



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 09:51 PM GMT

PDB ID : 1QXP
Title : Crystal Structure of a mu-like calpain
Authors : Pal, G.P.; Veyra, T.D.; Elce, J.S.; Jia, Z.
Deposited on : 2003-09-08
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

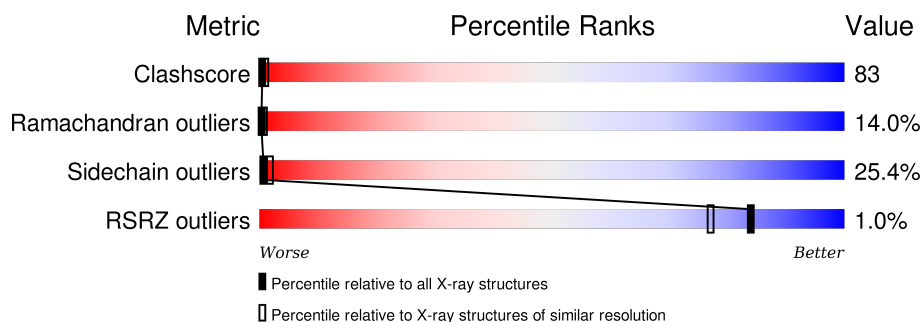
1 Overall quality at a glance

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	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	900	
1	B	900	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12368 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 mu-like calpain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	783	Total	C	N	O	S	0	0	0
			6053	3846	1037	1143	27			
1	B	788	Total	C	N	O	S	0	0	0
			6003	3830	1015	1129	29			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	SER	CYS	ENGINEERED	UNP P97571
B	105	SER	CYS	ENGINEERED	UNP P97571
A	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
A	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
A	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
A	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
A	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
A	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
A	702I	HIS	-	EXPRESSION TAG	UNP Q07009
A	702J	HIS	-	EXPRESSION TAG	UNP Q07009
A	702K	HIS	-	EXPRESSION TAG	UNP Q07009
A	702L	HIS	-	EXPRESSION TAG	UNP Q07009
A	702M	HIS	-	EXPRESSION TAG	UNP Q07009
A	702N	HIS	-	EXPRESSION TAG	UNP Q07009
B	702A	GLY	-	CLONING ARTIFACT	UNP Q07009
B	702B	LYS	-	CLONING ARTIFACT	UNP Q07009
B	702C	LEU	-	CLONING ARTIFACT	UNP Q07009
B	702D	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702E	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702F	ALA	-	CLONING ARTIFACT	UNP Q07009
B	702G	ILE	-	CLONING ARTIFACT	UNP Q07009
B	702H	GLU	-	CLONING ARTIFACT	UNP Q07009
B	702I	HIS	-	EXPRESSION TAG	UNP Q07009

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Chain	Residue	Modelled	Actual	Comment	Reference
B	702J	HIS	-	EXPRESSION TAG	UNP Q07009
B	702K	HIS	-	EXPRESSION TAG	UNP Q07009
B	702L	HIS	-	EXPRESSION TAG	UNP Q07009
B	702M	HIS	-	EXPRESSION TAG	UNP Q07009
B	702N	HIS	-	EXPRESSION TAG	UNP Q07009

