

wwPDB X-ray Structure Validation Summary Report (i)

Jan 3, 2024 - 09:54 am GMT

:	4ZIW
:	Crystal structure of AcrB deletion mutant in P21 space group
:	Ababou, A.; Koronakis, V.
:	2015-04-28
:	3.40 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7(2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R _{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 <=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				
			12%				
1	А	1044	47%	47%	5% •		
			10%				
1	В	1044	50%	45%	•		
			12%				
1	С	1044	47%	47%	5%•		
			16%				
1	D	1044	44%	50%	5% ••		
			17%				
1	Е	1044	47%	47%	5%•		

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Mol	Chain	Length	Quality of chain				
			17%				
1	\mathbf{F}	1044		46%	48%	5%•	

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	LMT	В	2000	-	-	-	Х
2	LMT	D	2000	Х	-	-	-
2	LMT	Е	1101	Х	-	-	Х



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 47532 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.

Mol	Chain	Residues		Α	toms			ZeroOcc	AltConf	Trace
1	Δ	1038	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	Л	1050	7893	5072	1306	1472	43	0	0	0
1	В	1030	Total	С	Ν	Ο	S	0	0	0
	D	1055	7900	5076	1307	1474	43	0	0	U
1	С	1035	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	U	1055	7867	5057	1299	1468	43		0	0
1	а	1038	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L I	D	1050	7893	5072	1306	1472	43	0	0	U
1	F	1037	Total	С	Ν	Ο	\mathbf{S}	0	0	0
L L		1037	7883	5066	1303	1471	43	0	0	0
1	1 F	1037	Total	С	Ν	Ο	S	0	0	0
	Ľ	1037	7883	5066	1303	1471	43		0	U

• Molecule 1 is a protein called Multidrug efflux pump subunit AcrB.

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	615	GLY	PHE	engineered mutation	UNP P31224
А	?	-	GLY	deletion	UNP P31224
А	?	-	PHE	deletion	UNP P31224
А	?	-	ALA	deletion	UNP P31224
А	?	-	GLY	deletion	UNP P31224
А	?	-	ARG	deletion	UNP P31224
В	615	GLY	PHE	engineered mutation	UNP P31224
В	?	-	GLY	deletion	UNP P31224
В	?	-	PHE	deletion	UNP P31224
В	?	-	ALA	deletion	UNP P31224
В	?	-	GLY	deletion	UNP P31224
В	?	-	ARG	deletion	UNP P31224
С	615	GLY	PHE	engineered mutation	UNP P31224
С	?	-	GLY	deletion	UNP P31224
C	?	-	PHE	deletion	UNP P31224
С	?	-	ALA	deletion	UNP P31224
С	?	-	GLY	deletion	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
С	?	-	ARG	deletion	UNP P31224
D	615	GLY	PHE	engineered mutation	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	PHE	deletion	UNP P31224
D	?	-	ALA	deletion	UNP P31224
D	?	-	GLY	deletion	UNP P31224
D	?	-	ARG	deletion	UNP P31224
Е	615	GLY	PHE	engineered mutation	UNP P31224
Е	?	-	GLY	deletion	UNP P31224
Е	?	-	PHE	deletion	UNP P31224
Е	?	-	ALA	deletion	UNP P31224
E	?	-	GLY	deletion	UNP P31224
Е	?	-	ARG	deletion	UNP P31224
F	615	GLY	PHE	engineered mutation	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	-	PHE	deletion	UNP P31224
F	?	-	ALA	deletion	UNP P31224
F	?	-	GLY	deletion	UNP P31224
F	?	_	ARG	deletion	UNP P31224

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• Molecule 2 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $\rm C_{24}H_{46}O_{11}).$



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
2	А	1	Total 35	C 24	0 11	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	1	Total C O	0	0
	D	Ĩ	35 24 11	0	0
2	С	1	Total C O	0	0
	U	1	35 24 11	0	0
0	р	1	Total C O	0	0
	D	1	35 24 11	0	0
2	Б	1	Total C O	0	0
	E	1	35 24 11	0	0
2	Б	1	Total C O	0	0
	Г	1	35 24 11	U	U

• Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total Ni 1 1	0	0
3	С	1	Total Ni 1 1	0	0
3	Е	1	Total Ni 1 1	0	0



3 Residue-property plots (i)

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.

















