



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 04:07 PM UTC

PDB ID : 1N6D / pdb_00001n6d
Title : Tricorn protease in complex with tetrapeptide chloromethyl ketone derivative
Authors : Kim, J.-S.; Groll, M.; Huber, R.; Brandstetter, H.
Deposited on : 2002-11-10
Resolution : 2.80 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
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

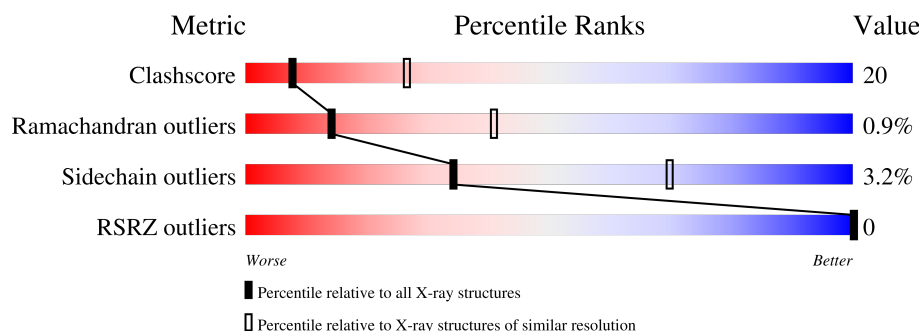
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	
1	B	1071	
1	C	1071	
1	D	1071	
1	E	1071	
1	F	1071	

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Mol	Chain	Length	Quality of chain
2	G	5	20%20%20%40%
2	H	5	20%20%20%40%
2	I	5	20%20%20%40%
2	J	5	20%20%20%40%
2	K	5	20%20%20%40%
2	L	5	20%20%20%40%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 49890 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.

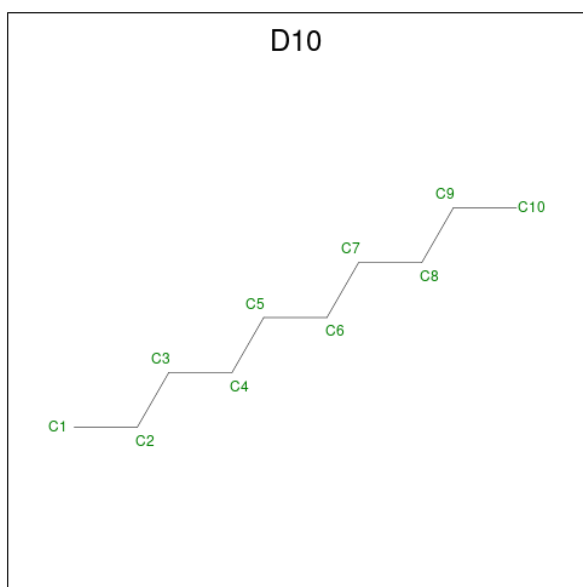
- Molecule 1 is a protein called Tricorn protease.

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
			8177	5196	1402	1551	28			
1	C	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	28			
1	D	1023	Total	C	N	O	S	94	0	0
			8177	5196	1402	1551	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
			8177	5196	1402	1551	28			

- Molecule 2 is a protein called RVRK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	5	Total	C	N	O	0	0	1
			39	24	11	4			
2	H	5	Total	C	N	O	0	0	1
			39	24	11	4			
2	I	5	Total	C	N	O	0	0	1
			39	24	11	4			
2	J	5	Total	C	N	O	0	0	1
			39	24	11	4			
2	K	5	Total	C	N	O	0	0	1
			39	24	11	4			
2	L	5	Total	C	N	O	0	0	1
			39	24	11	4			

- Molecule 3 is DECANE (CCD ID: D10) (formula: C₁₀H₂₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total C 10 10	0	0
3	H	1	Total C 10 10	0	0
3	I	1	Total C 10 10	0	0
3	J	1	Total C 10 10	0	0
3	K	1	Total C 10 10	0	0
3	L	1	Total C 10 10	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	106	Total O 106 106	0	0
4	G	4	Total O 4 4	0	0
4	B	88	Total O 88 88	0	0
4	C	88	Total O 88 88	0	0
4	I	2	Total O 2 2	0	0
4	D	79	Total O 79 79	0	0