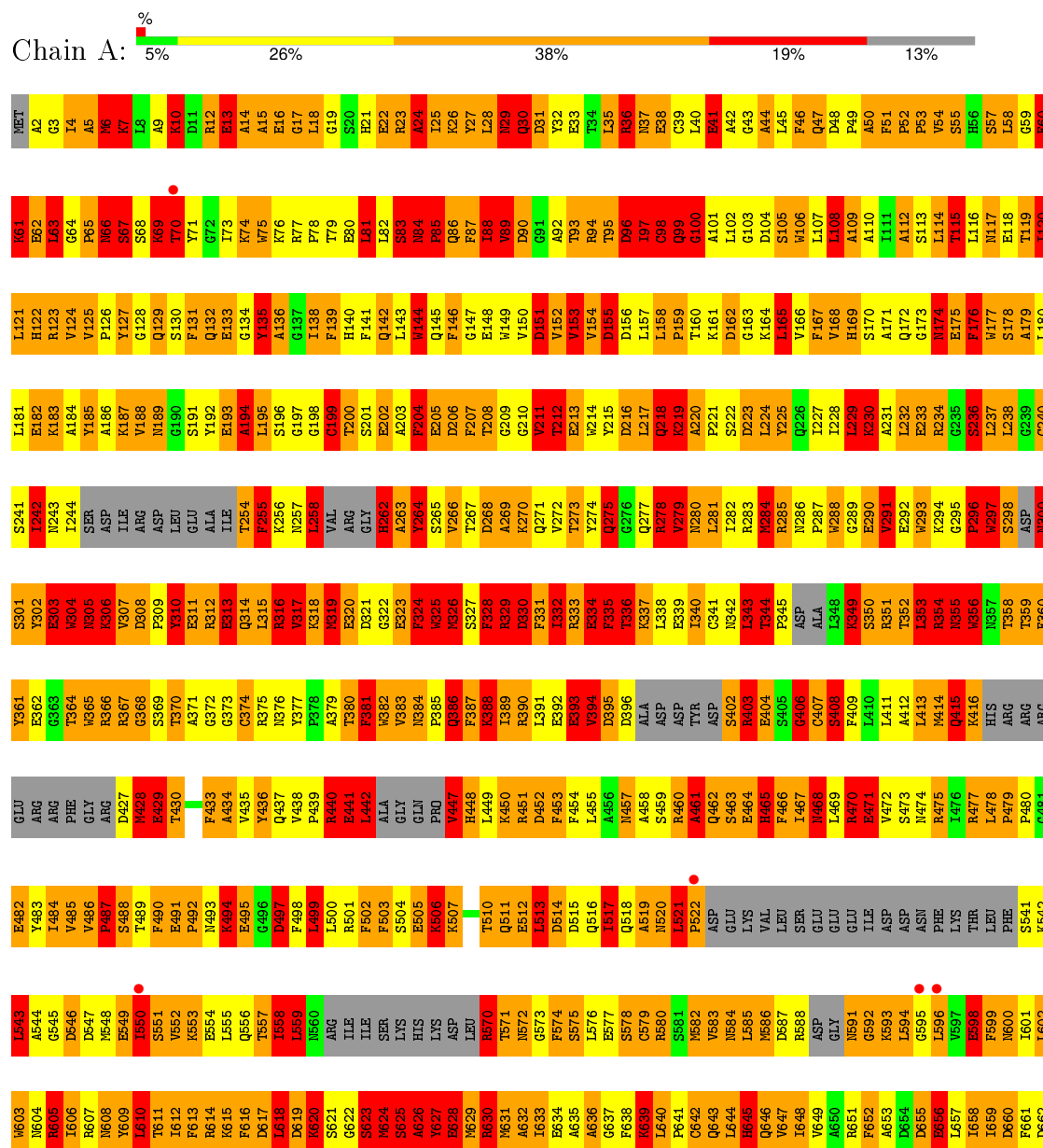
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	172	Total O 172 172	0	0
2	B	140	Total O 140 140	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: mu-like calpain