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V214 A215	017V	G220 G220	T222 P223	P224	L230	1235	A236	0237 T238	R239	L240 T241		E245	G247	K248	1249 1.250	L251	K252	V253 N754	Q255		R259	L262	R263	12 <mark>68</mark>	E269 L270		E273	1277	1278 A279	E280	F281	G283	0284 P285	A286	5287 G288	L289	1291	N 23 2
L293 A294	A297	L300 D301	T302 A303	Tank	R307	A308 E309	L310	A311 K312	M313	E314 P315	F316	F317	S319	G320	L321 K377	I323	V324	Y325	Y327	D328	T329 T330	P331	F332	K334	1335 8336		E339 V340	V341	K342 T343	L344	A347	I348	1349 1.350	V351	F352 L353	V354 M365	Y356	1007
F358 L359	N361	R363 A364	T365 L366	1367	T369	1370 A371	V372	P373 V374	V375	L376 L377	G378	T379 F380	000.1	A384	T390	N391	T392	L393 T394	M395	F396	G397	V399	L400 A401	I402	G403 L404	L405	V406 D407	D408	A409 I410	V411	V412 V413	E414	N415 V416		V419 M420	A421 E422	E423	1710
L425 P426	1421 1420	T431 R432	K433 S434	M435	I438	A441 ●	L442	V443 G444	1445	A446 M447	V448	L449	V452	F453	F469		S462	T463	A465	I466	Y467 R468	Q469	F470 S471	1472	T473		M478	S481	V482 L483	V484	A485	1487	L488	P490	A491 L492	C493	L497 VADB	N420
P499		G508	G511 F512	F513 CE14	W515	F516 N517	R518	M519 F520	E521	T524	H525	H526 V527	1027 T528	D529	S530 V531		1534	L535 R536	S537	T538	G539 R540	Y541	L542 V543	L544	Y545 L546	1547	1548	A553	Y554 L555	F556	V557 B558	L559	P560	L564	P565 D566	E567 DE68	0269 0569	0.00
V571	13/14 M575	Q577 L578	P579 A580	TE 83	0584 0584	E585 R586	T587	(1588 K589 ●	V590	L591 N592	E593	V594	Y597	Y598	L599	K601	E602	NEOR	0004	• <u>V609</u>	F610	V612	N613	0617	N618 T619	G620	I621 A622	F623	V624 S625	-	VI629	D631	R632 P633		N63/ K638	тела		A040
T647 R648	F650 5651	1652 1653	K654 D655	A656	L663	P664 A665	1666 1002	V 667 E 668	F669	G670 T671	A672	T673	F675	D676	T 679	1680 1680	D681	T 685	0000 0086	H687	E688 K689	L690	T691 0692	A 693	R694 N695	0696	L697	A 699	E700 A701	-	D706 M707	L708	V711	R712	P/13	E717	D718	L L L
P720 Q721	r / 22 K723 T794	D725 1726	D727 Q728	E729 4730		V /36 S737	1738	1741	N742	T743 T744	-	A747 A748	W749		V754 N755	D756	F757	I758 D769	R760		K764 K765	V766	Y767 V768	M769	S770 E771	A772	K773 Y774	R775	M776 L777	P778	D779 D780	1781	G782 D783	W784	Y785 V786	R787	M793	134
P7 95	A798	S800	802 R803	W804 ERAE	Y806	6807 8808			N815	G816	M820	E821 T822	1022 L823		K830 S831	H D D D D D D D D D D D D D D D D D D D	E834	A835 M836	E837	L838	M839 F.840	Q841	L842 A843	S844	K845 L846	-	Y852 D853	W854	M857	S858	Y859	S864	<mark>6865</mark>	Y872	S875	L876 T877		VOIS
F880 L881	0007 1883	L886 Y887	E888 S889	W890	1892	V896	M897	L898 V899	006A	P901 L902		1905 Cane	A907	L908	T909	R914	G915	L916 T917	1101	V920	Y921 F922	Q923	V924 G925	L926	L927 T928	T929	1930 6931	L932	8933 A934	K935	N936	1938	L939	V941	E942 F943	A944 Voaf		M340
K953	1955 1955 1956	E957 A958	<mark>T959</mark> L960	D961	V963	R964 M965	R966	L967 R968	P969	1970 L971	M972	T973	L975	A976	F977	M982	P983	L984 V985	1986	<mark>S987</mark>	T988	• 066V	6991 8992		A997 V998		G1005 M1006	V1007	T1008	T1010	V1011	A1013	T1014	F1016	V1017 P1018	V1019 E1030	F1021	1 7 7 7 7 N
V1023 V1024	R1026	S1029 R1030	K1031 N1032	E1033	I 1035	E1036 H1037	S1038	THR	VAL	ASP	HIS																											





