



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 09:50 PM UTC

PDB ID : 1N6F / pdb_00001n6f
Title : tricorn protease in complex with Z-Phe-diketo-Arg-Glu-Phe
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

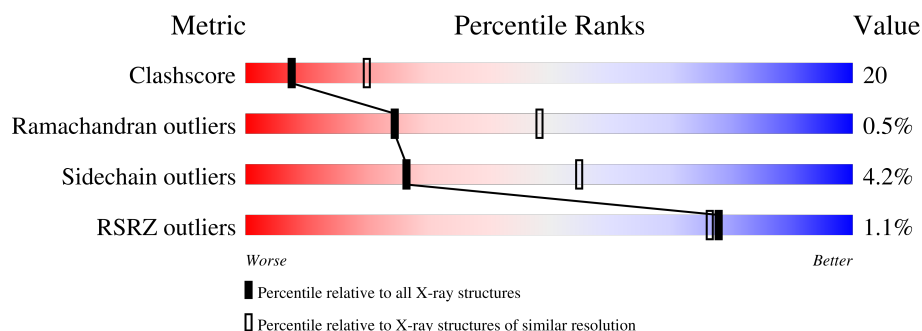
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1071	2% 63% 29% . .
1	B	1071	% 62% 30% . .
1	C	1071	% 58% 34% . .
1	D	1071	% 60% 32% . .
1	E	1071	% 62% 30% . .
1	F	1071	% 59% 33% . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DKT	A	1214	X	X	-	-
2	DKT	B	1214	X	X	-	-
2	DKT	C	1214	X	X	-	-
2	DKT	D	1214	X	X	-	-
2	DKT	E	1214	X	X	-	-
2	DKT	F	1214	X	X	-	-

2 Entry composition [i](#)

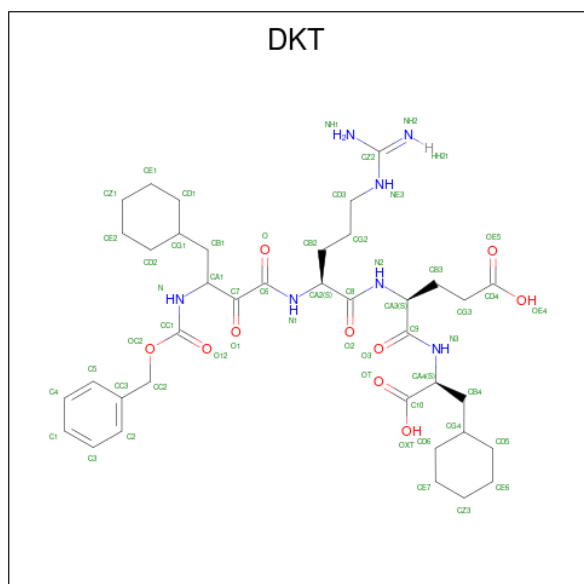
There are 3 unique types of molecules in this entry. The entry contains 50087 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called tricorn protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	B	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	D	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			
1	E	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	F	1023	Total	C	N	O	S	94	0	0
			8176	5196	1402	1550	28			

- Molecule 2 is 4-[2-(3-BENZYLOXYCARBONYLAMINO-4-CYCLOHEXYL-1-HYDROXY-2-OXO-BUTYLAMINO)-5-GUANIDINO-PENTANOYLAMINO]-4-(1-CARBOXY-2-CYCLOHEXYL-ETHYLCARBAMOYL)-BUTYRIC ACID (CCD ID: DKT) (formula: $C_{38}H_{57}N_7O_{10}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	38	7	10		
2	B	1	Total	C	N	O	0	0
			55	38	7	10		
2	C	1	Total	C	N	O	0	0
			55	38	7	10		
2	D	1	Total	C	N	O	0	0
			55	38	7	10		
2	E	1	Total	C	N	O	0	0
			55	38	7	10		
2	F	1	Total	C	N	O	0	0
			55	38	7	10		

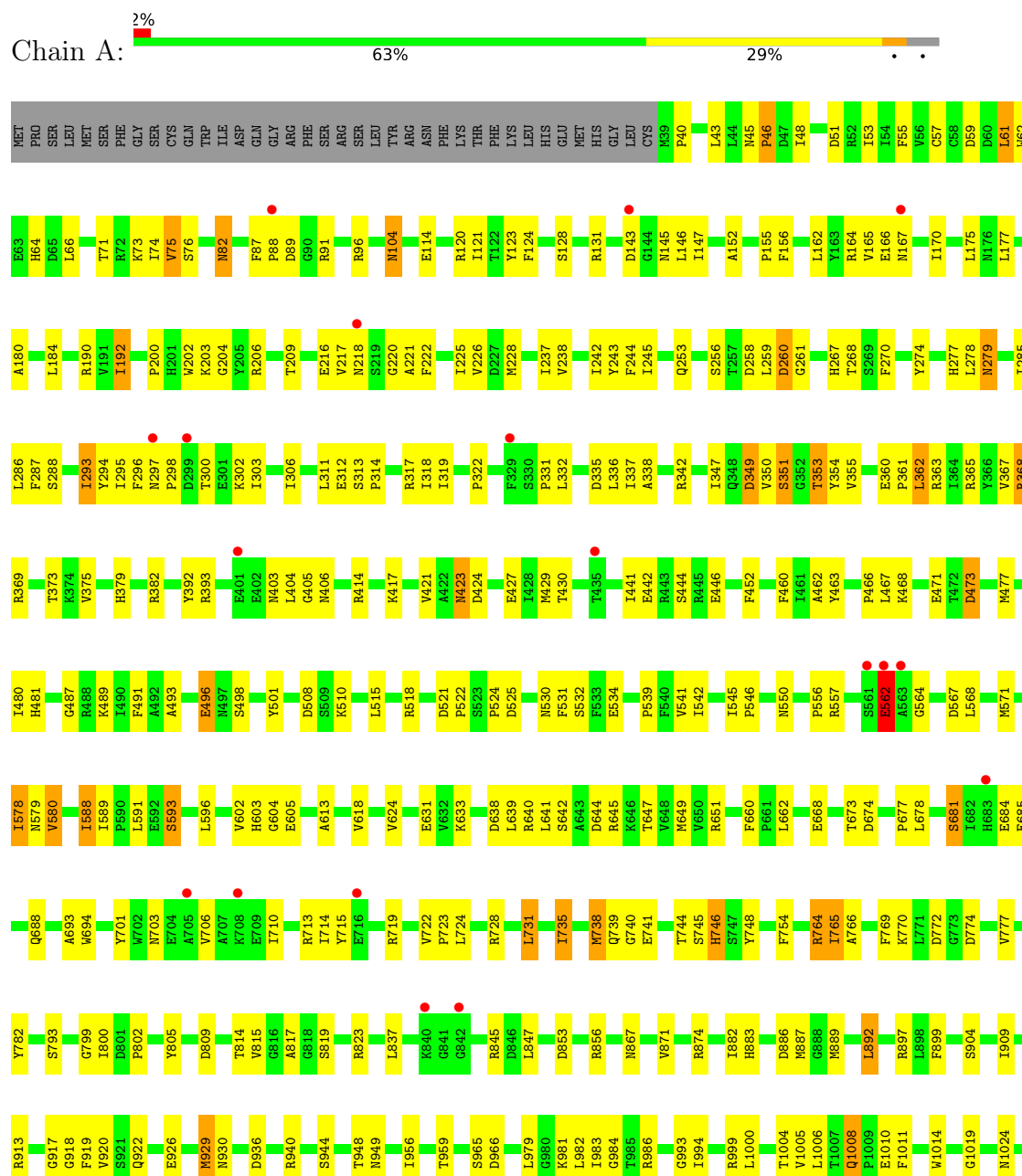
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	108	Total	O	0	0
			108	108		
3	C	136	Total	O	0	0
			136	136		
3	D	132	Total	O	0	0
			132	132		
3	E	105	Total	O	0	0
			105	105		
3	F	104	Total	O	0	0
			104	104		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: tricorn protease