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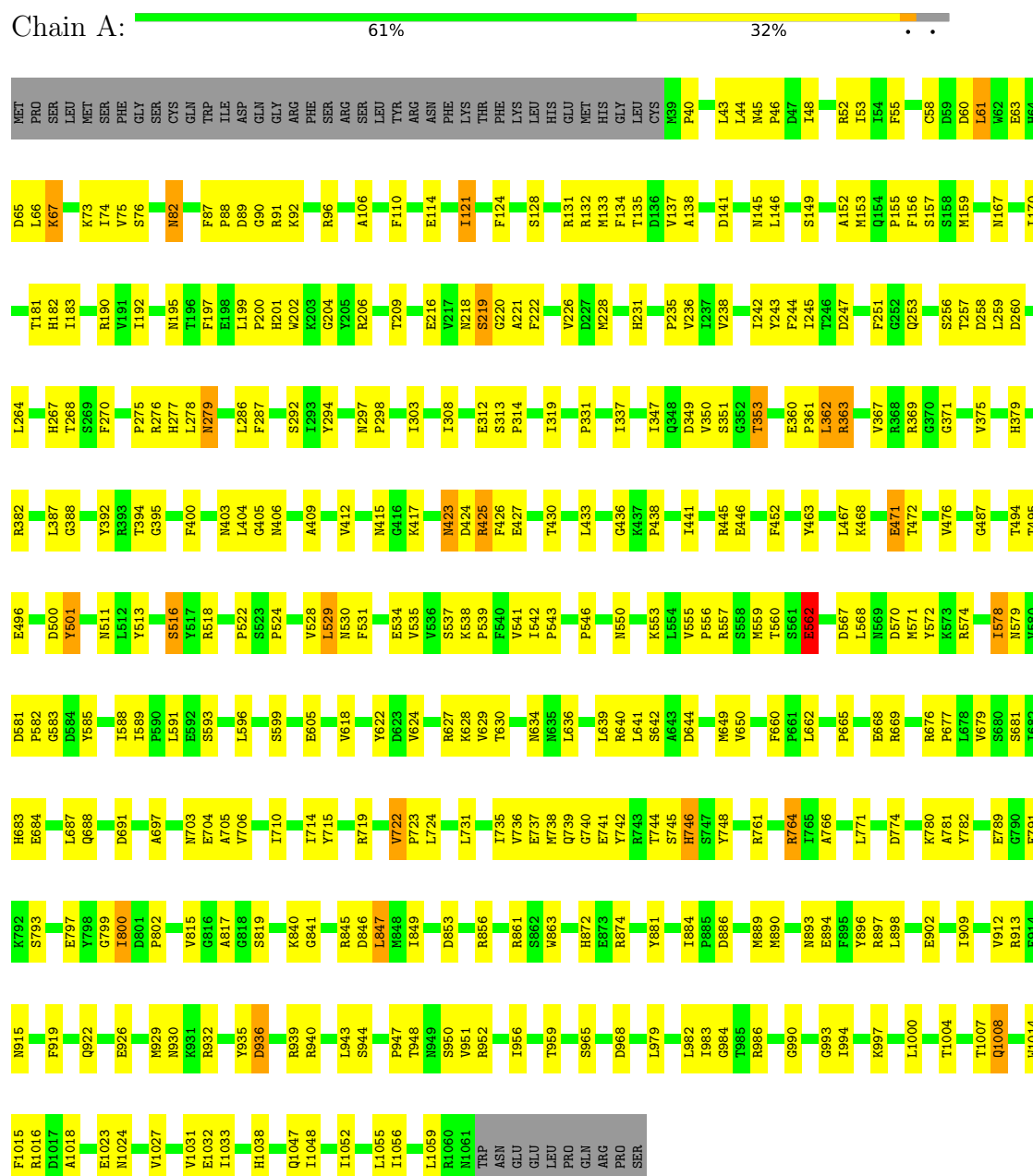
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	2	Total 2	O 2	0	0
4	E	89	Total 89	O 89	0	0
4	F	74	Total 74	O 74	0	0
4	L	2	Total 2	O 2	0	0

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 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.