L601	SER	G481	GLU	Y361	SER	S241	L181	L121	K81	ME1	S836	H776	GLU	S683
L602	LYS	E482	ARG	E362	TYR	I242	E182	H122	E82	ALA	ME1	D777	ALA	F664
M603	ALA	Y483	ARG	G363	ASP	I243	K183	L123	G14	ASN	ILE	S778	ASN	F665
M604	LEU	I484	F424	T364	ASP	I184	K184	V124	G64	GLU	ILE	D779	GLU	F666
I605	GLY	V485	G425	R365	LYS	ASP	Y185	V125	P85	ARG	ARG	T780	SER	C667
I606	ASP	V486	R426	R366	VAL	ASP	A186	P126	M66	GLY	ARG	T781	GLY	L668
R607	ASP	R487	D427	R367	ASP	ASP	K187	V127	S87	TYR	TYR	G782	GLU	V669
M608	MET	S488	M428	G368	D308	ARG	V188	Q128	S88	SER	ASP	K783	GLU	A670
Y609	GLU	T489	T430	S369	P309	ASP	M189	Q129	K69	ASP	ASP	L784	ARG	L671
T611	S551	E491	T370	A371	Y310	LEU	G190	F130	T70	GLN	T345	F785	GLN	E672
I612	V552	A492	G432	G372	R312	ALA	Y192	E132	Y71	PHE	T346	F786	PHE	L673
F613	K553	M493	F433	G373	E313	ILE	E193	E133	G72	ARG	G347	E787	ARG	L674
R614	E554	K494	A434	C374	Q314	THR	A194	G134	I73	LYS	M848	F788	LYS	F675
K615	L555	E495	V435	R375	L315	PHE	L195	Y135	K74	LEU	M849	F789	LEU	L676
F616	L556	G496	F436	N376	R316	K256	S196	A136	W75	VAL	D850	K790	VAL	L677
D617	T557	D497	Q437	Y377	V317	I257	S197	G137	K76	VAL	F851	Y791	F731	F678
L618	L558	F498	V438	P378	K318	L258	G197	E137	R77	GLY	D852	L792	GLY	K679
D619	L559	A499	P439	A379	M319	L259	C199	F139	P78	ARG	M853	L793	L733	D680
K620	M560	L500	R440	T380	E320	ARG	T200	H140	E80	GLY	F854	L794	A734	L681
S621	ARG	R501	R441	F381	D321	G261	S201	H141	L81	THR	S855	L795	G735	D682
G622	ILE	F502	L442	V382	E322	H262	E202	Q142	L82	ASP	S856	L796	D736	P683
S623	SER	F503	A443	V383	E323	A263	A203	L143	S83	THR	L858	K797	D737	E684
M624	SER	S504	G444	N384	F324	Y264	F204	Y144	M84	ARG	L859	K798	D738	M685
S625	LYS	E505	GLN	P385	H325	S265	E205	Q145	P85	THR	R860	Q800	E739	T686
A626	HIS	K506	P446	Q386	M326	Y266	D206	F146	Q86	VAL	L861	G801	S741	L688
Y627	LYS	R507	V447	R387	S327	T267	F207	G147	F87	THR	D862	L802	A742	L689
E628	ASP	A508	H448	K388	F328	D268	L268	E148	L88	THR	L863	L803	A743	Q690
M629	LEU	G509	L449	I389	R329	A269	G209	Y149	Y89	GLY	M864	L804	E744	L691
R630	LEU	T510	K450	R390	D330	K270	G210	V150	D90	ARG	F865	L805	L745	D692
M631	GLY	Q511	R451	L391	F331	Q271	V211	D151	G91	THR	R866	L806	M746	L693
A632	GLY	E512	D452	E392	I332	Y272	T212	V152	A82	GLY	A867	L807	M747	L694
I633	GLY	E513	F453	E393	R333	T273	E213	F153	T93	THR	F868	L808	I748	S695
E634	GLY	D514	F454	V394	E334	Y274	W214	V154	R89	THR	R869	L809	L749	L696
A635	LYS	D515	L455	D395	F335	Q275	Y215	D155	T95	THR	S870	L810	M750	L697
A636	LYS	Q516	A456	D396	T336	G276	D216	D156	D96	VAL	L871	S811	K751	S698
G637	LYS	I517	M457	A397	K337	Q277	L217	L157	I97	VAL	D872	G812	VAL	F699
R638	LYS	Q518	M458	D398	L338	R278	Q218	L158	C98	THR	K873	L812	VAL	S700
K639	GLY	A519	S459	D399	E339	Y279	K219	F159	C39	THR	M874	L813	THR	L701
L640	GLY	M520	R460	Y400	I340	N280	A220	T160	Q99	GLY	G875	L814	THR	L702
P641	LYS	L521	A461	D401	C341	L281	A221	K161	A101	GLY	T876	L815	ASP	GLY
C642	LYS	P522	Q462	S402	N342	L282	S222	D162	A42	LYS	G877	L816	P757	LYS
Q643	LYS	D523	S463	R403	R343	L283	D223	G163	L102	LYS	Q878	L817	D758	LEU
L644	LYS	E524	E464	E404	T344	N284	L224	K164	G103	GLY	I879	L818	L759	ALA
H645	LYS	K525	H465	S405	P345	N285	Y225	L165	S105	GLY	Q880	L819	K760	ALA
Q646	LYS	V526	F466	G406	D346	N286	Q226	V166	M106	THR	V881	L820	THR	ALA
V647	ARG	LEU	I467	C407	D347	N287	Q227	V167	F46	THR	V882	L821	THR	ALA
I648	ASP	SER	M468	F408	L348	N288	I227	F167	L107	ASP	M882	L822	ASP	ILE
V649	GLY	GLY	L469	S409	K349	N289	L229	H169	L108	GLY	I883	L823	G763	GLY
A650	GLY	GLY	R470	L410	S350	G289	K229	K169	A109	GLY	Q884	L824	F764	HIS
M651	ASN	GLY	E471	L411	R351	E290	K230	S170	A110	GLY	E885	L825	F765	HIS
F652	GLY	ILE	V472	A412	THR	E292	A231	A171	I111	GLY	W886	L826	I766	HIS
A653	LYS	ASP	S473	L413	LEU	E293	L232	Q172	A112	GLY	L887	L827	D767	HIS
D654	LYS	ASP	M474	M414	R354	N294	E233	G173	S113	GLY	Q888	L828	T768	HIS
D655	ASN	ASN	R475	Q415	N355	G295	R234	K174	V84	GLY	L889	L829	C769	HIS
E656	PHE	PHE	K476	K416	K356	P296	G235	E175	T115	GLY	T890	L830	R770	W710
L657	LYS	LYS	R477	H417	M357	N297	S236	F176	H56	GLY	M891	L831	S771	H711
L658	LYS	T538	L478	H418	T358	N298	L237	H177	N117	GLY	Y892	L832	M772	W712
L659	LYS	F539	P479	R418	T359	S298	L238	S178	E118	GLY	S893	L833	V773	W713
D660	LYS	F540	P480	ARG	F360	ASN	G239	L190	L120	GLY	Y894	L834	A774	W714
														L715

