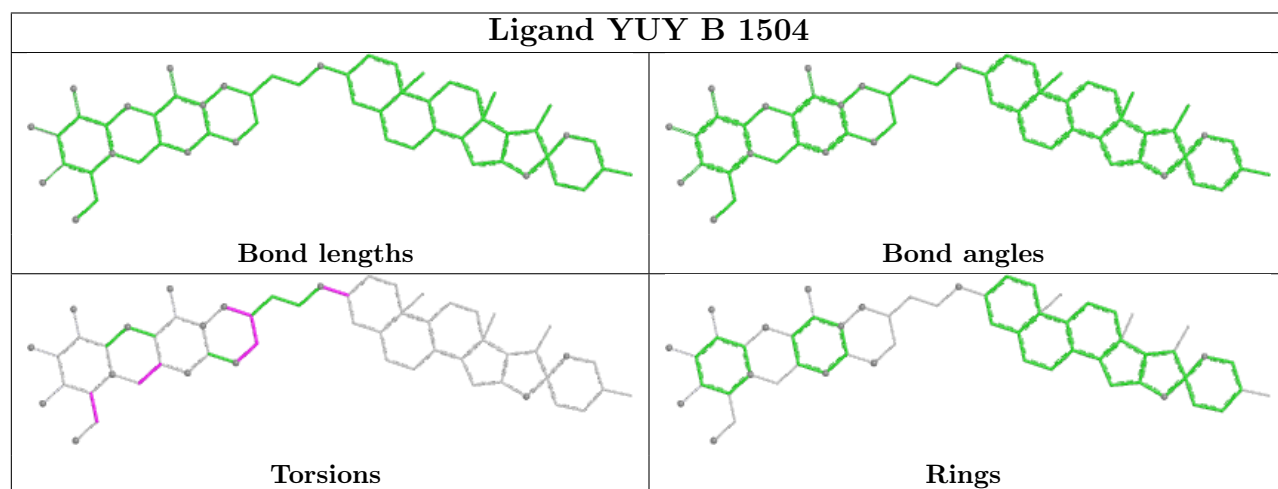
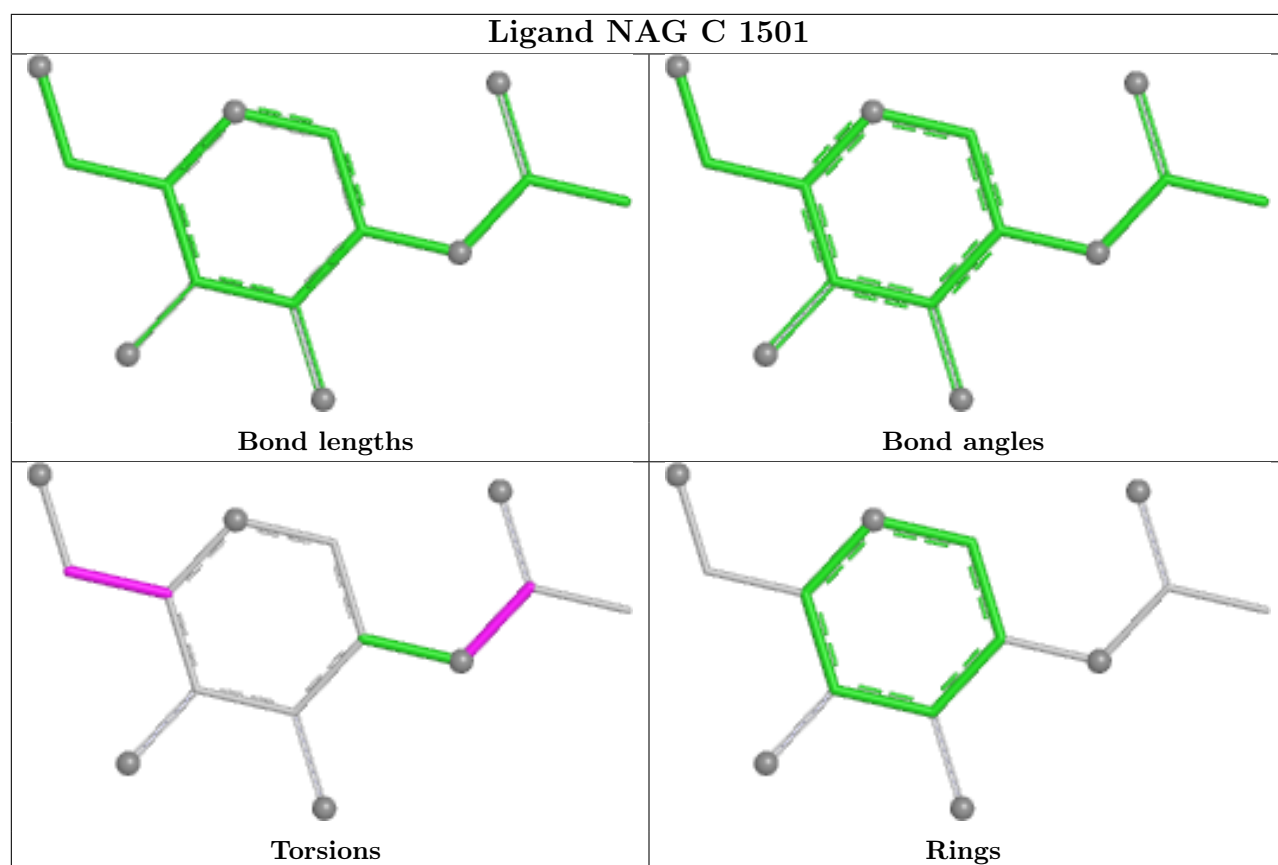


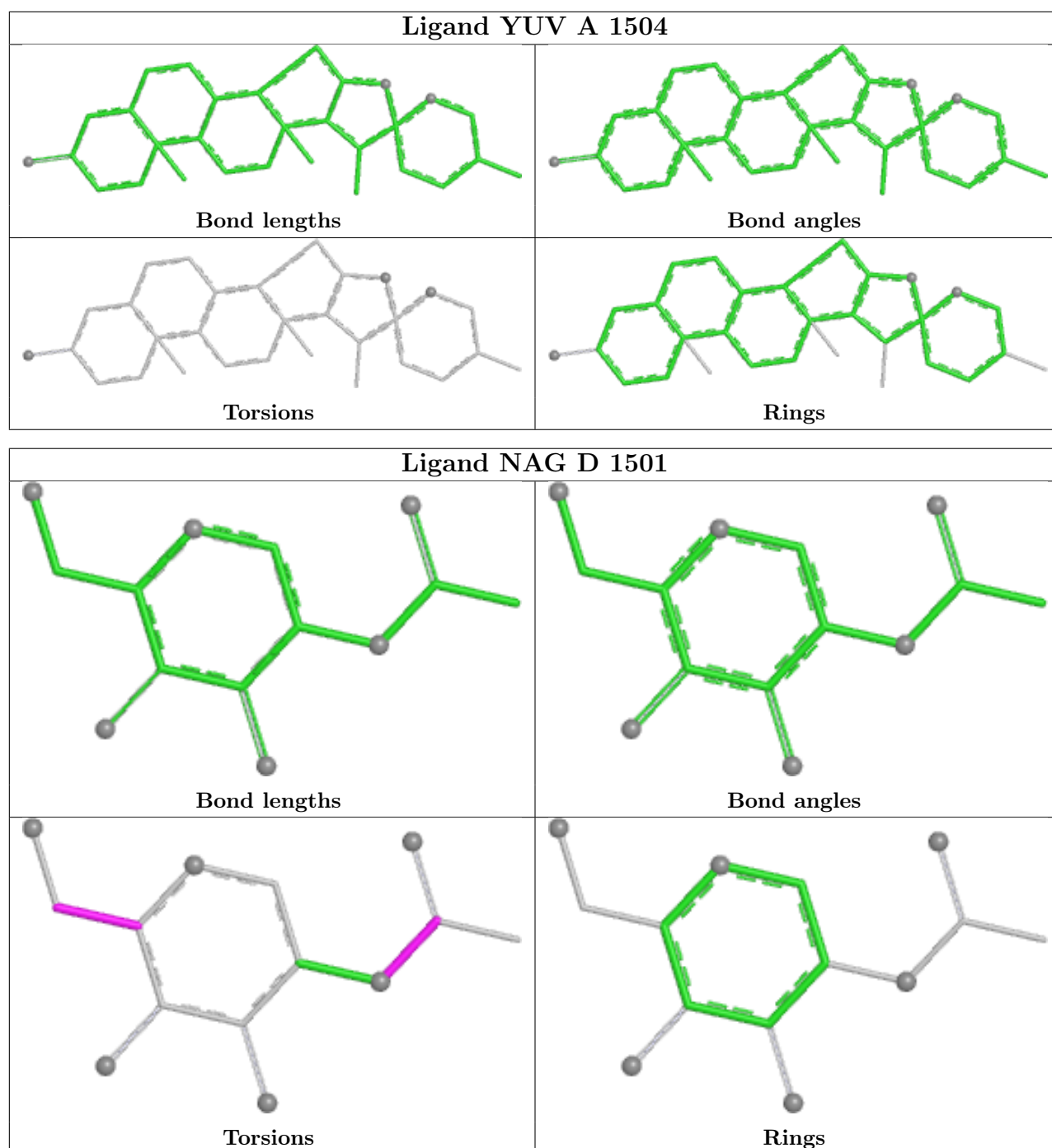
Ligand YUY A 1503











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-23747. 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.