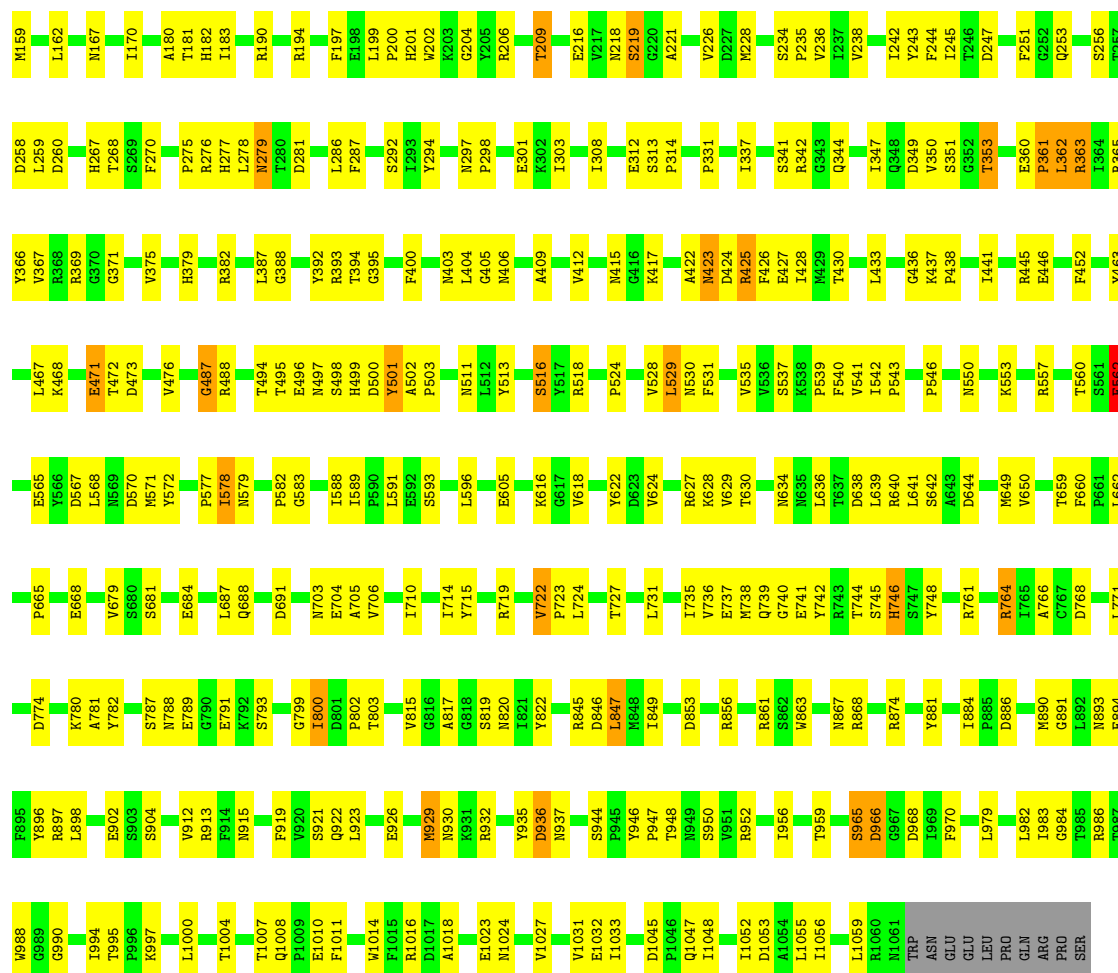
• Molecule 1: Tricorn protease



• Molecule 1: Tricorn protease

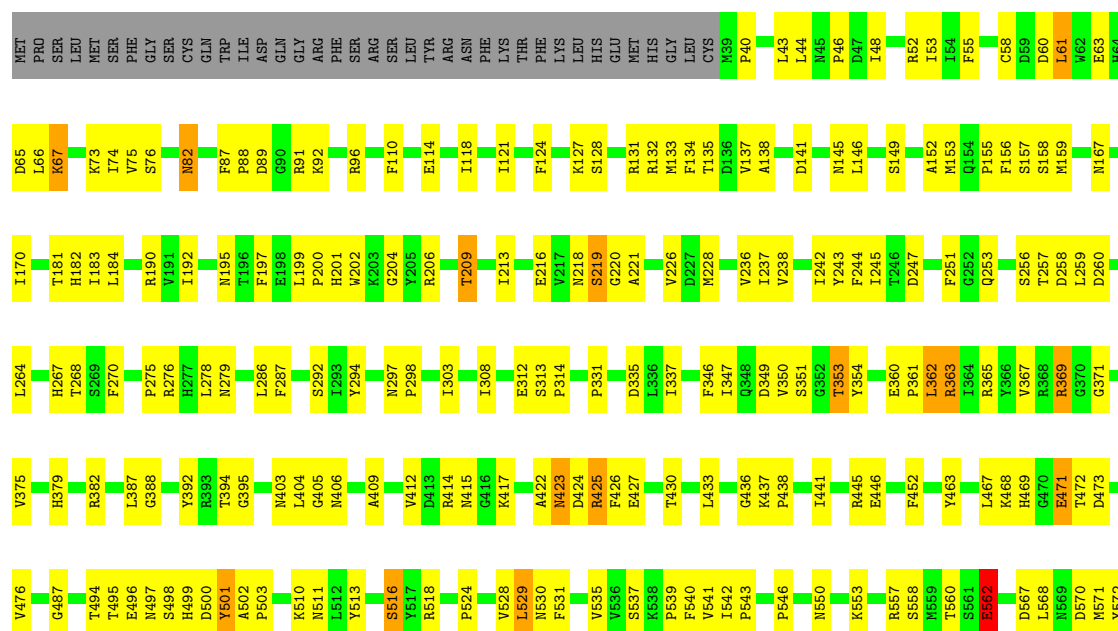
Chain B:  61% 32%

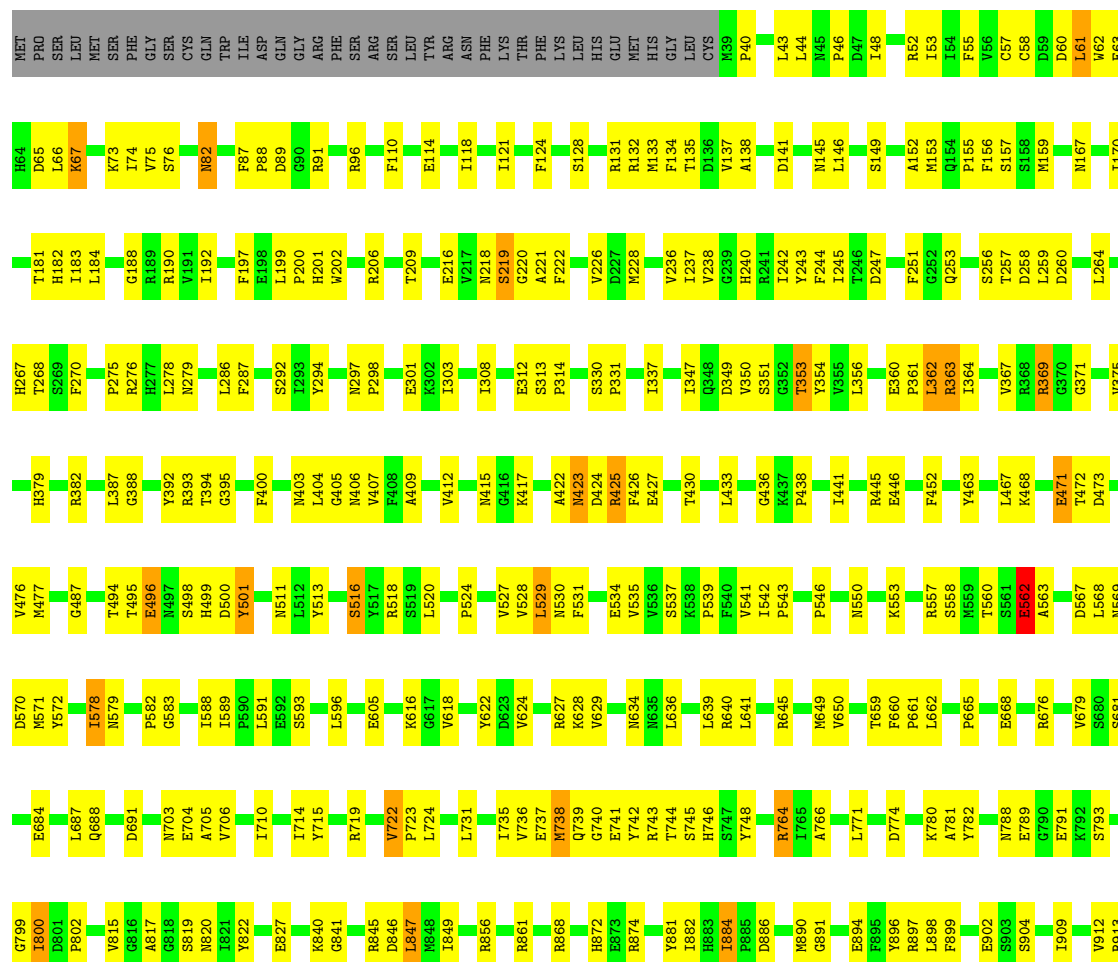
MET	PRO	SER	LEU	MET	SER	PHE	GLY	SER	CYS	GLN	TRP	TRP	ILE	ASP	GLN	ARG	PHE	SER	ARG	ARG	SER	LEU	TYR	ARG	ASN	PHE	LYS	THR	PHE	LYS	LEU	HIS	GLU	MET	HIS	GLY	LEU	CYS	R39	P40	L43	L44	N45	P46	D47	I48	R52	I53	I54	F55	C58	D59	D60	L61	W62	E63	D65	L66	K67	K73	I74	V75	S76	N82	F87	G88	G89	R91	K92	R96	S101	S102	L103	N104	F110	L1059	R1060	N1061	TRP	ASN	GLU	GLU	LEU	PRO	GLN	ARG	PRO	SER	D500	Y501	A502	P503	N511	L512	Y513	S516	Y517	R518	P522	S523	P524	V528	L529	N530	F531	E534	V535	V536	S537	D522	K538	P539	F540	V541	I542	P543	P546	N550	K553	L554	V555	P556	R557	S558	M559	T560	S561	E562	A563	D567	L568	N569	D570	M571	Y572	K573	R574	P577	S581	I578	N579	V580	D581	P582	G583	D584	Y585	I588	I589	P590	L591	E592	S593	L596	V600	E605	K616	G617	V618	Y622	D623	V624	R627	K628	V629	T630	N634	N635	L636	L639	R640	P641	D644	I665	A666	L667	P665	Y671	Y672	L673	K674	L675	M676	V677	F678	P679	L680	L681	L682	P683	L684	L685	L686	L687	Q688	D691	N703	E704	V706	I710	I714	Y715	R719	V722	P723	L724	L731	I735	V736	E737	M738	Q739	G740	E741	Y742	T744	S745	H746	Y748	R761	R764	I765	A766	L771	D774	K780	A781	Y782	S787	E791	K792	S793	E797	Y798	I800	D801	P802	V815	G816	A817	G818	S819	A829	G830	R845	D846	L847	P848	I849	D853	R856	R861	H872	Y881	I884	P885	D886	M889	G890	T891	R892	L893	T894	R895	G896	L897	L898	E902	I909	V912	R913	F914	N915	F919	Q922	E926	N929	N930	K931	R932	Y935	D936	R939	S944	P947	T948	S950	V951	R952	I956	T959	S965	D968	L969	F970	K976	L979	L982	G984	T985	R986	T987	Y988	G989	G990	G993	I994	T995	P996	K997	L1000	T1004	T1007	Q1008	W1014	E996	R997	F998	G999	H999	I999	L999	M999	N999	O999	P999	