• Molecule 1: mu-like calpain



Y835	S836	M837	I838	I839	R840	ARG	TYR	S843	G847	N848	M849	D850	F851	D852	N853	F854	I855	S856	C857	L858	V859	R860	L861	D862	A863	M864	F865	R866	A867	F868	R869	S870	L871	D872	K873	N874	G875	T876	G877	Q878	I879	Q880	V881	N882	I883	Q884	E885	W886	L887	Q888	L889	T890	M891	Y892	S893								
F661	D662	M663	F664	V665	R666	C667	L668	V669	R670	L671	E672	I673	L674	F675	K676	I677	F678	K679	Q680	L681	D682	P683	E684	N685	T686	G687	T688	I689	L691	Q690	D692	L693	I694	W696	L697	S698	F699	S700	V701	L702	GLY	LYS	LEU	ALA	ALA	ALA	ILE	ILE	GLU	HIS	HIS	HIS	HIS	HIS	Y710	H711	Y712	S713					
N714	ILE	GLU	ALA	N718	E719	S720	EO	GLU	E723	R724	Q725	F726	R727	K728	L729	F730	V731	Q732	L733	ALA	L881	GLY	ASP	ASP	W738	E739	V740	S741	A742	I689	T743	E744	L745	K746	ASN	ILE	LEU	ASN	LYS	VAL	VAL	THR	ARG	HIS	PRO	ASP	LEU	LEU	LYS	THR	ASP	THR	GLY	F764	G765	I766	D767	T768	C769	R770	S771	M772	V773
A774	V775	M776	D777	S778	D779	T780	T781	L784	G785	F786	E787	E788	F789	K790	Y791	L792	W793	N794	N795	I796	K797	K798	W799	Q800	G801	I802	TYR	LYS	R805	F806	E807	T808	D809	R810	S811	G812	THR	ILE	GLY	SER	ASN	GLU	LEU	P820	G821	A822	F823	E824	A825	A826	G827	F828	H829	L830	N831	Q832	H833	I834					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.74Å 184.60Å 86.37Å 90.00° 100.74° 90.00°	Depositor
Resolution (Å)	91.29 – 2.80 49.81 – 2.69	Depositor EDS
% Data completeness (in resolution range)	91.6 (91.29-2.80) 87.3 (49.81-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.311 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 98.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 55542 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12368	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	3.70	964/6177 (15.6%)	2.67	470/8354 (5.6%)
1	B	3.71	932/6128 (15.2%)	2.67	489/8288 (5.9%)
All	All	3.70	1896/12305 (15.4%)	2.67	959/16642 (5.8%)