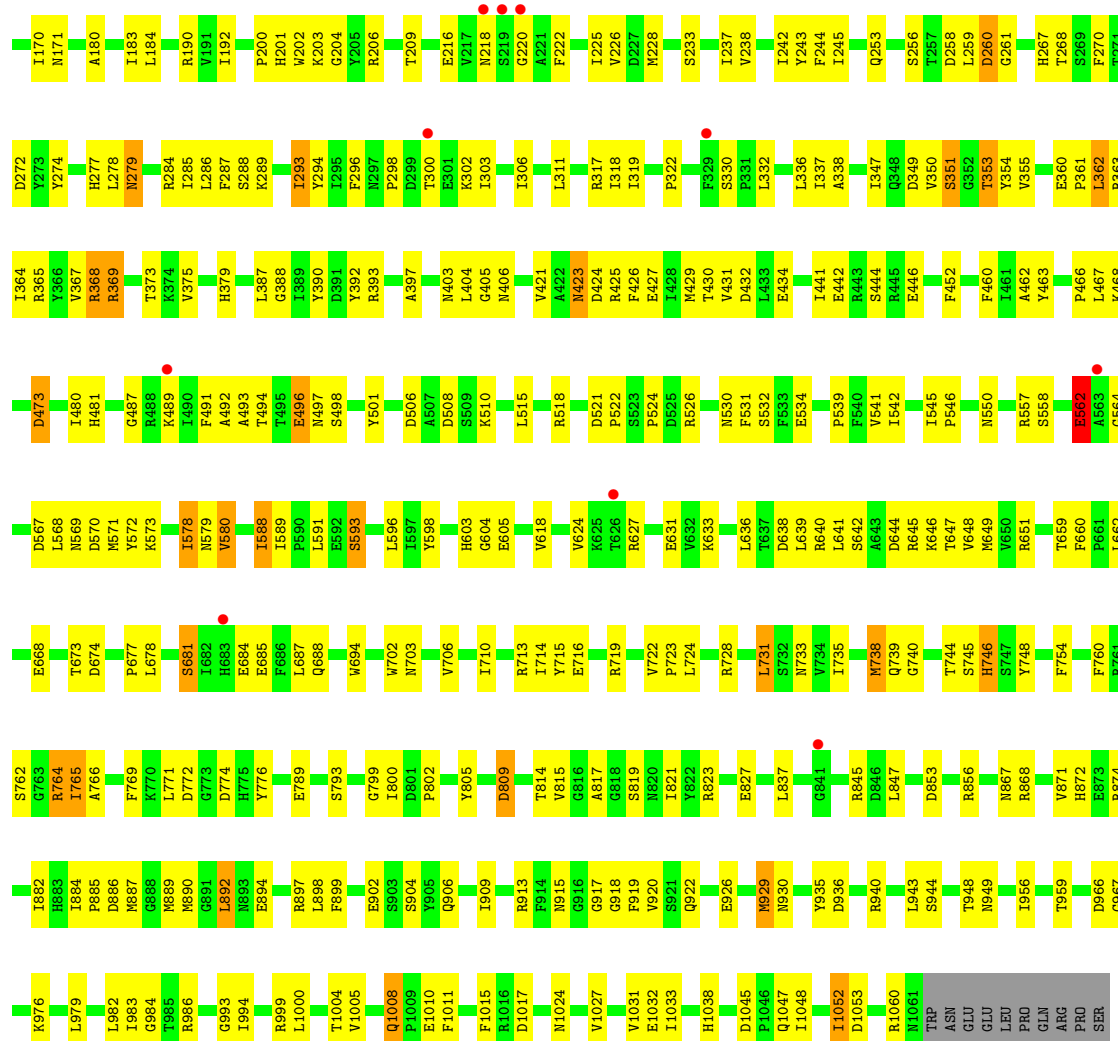


MET	PRO	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	ILE	ASP	GLN	GLY	ARG	PHE	SER	ARG	SER	LEU	TYR	ARG	ASN	PHE	LYS	THR	PHE	LYS	LEU	HIS	GLY	LEU	CYS	R39	P40	L43	L44	N45	P46	D47	I48	D51	R52	I53	I54	F55	V56	C57	C58	D59	D60	L61	W62																																													
E63	H64	D65	L66	T71	R72	K73	I74	W75	S76	N82	R85	F86	F87	P88	D89	G90	R91	R92	I93	R96	V97	N98	R99	M104	Y111	E114	I118	K119	R120	Y121	F124	G123	S125	S128	R131	D141	P142	D143	G144	N145	L146	A152	M153	Q154	P155	L166	N167																																																				
I242	Y243	F244	I245	Q253	S256	D258	L259	D260	G261	K262	L177	H277	L278	M279	I285	L286	F287	S288	K289	G388	L387	I389	Y390	D391	Y392	R393	A397	E301	K302	I303	I306	E307	L311	M228	P314	R317	I318	I319	P322	L332	I428	N429	F430	H431	V432	S433	F434	G435	L436	A437	M438	N439	I440	S441	R442	V443	W444	X445	Y446	Z447																																							
L336	I337	A338	F346	I347	Q348	D349	V350	G352	T353	Y354	E360	P361	R362	R363	I364	R365	Y366	V367	R368	R369	T373	K374	V375	H379	F386	L387	G388	I389	Y390	D391	Y392	R393	A397	E401	E402	N403	L404	G405	N406	V421	A422	N423	D424	R425	F426	E427	I428	N429	F430	H431	V432	S433	F434	G435	L436	A437	M438	N439	I440	S441	R442	V443	W444	X445	Y446	Z447																																	
E534	V535	V536	Q537	K538	F540	V541	I542	I545	P546	N550	R557	S558	M559	E563	G564	D567	L568	M571	P577	I578	W579	V580	G583	I588	I589	P590	L591	E592	S593	L596	H603	G604	E605	A613	V618	V624	S622	E631	V632	K633	D638	L641	S642	R645	Q646	T647	V648	M649	R651	T659	F660	P661	L662	E668	T673	D674	K675	P676	F677	L678	V679	S680	L681	D682	G683	M684	N685	I686	V687	W688	X689	Y690	Z691	AA692	AB693	AC694	AD695	AE696	AF697	AG698	AH699	AI700	AJ701	AK702	AL703	AM704	AN705	AO706	AP707	AQ708	AR709	AS710	AT711	AU712	AV713	AW714	AX715	AY716	AZ717
L641	S642	R645	Q646	T647	V648	M649	R651	T659	F660	P661	L662	E668	T673	D674	K675	P676	F677	L678	V679	S680	L681	D682	G683	M684	N685	I686	V687	W688	X689	Y690	Z691	AA692	AB693	AC694	AD695	AE696	AF697	AG698	AH699	AI700	AJ701	AK702	AL703	AM704	AN705	AO706	AP707	AQ708	AR709	AS710	AT711	AU712	AV713	AW714	AX715	AY716	AZ717																																										
E737	M738	Q739	G740	E741	T744	S745	H746	S747	Y748	F754	F760	R761	G762	R763	R764	I765	A766	C767	D768	F769	K770	L771	D772	G773	D774	H775	Y776	V777	V778	A779	K780	A781	Y782	Y786	S787	N788	E789	G790	E791	K792	S793	F796	G799	I800	D801	P802	G803	R804	Y805	D809	T814	V815	W816	X817	Y818	Z819	AA820	AB821	AC822	AD823	AE824	AF825	AG826	AH827	AI828	AJ829	AK830	AL831	AM832	AN833	AO834	AP835	AQ836	AR837	AS838	AT839	AU840	AV841	AW842	AX843	AY844	AZ845																	
Q816	A817	Q818	S819	R823	L837	R845	L846	L847	D853	R856	F857	I858	R861	N867	R868	R869	Y870	V871	R874	M887	K888	M889	M890	Q891	L892	N893	E894	L898	F899	S904	Y905	Q906	I909	V912	R913	F914	G916	G917	G918	F919	V920	S921	Q922	E926	M929	N930	D936	R939	R940	S944	T948	N949	G953	K954	I955	I956	T959	N960	G964	S965	D966	T969	F970	K975	K976	L977	G978	L979	L982	R983	G984	R985	R986	G993	I994	R999	L1000	T1004	V1005	Q1008	P1009	E1010	F1011	W1014	D1017	A1018	G1019												
N1024	V1027	D1028	V1031	E1032	I1033	H1038	D1045	F1046	Q1047	I1048	D1049	Y1050	A1051	I1052	D1053	N1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	PRO	SER																																																																								