Q999	R999	S999	T999	V999	W999	X999	Y999	Z999	A000	C000	G000	I000	L000	N000	O000	P000	Q000	R000	S000	T000	V000	W000	X000	Y000	Z000	A001	C001	G001	I001	L001	N001	O001	P001	Q001	R001	S001	T001	V001	W001	X001	Y001	Z001	A002	C002	G002	I002	L002	N002	O002	P002	Q002	R002	S002	T002	V002	W002	X002	Y002	Z002	A003	C003	G003	I003	L003	N003	O003	P003	Q003	R003	S003	T003	V003	W003	X003	Y003	Z003	A004	C004	G004	I004	L004	N004	O004	P004	Q004	R004	S004	T004	V004	W004	X004	Y004	Z004	A005	C005	G005	I005	L005	N005	O005	P005	Q005	R005	S005	T005	V005	W005	X005	Y005	Z005	A006	C006	G006	I006	L006	N006	O006	P006	Q006	R006	S006	T006	V006	W006	X006	Y006	Z006	A007	C007	G007	I007	L007	N007	O007	P007	Q007	R007	S007	T007	V007	W007	X007	Y007	Z007	A008	C008	G008	I008	L008	N008	O008	P008	Q008	R008	S008	T008	V008	W008	X008	Y008	Z008	A009	C009	G009	I009	L009	N009	O009	P009	Q009	R009	S009	T009	V009	W009	X009	Y009	Z009	A010	C010	G010	I010	L010	N010	O010	P010	Q010	R010	S010	T010	V010	W010	X010	Y010	Z010	A011	C011	G011	I011	L011	N011	O011	P011	Q011	R011	S011	T011	V011	W011	X011	Y011	Z011	A012	C012	G012	I012	L012	N012	O012	P012	Q012	R012	S012	T012	V012	W012	X012	Y012	Z012	A013	C013	G013	I013	L013	N013	O013	P013	Q013	R013	S013	T013	V013	W013	X013	Y013	Z013	A014	C014	G014	I014	L014	N014	O014	P014	Q014	R014	S014	T014	V014	W014	X014	Y014	Z014	A015	C015	G015	I015	L015	N015	O015	P015	Q015	R015	S015	T015	V015	W015	X015	Y015	Z015	A016	C016	G016	I016	L016	N016	O016	P016	Q016	R016	S016	T016	V016	W016	X016	Y016	Z016	A017	C017	G017	I017	L017	N017	O017	P017	Q017	R017	S017	T017	V017	W017	X017	Y017	Z017	A018	C018	G018	I018	L018	N018	O018	P018	Q018	R018	S018	T018	V018	W018	X018	Y018	Z018	A019	C019	G019	I019	L019	N019	O019	P019	Q019	R019	S019	T019	V019	W019	X019	Y019	Z019	A020	C020	G020	I020	