N68	02N	G71 172	D73	N74 L75	M76 Y77	M78	N81	582	284 S84	T85	G86 T87	V88	089 100	T91	L92 T02	193 F94	E95	S96	D101	1102 1103	0104	V105	V107	Q108	K110	L111 Q112	L113	A114 M115	P116	L118	P119 0120	E121	0122 0123	Q124 D125	G126	V127 S128	V129 E130 K131	
S132	S134	<mark>S135</mark>	V139	I143	N144 T145	D146	G14/ T148	M149 T160	0151	E152	D153 1154		V158	M162	K163	A165		R168 T169	S170	G171	Q176	L177 E178	G179	S180	M184	R185 I186	W187	M1 88 N1 89	E1 93	L193	F196	Q197	L198 T199	P200 V201		907.I	N211 A212 Q213	
V214	A215 A216	G217 D218	L219	T222	P223	V225	q228	0229 1230		12 <mark>34</mark>	037	T238	R239 1240	0527	T243	F246	G247	K248 T249	L250	L251	2024	R259	V260 L261	L262	A266	K267 1268		6272 E273	N274 V275		1278 A279	E280	F281 N282	G283 0284		528/ G288	L289 L293	
A294	N298	na01	T302	A303 A304	R307		A311 K312	M313 E314	F315		S319 C320	L321	K322	P326	Y327	1329		V333	1337	H338	V340	V341	T343	L344 V345	E346	A347 I348	1349	L350 V351	F352	M355	Y356 L357	F358	L359 Q360	N361 F362	R363	A364 T365	L366	
T369	A371	V372	V374	V375 L376	T379	F380	A381 V382	L383 A304	A 304	13 <mark>9</mark> 0	N391 T392	L393	T394 M305	F396	G397	V399	L400	A401	G403	L404	V406	D407	A409	I410	V412	V413 E414	N415	V410 E417	R418 V419	M420	A421 E422	E423	6424 L425	K428	E429	A430 T431	S434 M435	
	6440 G440	A441	V443	6444 1445	A446 • M447	V448	L449	V452 EAE2	V454	P455	M456 A457	F458	F459	G461	S462	1403 G464	A465	I466	R468	Q469 E470	5471 S471	I472 T473	1473 •	V475 S476	A477	M478	L480	2481 V482	L483 V484	A485	L486 1487	L488	1489 P490	A491 L492	C493	A494 T495	M496 L497	•
I500	K502	G503	HEOS	G506 E507	G508 K509	K510	G511 F512	F513 C514	V515	F516	N517 R518	M519	F520 E521	K522	8523 #504	1 324 H525	H526	Y527 T528	D529	S530 VE24	TCOA	L535 D526	S537	T538 (539	R540	<mark>Y541</mark> L542	V543	L544 Y545	L546 T547	1548	V549 V550		A553	V557 R558	L559	P960	F563 L564 P565	