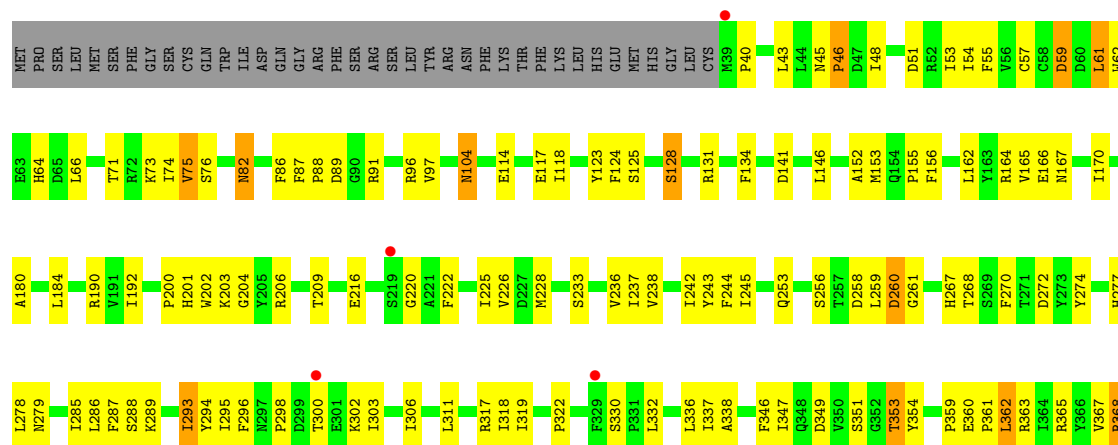
• Molecule 1: tricorn protease

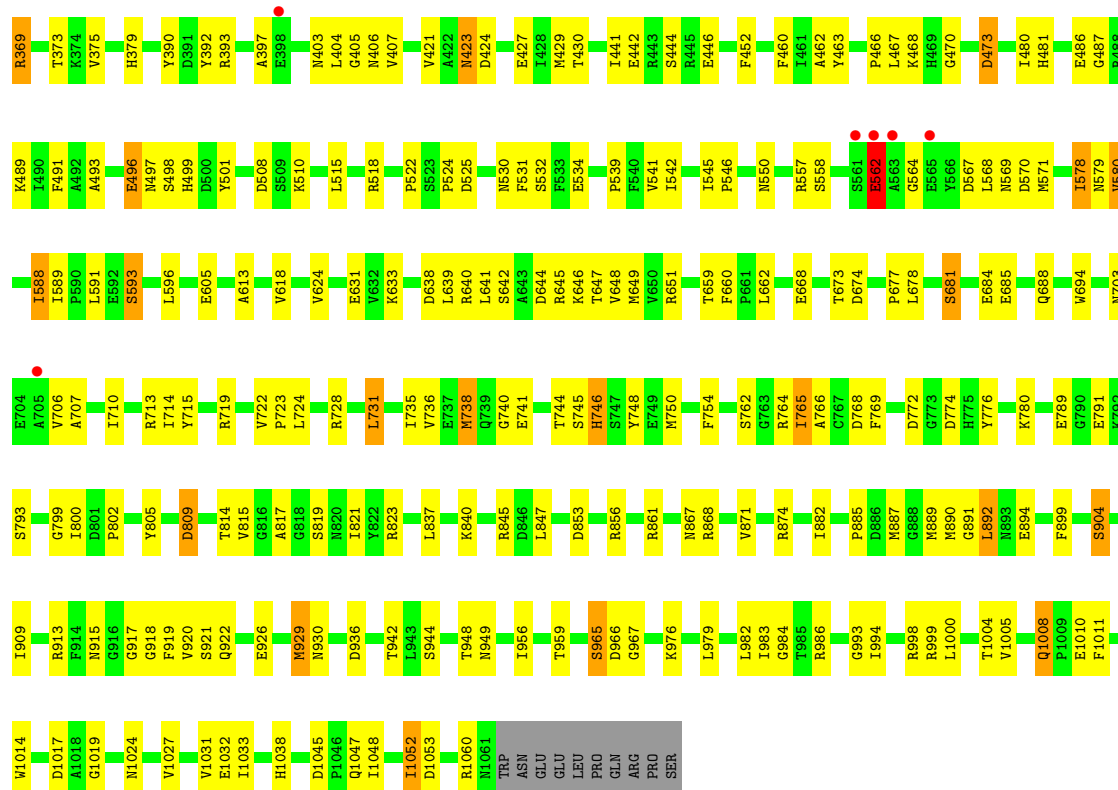


MET	PRO	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	ILE	ASP	GLN	GLY	ARG	PHE	SER	ARG	SER	LEU	TYR	ASN	ASN	PHE	LYS	THR	PHE	LYS	LEU	HIS	GLU	MET	HIS	GLY	LEU	CYS	R39	P40	L43	L44	N45	P46	D47	I48	D51	R52	I53	I54	F55	V56	C57	C58	D59	D60	L61	W62																													
E63	H64	D65	L66	T71	R72	K73	I74	W75	S76	N82	R85	F86	F87	P88	D89	G90	R91	R96	V97	N98	R99	M104	Y109	E114	E117	I118	K119	R120	Y123	S125	S128	R131	D141	P142	G144	N145	L146	A152	M153	Q154	P155	L166	N167	I170	V173	P174	L175	H176	L177	A180	T267	R268	S269	F270	R189	R190	R191	Y192	T196	F197	P200	H201	W202	K203	G204	K205	R206	T209	E216	V217	N218	S219	A221	F222	I225	V226	D227	H228	H231	V232	S233	R234	I318	I319	P322	L332
L336	I337	A338	F346	I347	Q348	D349	V350	L351	G352	T353	Y354	E360	L361	L362	R363	I364	R365	Y366	V367	R368	R369	T373	K374	V375	H379	F386	L387	G388	I389	Y390	D391	Y392	R393	A397	E401	E402	N403	L404	G405	N406	V421	A422	N423	D424	R425	F426	E427	I428	T430																																					
E434	V440	I441	E442	R443	S444	R445	E446	A447	M448	F452	F460	L461	A462	Y463	P466	L467	K468	D473	T480	H481	G487	R488	K489	L490	F491	A492	A493	E496	M497	S498	Y501	D508	S509	K510	L515	R518	D521	P522	S523	P524	N530	F531	S532	F533																																										
E534	V535	V536	Q537	K538	F540	V541	I542	I545	P546	N550	R557	S558	M559	E563	G564	D567	L568	M571	P577	I578	W579	V580	G583	I588	I589	P590	L591	E592	S593	L596	H603	G604	E605	A613	V618	V624	S622	E631	V632	K633	D638																																													
L641	S642	R645	Q646	T647	V648	M649	R651	T659	F660	P661	L662	E668	T673	D674	K675	P677	F678	V679	L680	S681	E684	I685	F686	L687	Q688	M689	A689	Y690	W694	N703	V706	I710	R713	I714	Y715	R719	V722	P723	L724	R728	L731	V734																																												
E737	M738	Q739	G740	E741	T744	S745	H746	S747	Y748	F754	F760	R761	G762	R763	R764	I765	A766	C767	D768	F769	K770	L771	D772	G773	D774	H775	Y776	V777	V778	A779	K780	A781	Y782	Y786	S787	N788	E789	G790	E791	K792	S793	F796	G799	I800	D801	P802	G803	R804	Y805	D809	T814	V815																																		
Q816	A817	Q818	S819	R823	L837	R845	L846	L847	D853	R856	F857	I858	R861	N867	R868	R869	Y870	V871	R874	M887	K888	M889	M890	Q891	L892	N893	E894	L898	F899	S904	Y905	Q906	I909	V912	R913	F914	G916	G917	G918	F919	V920	S921	Q922	E926																																										
M929	N930	D936	R939	R940	S944	T948	N949	G953	K954	I955	I956	T959	N960	G964	S965	D966	T969	F970	K975	K976	L977	G978	L979	L982	R983	G984	R985	R986	G993	I994	R999	L1000	T1004	V1005	Q1008	P1009	E1010	F1011	W1014	D1017	A1018	G1019																																												
M1024	V1027	D1028	V1031	E1032	I1033	H1038	D1045	F1046	Q1047	I1048	D1049	Y1050	A1051	I1052	D1053	N1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	PRO	SER																																																											