L020	N020	O020	P020	Q020	R020	S020	T020	V020	W020	X020	Y020	Z020	A021	C021	G021	I021	L021	N021	O021	P021	Q021	R021	S021	T021	V021	W021	X021	Y021	Z021	A022	C022	G022	I022	L022	N022	O022	P022	Q022	R022	S022	T022	V022	W022	X022	Y022	Z022	A023	C023	G023	I023	L023	N023	O023	P023	Q023	R023	S023	T023	V023	W023	X023	Y023	Z023	A024	C024	G024	I024	L024	N024	O024	P024	Q024	R024	S024	T024	V024	W024	X024	Y024	Z024	A025	C025	G025	I025	L025	N025	O025	P025	Q025	R025	S025	T025	V025	W025	X025	Y025	Z025	A026	C026	G026	I026	L026	N026	O026	P026	Q026	R026	S026	T026	V026	W026	X026	Y026	Z026	A027	C027	G027	I027	L027	N027	O027	P027	Q027	R027	S027	T027	V027	W027	X027	Y027	Z027	A028	C028	G028	I028	L028	N028	O028	P028	Q028	R028	S028	T028	V028	W028	X028	Y028	Z028	A029	C029	G029	I029	L029	N029	O029	P029	Q029	R029	S029	T029	V029	W029	X029	Y029	Z029	A030	C030	G030	I030	L030	N030	O030	P030	Q030	R030	S030	T030	V030	W030	X030	Y030	Z030	A031	C031	G031	I031	L031	N031	O031	P031	Q031	R031	S031	T031	V031	W031	X031	Y031	Z031	A032	C032	G032	I032	L032	N032	O032	P032	Q032	R032	S032	T032	V032	W032	X032	Y032	Z032	A033	C033	G033	I033	L033	N033	O033	P033	Q033	R033	S033	T033	V033	W033	X033	Y033	Z033	A034	C034	G034	I034	L034	N034	O034	P034	Q034	R034	S034	T034	V034	W034	X034	Y034	Z034	A035	C035	G035	I035	L035	N035	O035	P035	Q035	R035	S035	T035	V035	W035	X035	Y035	Z035	A036	C036	G036	I036	L036	N036	O036	P036	Q036	R036	S036	T036	V036	W036	X036	Y036	Z036	A037	C037	G037	I037	L037	N037	O037	P037	Q037	R037	S037	T037	V037	W037	X037	Y037	Z037	A038	C038	G038	I038	L038	N038	O038	P038	Q038	R038	S038	T038	V038	W038	X038	Y038	Z038	A039	C039	G039	I039	L039	N039	O039	P039	Q039	R039	S039	T039	V039	W039	X039	Y03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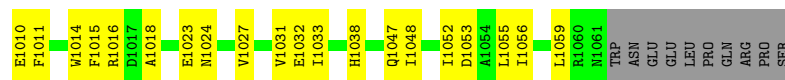