D566	V571	F572 M573	T574	M575 V576	Q577		A582 T583	Q584 5585	E262 R586	T587	0588 K589	V590	L591	E593	V594	1090	Y598	L599 TEAD	K601	E602 V603	N604	N605 V605	000	F610 A611	V612	N613 G614	G615	0100 0617	N618 T619	G620	1621 A622		97.9S	D631 R632	P633	K638	V639 E640 A641	
I642	1043 M644	R645 A646	T647	R648 A649	F650	I653	K654 D655	A656 Meez	V658	F659	NEGO	L663	P664	I666	V667	<u>гооо</u> Г669	G670	T671	T673	G674 •	D676	F677 F678	E0/8	1680 D681	0682	A683 G684	L685	4080 H687	E688 K689	L690	T691 Q692	A693	K694 N695	0696 1697		00 E	K703 D706	
M707		V711 • R712 •	P713	N714 G715	D718	T7 19	0721 0721	F7 22 V7 33	N/ 23	D7 25	I726	0728	1730		1741	N1 4.2	W7 49	N7 55	D756	F757 T7E0	1/ 30 D759	1 2	KI 02	V766	S770	E771 A772	K773	r / / 4 R775	P778	D779	D780 1781		W/ 84 Y7 85	V786 R787		ur 92 M793	V794 P795 F796	
S797	V130	S801 S803	R803	<mark>W804</mark> E805	2808 808	P809	K810 L811	E812 De13	CTON	<mark>G816</mark>	L817	M820	E821	1022 L823	G824	4020 A826	A827	P828	K830	S831	1032 G833	E834	Ac33 M836	E837 1.838		L842	K845		V850	Y852	D853 V854	T855	G856 M857	S858 Y859	q 860	E861 R862	L863 S864	
(1867	P869	S870 1.871	Y872	<mark>8875</mark>	L876 T877	V878	V8/9 F880	L881	L883	A884	V887	E888	S889 14600	8891	1892 2002	F033	5895	V896 M897	L898	V899	P901	L902	V904	1905	1909	A910 A911		K914 G915	L916 T917	N918	D919 V920		4923 V924	L927	T928	1929	G931 L932 S933	
A934	N936	A937 T938	1939	1940 V941	K945	D946	L94/ M948	KOE3	6954	L955	1956	T959	L960	1961 A962	V963	M965	R966	L967 R968	P969	1970 1971	M972	T973	59/4 L975	A976	1978	L979 G980	V981	P983	L984 V985	1986	060 <mark>0</mark>		V1 002 M1 003	M1 006	V1007	A1 008	T1010 • V1011 • L1012 •	
A1013	F1015	F1016	P1018	V1019 F1020	F1021 V1022	V1023	V1024	F1028	R1030	K1031	N1032 F1033	D1034	I1035	S1038	HIS	VAL	ASP	HIS	2111																			