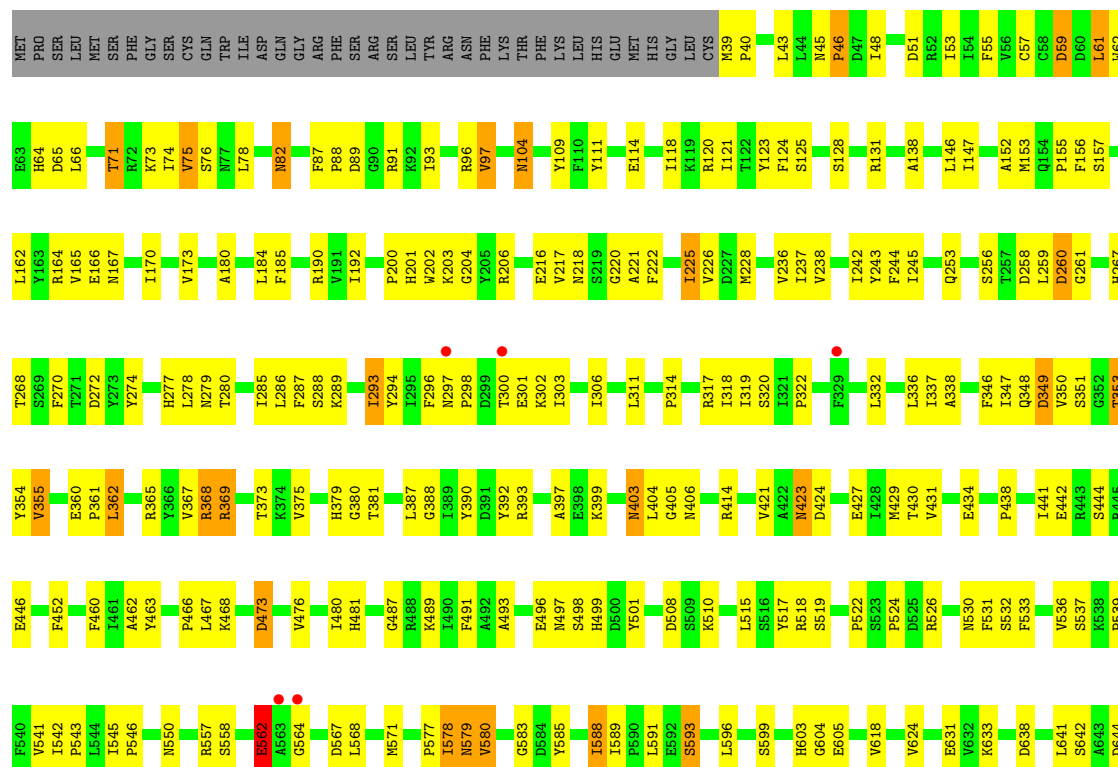


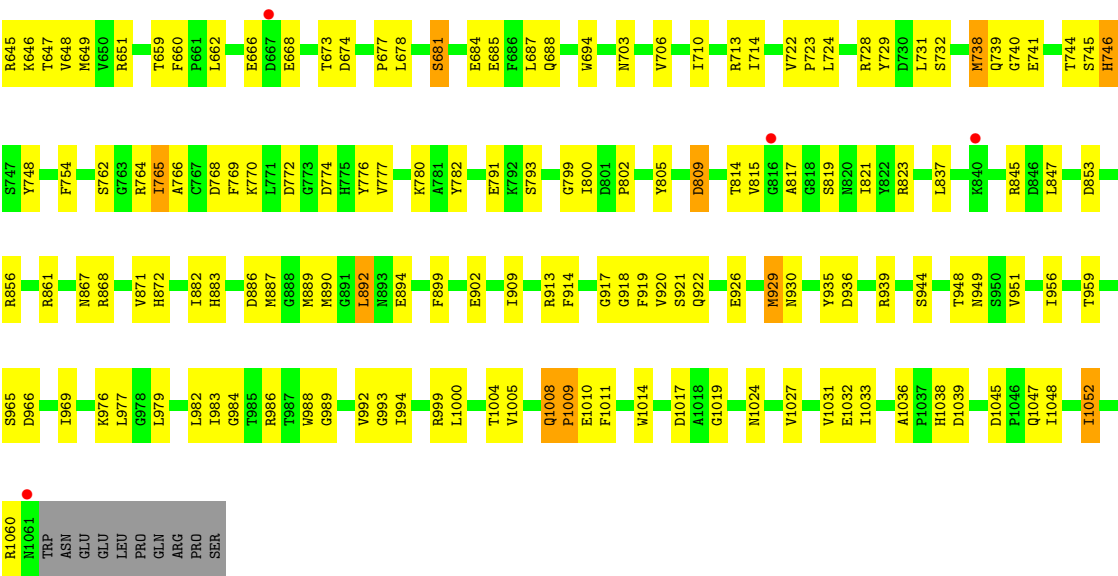
• Molecule 1: tricorn protease





• Molecule 1: tricorn protease





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.67Å 244.55Å 158.32Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	85.8 (6.00-2.70) 77.0 (6.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.247 , 0.280 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.682	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.52 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.054 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	50087	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DKT

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	0.64	1/8367 (0.0%)	0.94	12/11311 (0.1%)
1	B	0.65	0/8366	0.94	13/11310 (0.1%)
1	C	0.61	1/8366 (0.0%)	0.94	11/11310 (0.1%)
1	D	0.62	0/8366	0.94	10/11310 (0.1%)
1	E	0.62	1/8367 (0.0%)	0.94	12/11311 (0.1%)
1	F	0.60	0/8366	0.94	13/11310 (0.1%)
All	All	0.62	3/50198 (0.0%)	0.94	71/67862 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	MET	SD-CE	5.36	1.93	1.79
1	E	153	MET	SD-CE	5.22	1.92	1.79
1	A	477	MET	SD-CE	-5.15	1.66	1.79

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	746	HIS	N-CA-C	6.87	120.97	111.90
1	B	1052	ILE	CB-CA-C	-6.78	103.34	111.81
1	C	1052	ILE	CB-CA-C	-6.76	103.36	111.81
1	E	1052	ILE	CB-CA-C	-6.59	103.57	111.81
1	D	746	HIS	N-CA-C	6.42	120.26	111.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8177	0	8003	310	0
1	B	8176	0	8000	307	0
1	C	8176	0	8000	399	0
1	D	8176	0	8000	332	0
1	E	8177	0	8003	316	0
1	F	8176	0	8000	371	0
2	A	55	0	46	20	0
2	B	55	0	46	7	0
2	C	55	0	46	8	0
2	D	55	0	46	8	0
2	E	55	0	46	18	0
2	F	55	0	46	11	0
3	A	114	0	0	36	0
3	B	108	0	0	38	0
3	C	136	0	0	94	0
3	D	132	0	0	54	0
3	E	105	0	0	24	0
3	F	104	0	0	87	0
All	All	50087	0	48282	1943	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 20.

The worst 5 of 1943 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:965:SER:HB3	2:A:1214:DKT:C7	1.23	1.62
1:F:965:SER:CB	2:F:1214:DKT:O1	1.64	1.46
1:A:965:SER:CB	2:A:1214:DKT:O1	1.63	1.46
1:E:965:SER:CB	2:E:1214:DKT:O1	1.64	1.43
1:E:965:SER:CB	2:E:1214:DKT:C7	2.02	1.38

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	950 (93%)	66 (6%)	5 (0%)	24	48
1	B	1021/1071 (95%)	948 (93%)	68 (7%)	5 (0%)	24	48
1	C	1021/1071 (95%)	947 (93%)	69 (7%)	5 (0%)	24	48
1	D	1021/1071 (95%)	955 (94%)	61 (6%)	5 (0%)	24	48
1	E	1021/1071 (95%)	951 (93%)	65 (6%)	5 (0%)	24	48
1	F	1021/1071 (95%)	946 (93%)	69 (7%)	6 (1%)	21	44
All	All	6126/6426 (95%)	5697 (93%)	398 (6%)	31 (0%)	24	48

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
1	B	579	ASN
1	C	579	ASN
1	D	579	ASN
1	E	579	ASN

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	847 (96%)	36 (4%)	27	56
1	B	882/928 (95%)	845 (96%)	37 (4%)	26	55
1	C	882/928 (95%)	843 (96%)	39 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	882/928 (95%)	843 (96%)	39 (4%)	25	53
1	E	883/928 (95%)	847 (96%)	36 (4%)	27	56
1	F	882/928 (95%)	845 (96%)	37 (4%)	26	55
All	All	5294/5568 (95%)	5070 (96%)	224 (4%)	26	55

5 of 224 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	75	VAL
1	F	892	LEU
1	D	772	ASP
1	F	847	LEU
1	F	311	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 192 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	635	ASN
1	E	499	HIS
1	D	867	ASN
1	E	104	ASN
1	E	733	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	DKT	B	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	C	1214	-	55,57,57	3.84	26 (47%)	66,74,74	5.26	38 (57%)
2	DKT	F	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	D	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	E	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)
2	DKT	A	1214	-	55,57,57	3.85	26 (47%)	66,74,74	5.27	38 (57%)

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	DKT	B	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	C	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	F	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	D	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	E	1214	-	1/1/14/19	27/61/77/77	0/3/3/3
2	DKT	A	1214	-	1/1/14/19	27/61/77/77	0/3/3/3

The worst 5 of 156 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1214	DKT	C4-C5	9.77	1.55	1.38
2	D	1214	DKT	C4-C5	9.77	1.55	1.38
2	A	1214	DKT	C4-C5	9.72	1.55	1.38
2	E	1214	DKT	C4-C5	9.72	1.55	1.38
2	F	1214	DKT	C4-C5	9.70	1.55	1.38

The worst 5 of 228 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1214	DKT	CG1-CB1-CA1	20.45	142.02	114.52
2	F	1214	DKT	CG1-CB1-CA1	20.44	142.00	114.52
2	B	1214	DKT	CG1-CB1-CA1	20.42	141.98	114.52
2	E	1214	DKT	CG1-CB1-CA1	20.42	141.98	114.52
2	D	1214	DKT	CG1-CB1-CA1	20.42	141.97	114.52

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1214	DKT	CA1
2	B	1214	DKT	CA1
2	C	1214	DKT	CA1
2	D	1214	DKT	CA1
2	E	1214	DKT	CA1

5 of 162 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1214	DKT	N-CC1-OC2-CC2
2	A	1214	DKT	O12-CC1-OC2-CC2
2	A	1214	DKT	CC3-CC2-OC2-CC1
2	A	1214	DKT	N-CA1-CB1-CG1
2	A	1214	DKT	C6-C7-CA1-N