• Molecule 1: Tricorn protease

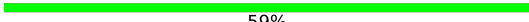
Chain D: 59% 34%

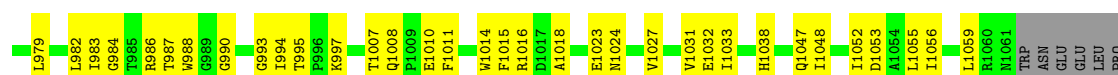
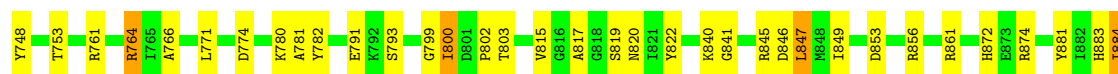
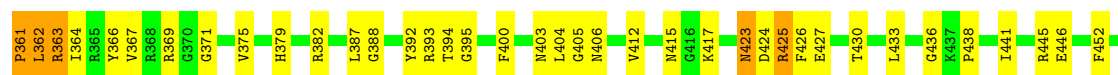
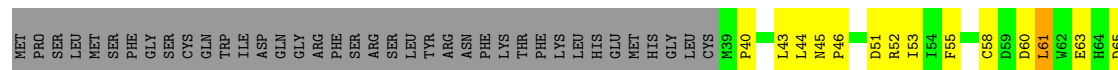