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
1	A	0	45
1	B	0	39
All	All	0	84

The worst 5 of 1896 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	SER	CA-CB	28.73	1.96	1.52
1	A	339	GLU	CD-OE1	23.66	1.51	1.25
1	A	320	GLU	CD-OE2	20.06	1.47	1.25
1	B	429	GLU	CD-OE1	19.54	1.47	1.25
1	A	811	SER	CA-CB	-18.37	1.25	1.52

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	ARG	NE-CZ-NH1	-29.77	105.41	120.30
1	A	329	ARG	NE-CZ-NH1	26.14	133.37	120.30
1	A	329	ARG	NE-CZ-NH2	-24.17	108.22	120.30
1	B	514	ASP	CB-CG-OD2	-18.56	101.59	118.30
1	A	285	ARG	NE-CZ-NH2	-15.96	112.32	120.30

There are no chirality outliers.

5 of 84 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ILE	Mainchain
1	A	152	VAL	Mainchain
1	A	24	ALA	Mainchain
1	A	29	ASN	Mainchain
1	A	99	GLN	Mainchain,Peptide

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	6053	0	5615	959	3
1	B	6003	0	5477	969	1
2	A	172	0	0	53	1
2	B	140	0	0	45	1
All	All	12368	0	11092	1928	3

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 83.

The worst 5 of 1928 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:583:VAL:CB	1:A:583:VAL:CA	1.74	1.65
1:B:0:GLU:CA	1:B:0:GLU:CB	1.75	1.64
1:B:786:PHE:CA	1:B:786:PHE:CB	1.74	1.64
1:A:550:ILE:CB	1:A:550:ILE:CA	1.75	1.64
1:B:8:LEU:CD2	1:B:8:LEU:CG	1.76	1.63

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:ASN:OD1	2:B:1033:HOH:O[1_454]	1.56	0.64
1:A:442:LEU:CD2	2:A:922:HOH:O[1_455]	1.95	0.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:ASN:OD1	1:B:303:GLU:N[2_656]	2.08	0.12

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	747/900 (83%)	500 (67%)	143 (19%)	104 (14%)	0	1
1	B	748/900 (83%)	497 (66%)	146 (20%)	105 (14%)	0	1
All	All	1495/1800 (83%)	997 (67%)	289 (19%)	209 (14%)	0	1

5 of 209 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	VAL
1	A	60	PHE
1	A	63	LEU
1	A	67	SER
1	A	83	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	606/782 (78%)	459 (76%)	147 (24%)	1	2
1	B	584/782 (75%)	429 (74%)	155 (26%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1190/1564 (76%)	888 (75%)	302 (25%)	1 2

5 of 302 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	111	ILE
1	B	701	VAL
1	A	874	ASN
1	B	41	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	853	ASN
1	B	47	GLN
1	B	646	GLN
1	A	878	GLN
1	A	888	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	783/900 (87%)	-0.35	5 (0%) 90 86	16, 49, 81, 98	0
1	B	788/900 (87%)	-0.32	11 (1%) 78 69	17, 51, 84, 102	0
All	All	1571/1800 (87%)	-0.33	16 (1%) 84 77	16, 50, 83, 102	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	587	ASP	3.8
1	B	596	LEU	3.8
1	A	596	LEU	3.4
1	B	712	TYR	3.3
1	B	402	SER	3.3

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.