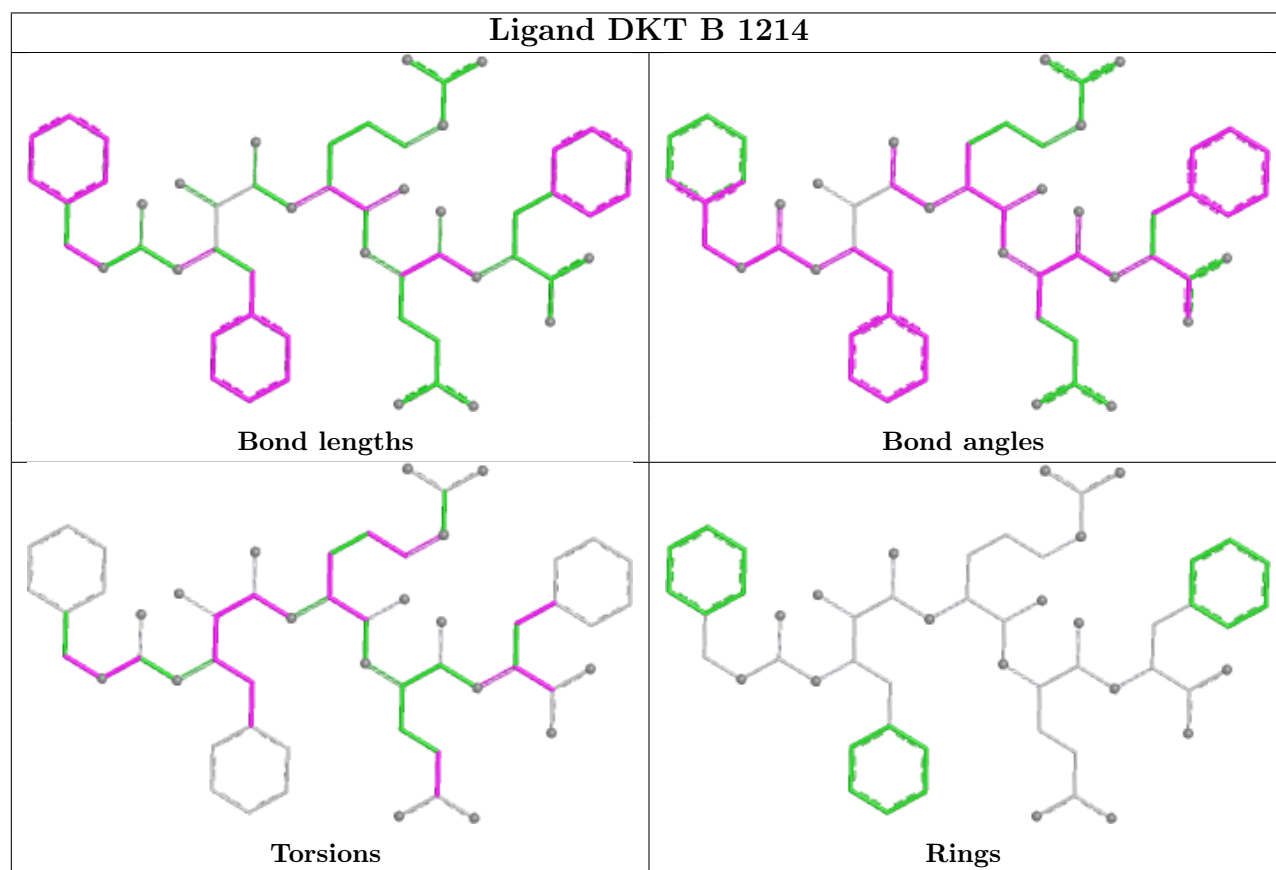
There are no ring outliers.

6 monomers are involved in 72 short contacts:

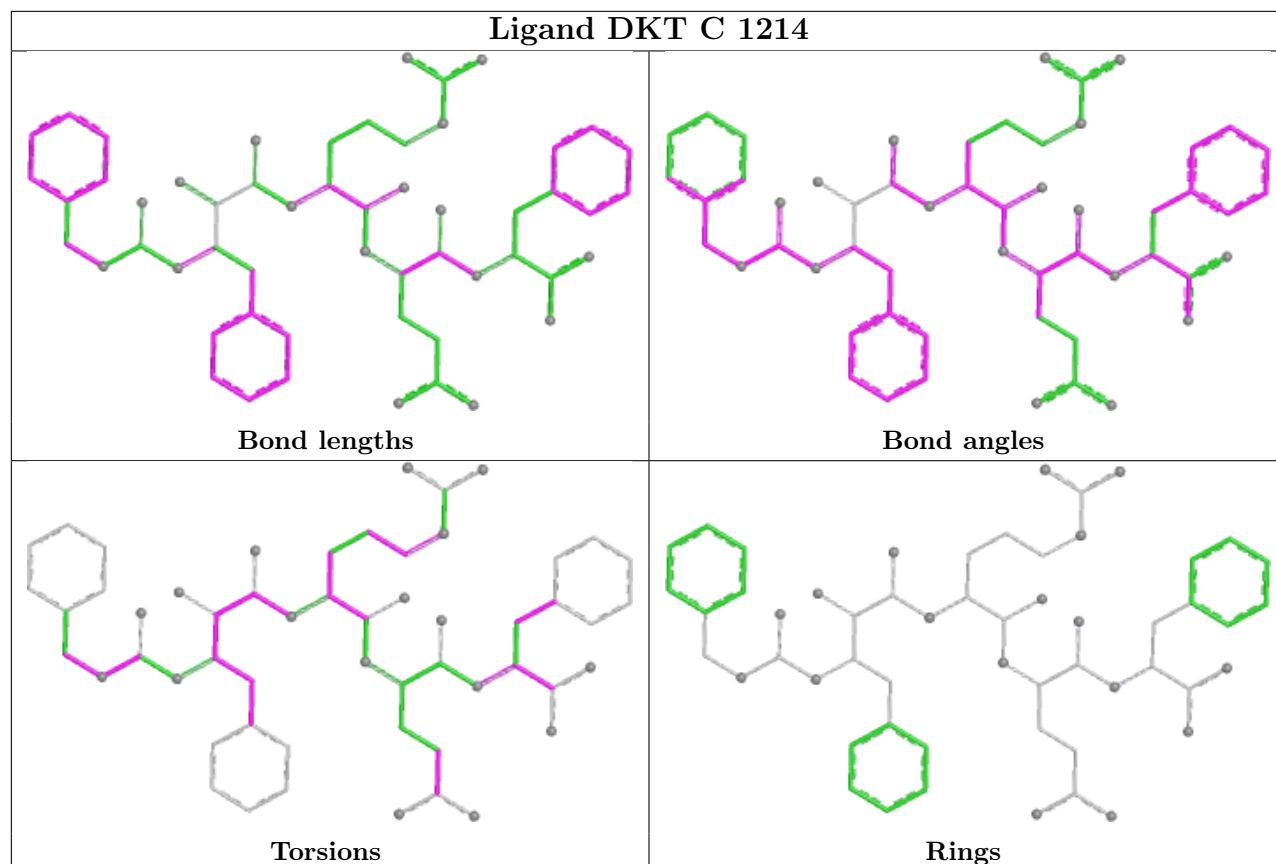
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1214	DKT	7	0
2	C	1214	DKT	8	0
2	F	1214	DKT	11	0
2	D	1214	DKT	8	0
2	E	1214	DKT	18	0
2	A	1214	DKT	20	0

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

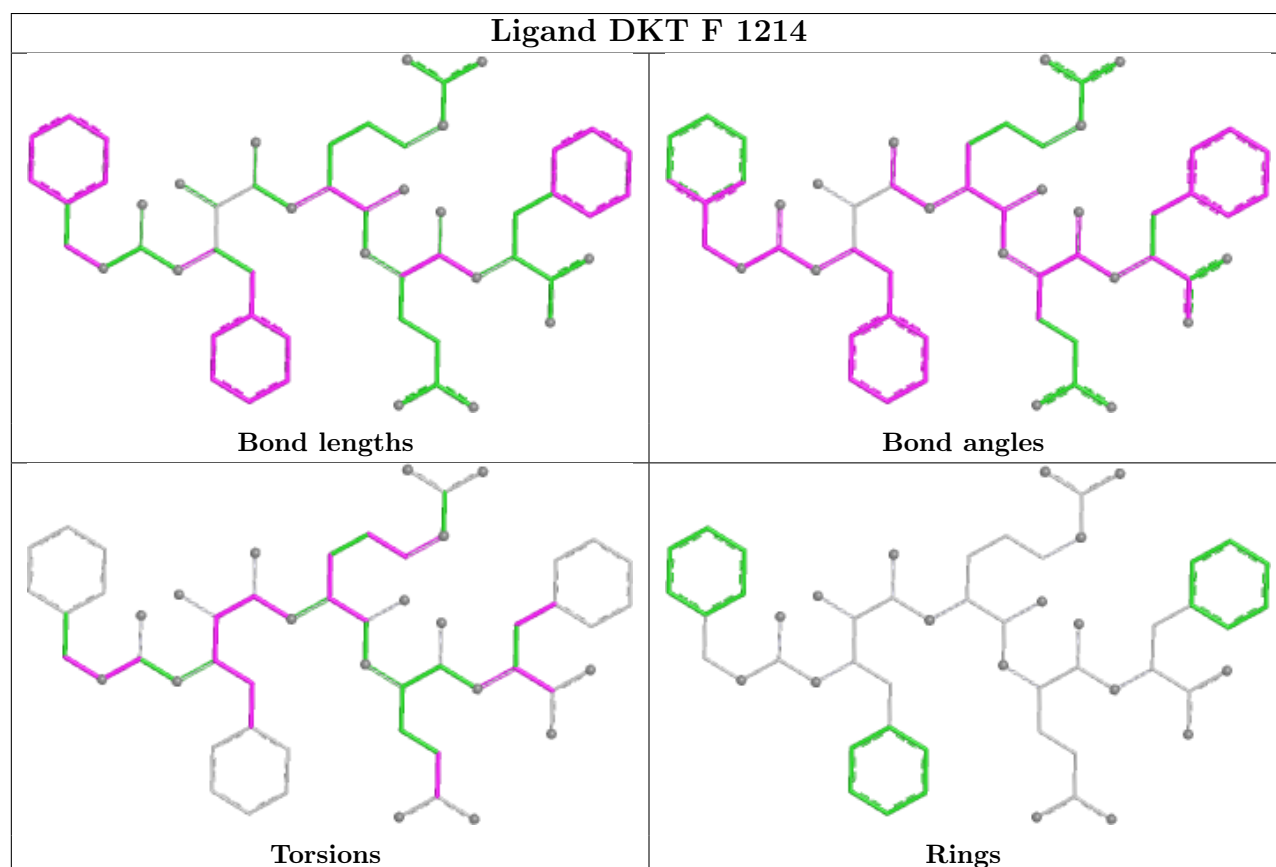
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