• Molecule 1: Tricorn protease

Chain F:  59%  34%



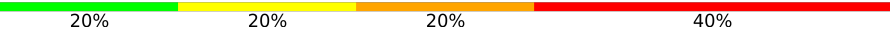
GLN
ARG
PRO
SER

• Molecule 2: RVRK

Chain G:  20% 20% 20% 40%

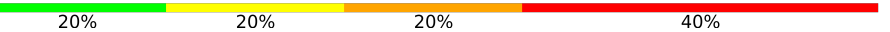


• Molecule 2: RVRK

Chain H:  20% 20% 20% 40%

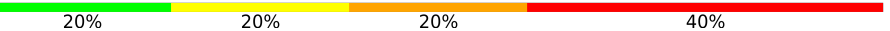


• Molecule 2: RVRK

Chain I:  20% 20% 20% 40%



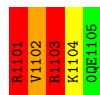
• Molecule 2: RVRK

Chain J:  20% 20% 20% 40%

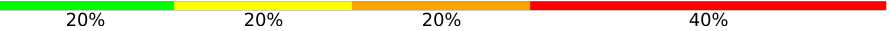


• Molecule 2: RVRK

Chain K:  20% 20% 20% 40%



• Molecule 2: RVRK

Chain L:  20% 20% 20% 40%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.44Å 245.43Å 159.40Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	6.00 – 2.80 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	88.7 (6.00-2.80) 75.4 (6.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.66 (at 2.71Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.285 , 0.315 0.273 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	32.2	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 12.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.079 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	49890	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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: 0QE, D10

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	0.61	1/8367 (0.0%)	0.92	12/11311 (0.1%)
1	B	0.61	1/8367 (0.0%)	0.93	18/11311 (0.2%)
1	C	0.58	1/8367 (0.0%)	0.92	14/11311 (0.1%)
1	D	0.60	1/8367 (0.0%)	0.92	12/11311 (0.1%)
1	E	0.59	1/8367 (0.0%)	0.92	11/11311 (0.1%)
1	F	0.59	1/8367 (0.0%)	0.91	14/11311 (0.1%)
2	G	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	H	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	I	2.77	2/37 (5.4%)	5.63	10/46 (21.7%)
2	J	2.76	2/37 (5.4%)	5.62	10/46 (21.7%)
2	K	2.76	2/37 (5.4%)	5.63	10/46 (21.7%)
2	L	2.77	2/37 (5.4%)	5.63	10/46 (21.7%)
All	All	0.62	18/50424 (0.0%)	0.99	141/68142 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	G	0	3
2	H	0	3
2	I	0	3
2	J	0	3
2	K	0	3
2	L	0	3
All	All	0	18

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1103	ARG	N-CA	-12.40	1.30	1.45
2	L	1103	ARG	N-CA	-12.36	1.30	1.45
2	H	1103	ARG	N-CA	-12.33	1.30	1.45
2	J	1103	ARG	N-CA	-12.33	1.30	1.45
2	K	1103	ARG	N-CA	-12.33	1.30	1.45

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1101	ARG	CA-C-N	18.84	139.36	121.65
2	G	1101	ARG	C-N-CA	18.84	139.36	121.65
2	H	1101	ARG	CA-C-N	18.83	139.35	121.65
2	H	1101	ARG	C-N-CA	18.83	139.35	121.65
2	I	1101	ARG	CA-C-N	18.81	139.34	121.65

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1101	ARG	Sidechain
2	G	1102	VAL	Mainchain
2	G	1103	ARG	Sidechain
2	H	1101	ARG	Sidechain
2	H	1102	VAL	Mainchain

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	8177	0	8002	311	0
1	B	8177	0	8002	315	0
1	C	8177	0	8002	345	0
1	D	8177	0	8002	345	0
1	E	8177	0	8002	334	0
1	F	8177	0	8002	347	0
2	G	39	0	47	8	0
2	H	39	0	47	5	0
2	I	39	0	47	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	39	0	47	7	0
2	K	39	0	47	5	0
2	L	39	0	47	8	0
3	G	10	0	20	2	0
3	H	10	0	20	3	0
3	I	10	0	20	4	0
3	J	10	0	20	3	0
3	K	10	0	20	4	0
3	L	10	0	20	4	0
4	A	106	0	0	16	0
4	B	88	0	0	23	0
4	C	88	0	0	40	0
4	D	79	0	0	32	0
4	E	89	0	0	26	0
4	F	74	0	0	40	0
4	G	4	0	0	3	0
4	I	2	0	0	2	0
4	J	2	0	0	3	0
4	L	2	0	0	3	0
All	All	49890	0	48414	1929	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 1929 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)
2:I:1103:ARG:CB	2:I:1103:ARG:CG	1.77	1.63
2:G:1103:ARG:CB	2:G:1103:ARG:CG	1.77	1.62
2:H:1103:ARG:CG	2:H:1103:ARG:CB	1.77	1.57
2:K:1103:ARG:CB	2:K:1103:ARG:CG	1.77	1.57
2:J:1103:ARG:CB	2:J:1103:ARG:CG	1.77	1.56