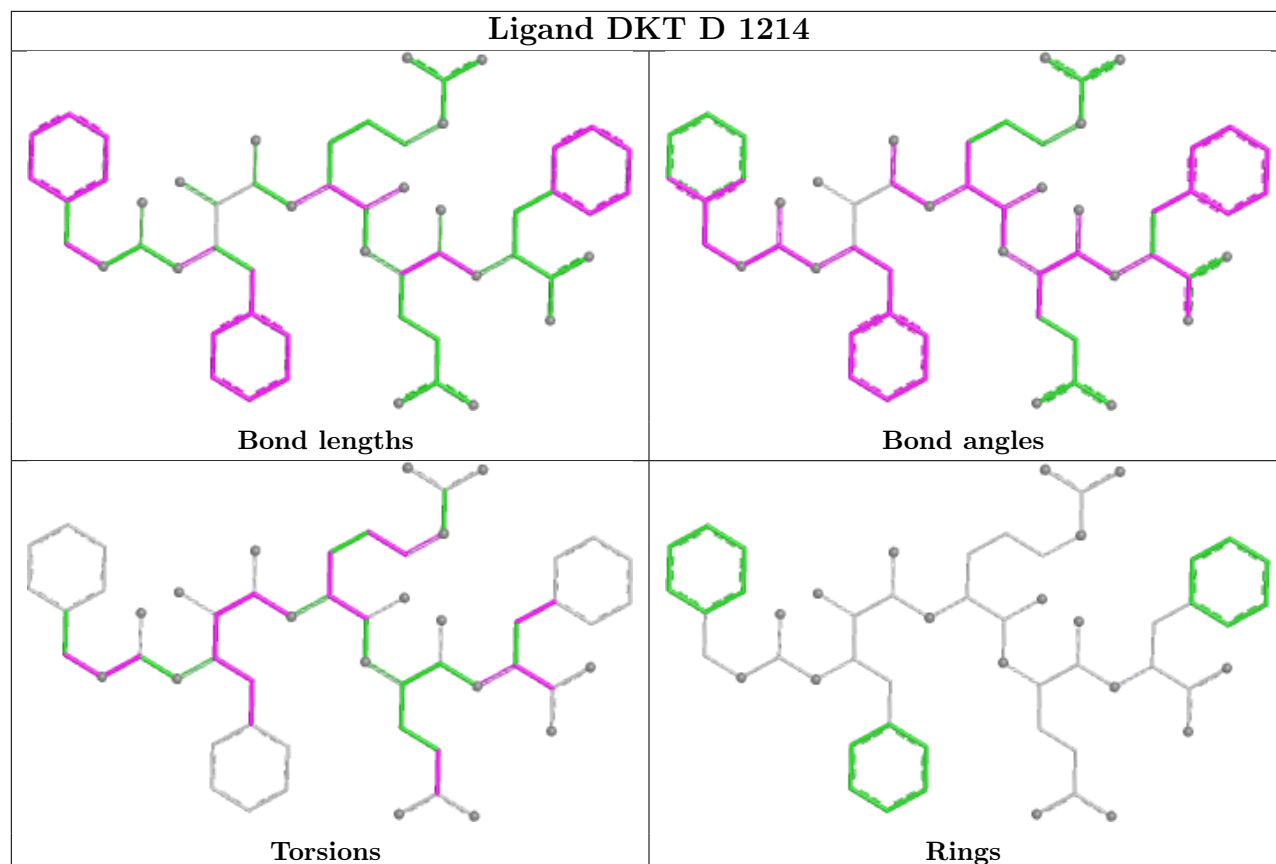
Ligand DKT C 1214



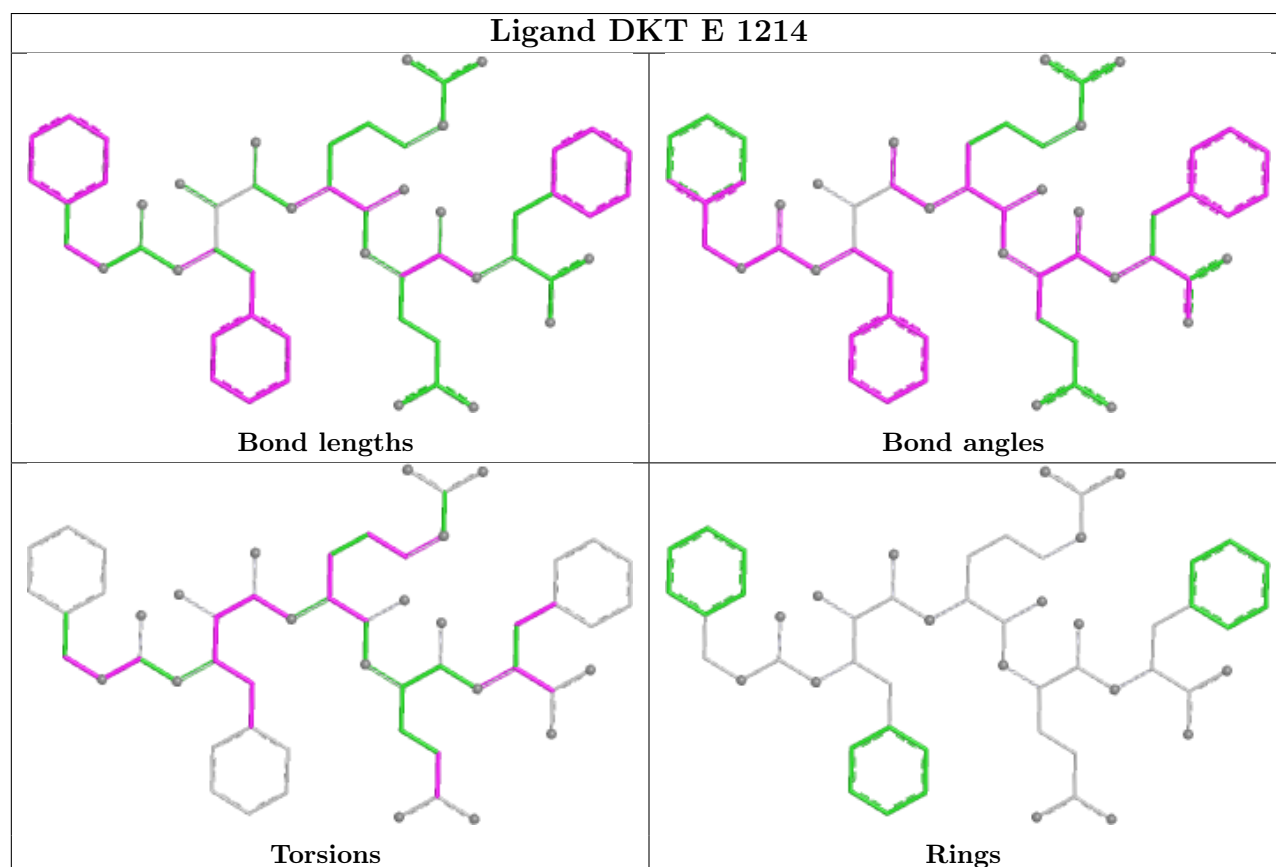
Ligand DKT F 1214

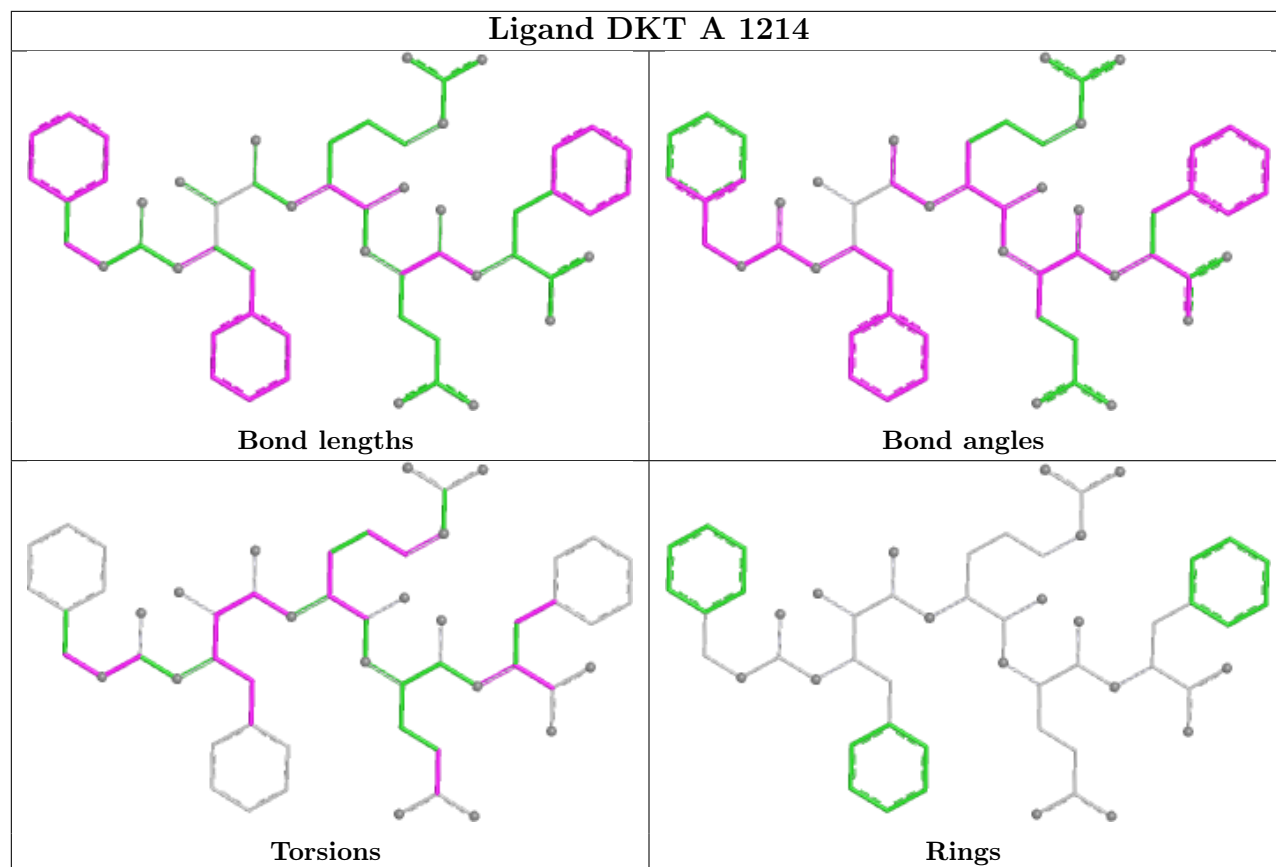


Ligand DKT D 1214



Ligand DKT E 1214





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1023/1071 (95%)	-0.28	18 (1%) 67 65	7, 34, 57, 85	20 (1%)
1	B	1023/1071 (95%)	-0.30	11 (1%) 78 76	7, 34, 57, 85	20 (1%)
1	C	1023/1071 (95%)	-0.13	10 (0%) 79 78	7, 39, 60, 85	20 (1%)
1	D	1023/1071 (95%)	-0.28	10 (0%) 79 78	7, 35, 58, 84	20 (1%)
1	E	1023/1071 (95%)	-0.29	10 (0%) 79 78	7, 35, 58, 83	20 (1%)
1	F	1023/1071 (95%)	-0.18	9 (0%) 81 80	7, 38, 60, 85	20 (1%)
All	All	6138/6426 (95%)	-0.24	68 (1%) 78 76	7, 36, 59, 85	120 (1%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	220	GLY	4.2
1	B	842	GLY	4.1
1	A	562	GLU	4.0
1	C	562	GLU	4.0
1	D	218	ASN	3.9

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

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

6.3 Carbohydrates [i](#)

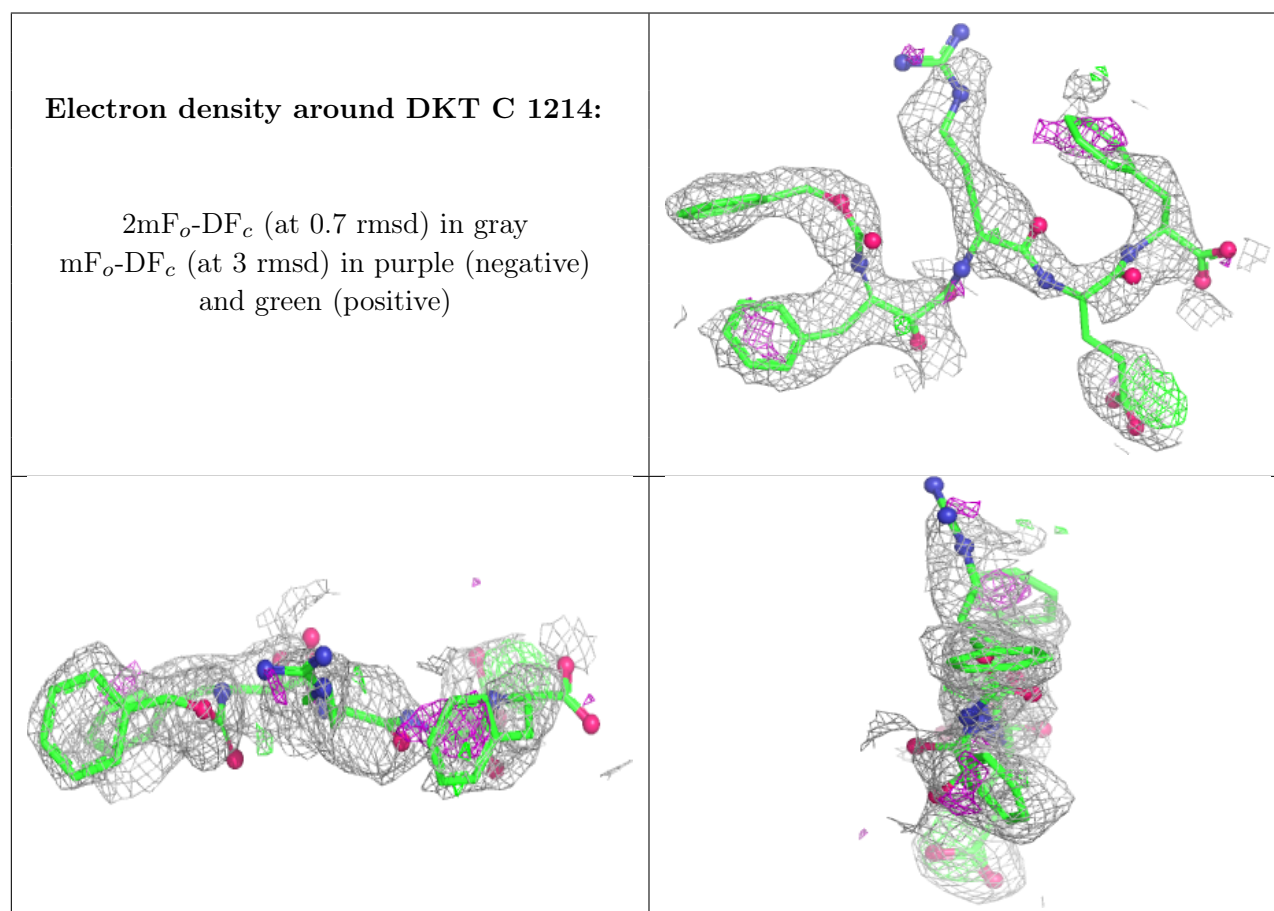
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