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	B	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	C	1021/1071 (95%)	930 (91%)	80 (8%)	11 (1%)	11	36
1	D	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	E	1021/1071 (95%)	934 (92%)	78 (8%)	9 (1%)	14	41
1	F	1021/1071 (95%)	930 (91%)	81 (8%)	10 (1%)	12	38
2	G	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	H	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	I	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	J	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	K	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
2	L	2/5 (40%)	1 (50%)	1 (50%)	0	100	100
All	All	6138/6456 (95%)	5602 (91%)	479 (8%)	57 (1%)	14	41

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	SER
1	C	219	SER
1	C	562	GLU
1	D	219	SER
1	E	219	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	883/928 (95%)	855 (97%)	28 (3%)	34	70
1	B	883/928 (95%)	856 (97%)	27 (3%)	35	70
1	C	883/928 (95%)	857 (97%)	26 (3%)	37	73
1	D	883/928 (95%)	855 (97%)	28 (3%)	34	70
1	E	883/928 (95%)	854 (97%)	29 (3%)	33	69
1	F	883/928 (95%)	856 (97%)	27 (3%)	35	70
2	G	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	H	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	I	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	J	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	K	4/4 (100%)	3 (75%)	1 (25%)	0	2
2	L	4/4 (100%)	3 (75%)	1 (25%)	0	2
All	All	5322/5592 (95%)	5151 (97%)	171 (3%)	34	70

5 of 171 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	82	ASN
1	F	44	LEU
1	E	313	SER
1	E	578	ILE
1	F	353	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 189 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	703	ASN
1	E	611	GLN
1	D	893	ASN
1	E	145	ASN
1	E	930	ASN

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](#)

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	$\# Z > 2$
3	D10	G	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	J	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	I	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	K	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	H	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)
3	D10	L	2101	-	9,9,9	0.56	0	8,8,8	1.06	1 (12%)

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
3	D10	G	2101	-	-	3/7/7/7	-
3	D10	J	2101	-	-	3/7/7/7	-
3	D10	I	2101	-	-	3/7/7/7	-
3	D10	K	2101	-	-	3/7/7/7	-
3	D10	H	2101	-	-	3/7/7/7	-
3	D10	L	2101	-	-	3/7/7/7	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2101	D10	C1-C2-C3	-2.13	98.96	113.36
3	L	2101	D10	C1-C2-C3	-2.13	98.98	113.36
3	H	2101	D10	C1-C2-C3	-2.13	98.98	113.36
3	K	2101	D10	C1-C2-C3	-2.13	98.99	113.36
3	I	2101	D10	C1-C2-C3	-2.12	99.01	113.36

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2101	D10	C4-C5-C6-C7
3	H	2101	D10	C4-C5-C6-C7
3	I	2101	D10	C4-C5-C6-C7
3	J	2101	D10	C4-C5-C6-C7
3	K	2101	D10	C4-C5-C6-C7

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	2101	D10	2	0
3	J	2101	D10	3	0
3	I	2101	D10	4	0
3	K	2101	D10	4	0
3	H	2101	D10	3	0
3	L	2101	D10	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1023/1071 (95%)	-1.44	0 100 100	8, 35, 56, 80	20 (1%)
1	B	1023/1071 (95%)	-1.46	0 100 100	8, 35, 56, 79	20 (1%)
1	C	1023/1071 (95%)	-1.33	0 100 100	8, 38, 57, 80	20 (1%)
1	D	1023/1071 (95%)	-1.42	0 100 100	8, 36, 56, 79	20 (1%)
1	E	1023/1071 (95%)	-1.43	0 100 100	8, 35, 56, 80	20 (1%)
1	F	1023/1071 (95%)	-1.37	0 100 100	8, 38, 57, 80	20 (1%)
2	G	4/5 (80%)	-1.36	0 100 100	36, 39, 40, 42	0
2	H	4/5 (80%)	-1.58	0 100 100	36, 39, 40, 42	0
2	I	4/5 (80%)	-1.44	0 100 100	36, 39, 40, 42	0
2	J	4/5 (80%)	-1.34	0 100 100	36, 39, 40, 42	0
2	K	4/5 (80%)	-1.44	0 100 100	36, 39, 40, 42	0
2	L	4/5 (80%)	-1.61	0 100 100	36, 39, 40, 42	0
All	All	6162/6456 (95%)	-1.41	0 100 100	8, 36, 56, 80	120 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	D10	L	2101	10/10	0.91	0.12	0,0,0,0	0
3	D10	J	2101	10/10	0.94	0.11	0,0,0,0	0
3	D10	I	2101	10/10	0.94	0.11	0,0,0,0	0
3	D10	H	2101	10/10	0.95	0.10	0,0,0,0	0
3	D10	G	2101	10/10	0.95	0.09	0,0,0,0	0
3	D10	K	2101	10/10	0.96	0.11	0,0,0,0	0

6.5 Other polymers [i](#)

There are no such residues in this entry.