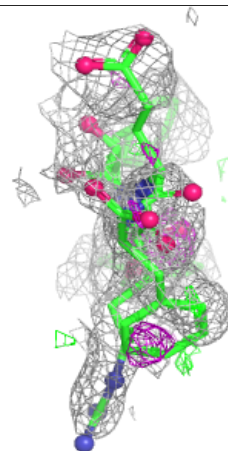
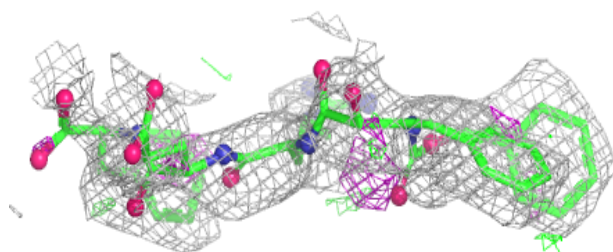
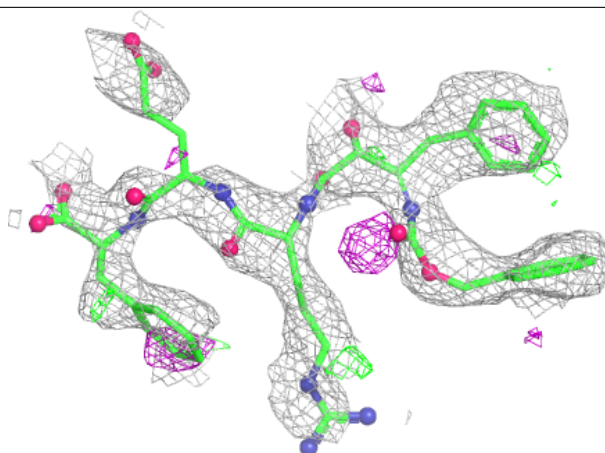
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	DKT	C	1214	55/55	0.69	0.14	41,57,73,74	0
2	DKT	F	1214	55/55	0.70	0.14	41,57,73,74	0
2	DKT	E	1214	55/55	0.71	0.14	41,57,73,74	0
2	DKT	D	1214	55/55	0.75	0.12	41,57,73,74	0
2	DKT	B	1214	55/55	0.76	0.13	41,57,73,74	0
2	DKT	A	1214	55/55	0.78	0.13	41,57,73,74	0

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



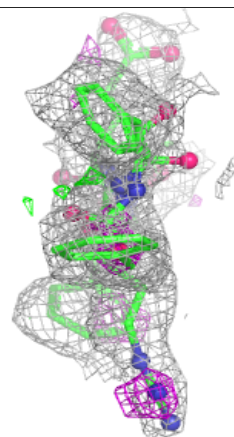
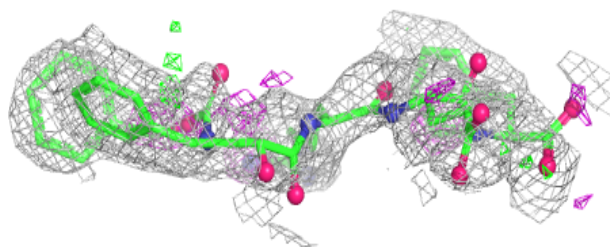
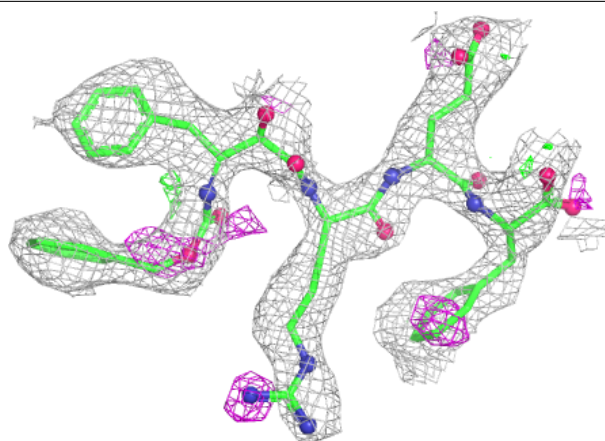
Electron density around DKT F 1214:

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



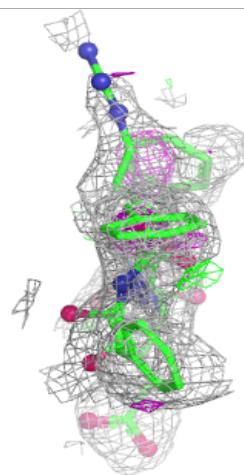
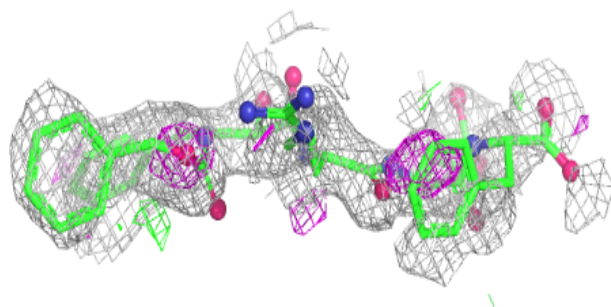
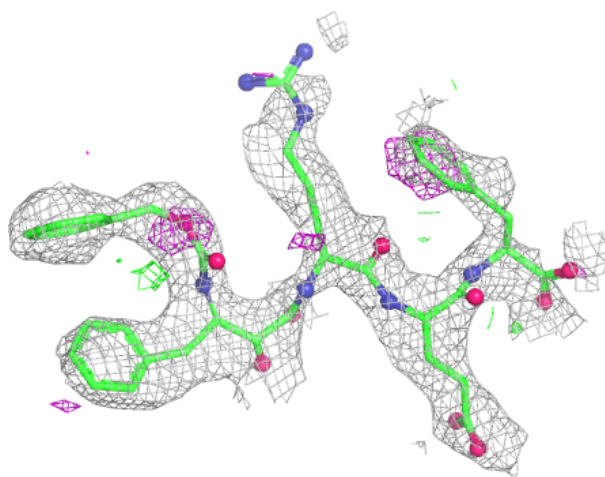
Electron density around DKT E 1214:

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



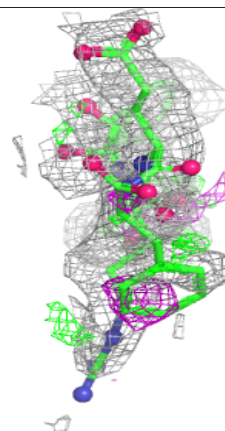
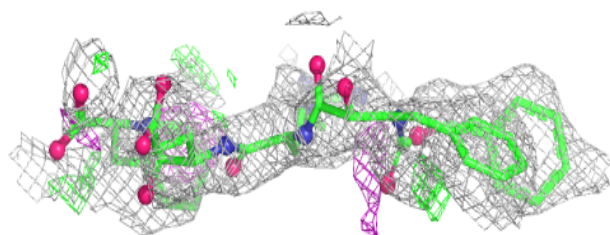
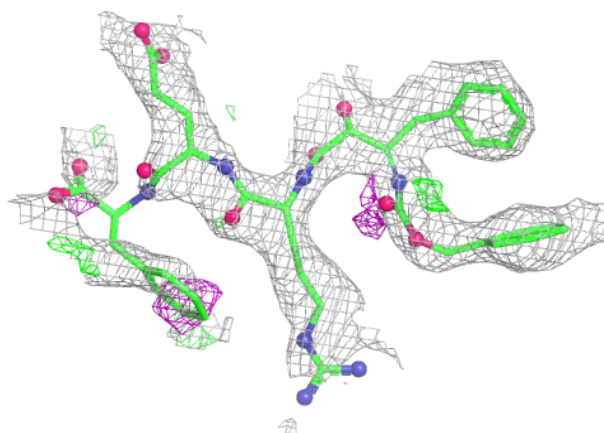
Electron density around DKT D 1214:

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



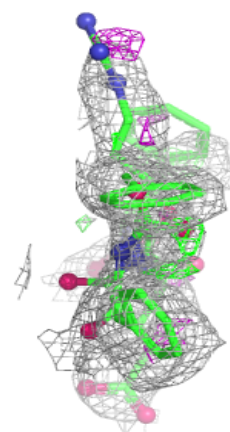
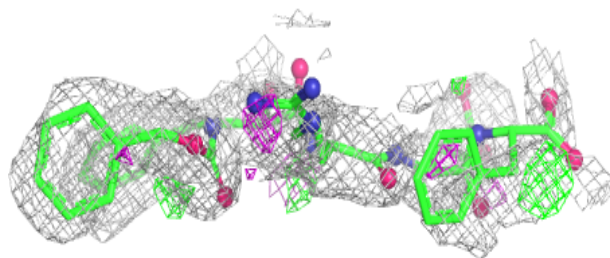
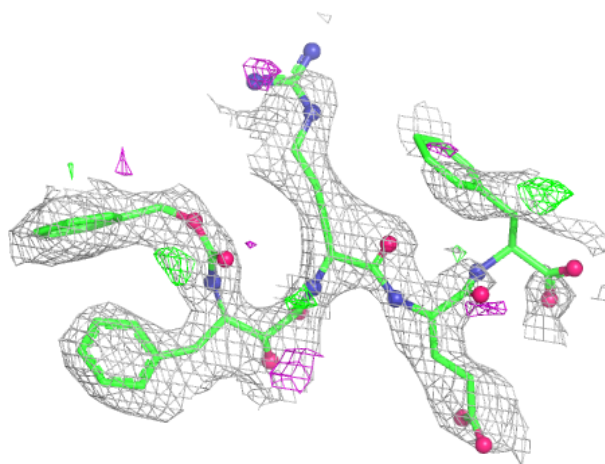
Electron density around DKT B 1214:

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



Electron density around DKT A 1214:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.