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	152.07Å 157.78Å 219.39Å	Depositor
a, b, c, α , β , γ	90.00° 93.14° 90.00°	Depositor
Bosolution (Å)	20.00 - 3.40	Depositor
	109.53 - 3.40	EDS
% Data completeness	99.8 (20.00-3.40)	Depositor
(in resolution range)	97.9(109.53-3.40)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.93 (at 3.41 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
B.B.	0.275 , 0.349	Depositor
II, II, <i>free</i>	0.285 , 0.354	DCC
R_{free} test set	7110 reflections (5.00%)	wwPDB-VP
Wilson B-factor $(Å^2)$	98.9	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.26 , 74.0	EDS
L-test for twinning ²	$ < L >=0.39, < L^2>=0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	EDS
Total number of atoms	47532	wwPDB-VP
Average B, all atoms $(Å^2)$	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 47.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8623e-05.

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.



¹Intensities estimated from amplitudes.

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: NI, LMT

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).

Mal	Chain	Bo	nd lengths	B	ond angles
	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.65	1/8043~(0.0%)	0.89	11/10922~(0.1%)
1	В	0.65	1/8050~(0.0%)	0.89	9/10932~(0.1%)
1	С	0.67	1/8015~(0.0%)	0.91	9/10884~(0.1%)
1	D	0.60	1/8043~(0.0%)	0.89	15/10922~(0.1%)
1	Е	0.60	1/8032~(0.0%)	0.87	12/10907~(0.1%)
1	F	0.60	0/8032	0.89	7/10907~(0.1%)
All	All	0.63	5/48215~(0.0%)	0.89	63/65474~(0.1%)

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	А	0	3
1	В	0	2
1	С	0	1
1	D	0	1
1	F	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	D	515	TRP	CB-CG	7.50	1.63	1.50
1	А	515	TRP	CB-CG	6.68	1.62	1.50
1	Е	515	TRP	CB-CG	5.77	1.60	1.50
1	В	515	TRP	CB-CG	5.72	1.60	1.50
1	С	515	TRP	CB-CG	5.07	1.59	1.50

The worst 5 of 63 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	939	LEU	CA-CB-CG	-8.38	96.02	115.30
1	С	529	ASP	CB-CG-OD1	8.07	125.56	118.30
1	F	529	ASP	CB-CG-OD1	7.98	125.48	118.30
1	А	529	ASP	CB-CG-OD1	7.69	125.22	118.30
1	D	350	LEU	CA-CB-CG	-7.26	98.61	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	Group
1	А	1033	GLU	Peptide
1	А	1034	ASP	Peptide
1	А	1036	GLU	Peptide
1	В	1033	GLU	Peptide
1	В	1035	ILE	Peptide

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	А	7893	0	8034	457	0
1	В	7900	0	8041	384	0
1	С	7867	0	8015	444	0
1	D	7893	0	8034	515	0
1	Е	7883	0	8027	461	0
1	F	7883	0	8027	477	0
2	А	35	0	46	4	0
2	В	35	0	46	3	0
2	С	35	0	46	1	0
2	D	35	0	46	3	0
2	Е	35	0	46	8	0
2	F	35	0	46	1	0
3	А	1	0	0	0	0
3	С	1	0	0	0	0
3	Е	1	0	0	0	0
All	All	47532	0	48454	2651	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 28.

The worst 5 of 2651 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:E:536:ARG:NE	2:E:1101:LMT:O3B	1.81	1.13
1:A:424:GLY:HA3	1:A:502:LYS:HG2	1.38	1.04
1:D:954:GLY:HA2	1:D:1034:ASP:H	1.23	1.03
1:C:686:GLY:HA3	1:C:689:LYS:HD3	1.42	1.01
1:D:533:GLY:HA2	1:D:536:ARG:HD3	1.48	0.95

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	Perc	entiles
1	А	1036/1044~(99%)	942 (91%)	79 (8%)	15 (1%)	11	37
1	В	1037/1044~(99%)	942 (91%)	85 (8%)	10 (1%)	15	46
1	С	1033/1044 (99%)	931 (90%)	84 (8%)	18 (2%)	9	34
1	D	1036/1044 (99%)	934 (90%)	83 (8%)	19 (2%)	8	32
1	Е	1035/1044~(99%)	937~(90%)	87 (8%)	11 (1%)	14	44
1	F	1035/1044~(99%)	926 (90%)	84 (8%)	25 (2%)	6	28
All	All	6212/6264~(99%)	5612 (90%)	502 (8%)	98 (2%)	9	34

5 of 98 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	672	ALA
1	А	986	ILE
1	А	1029	SER
1	А	1033	GLU
1	В	617	GLN



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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	846/852~(99%)	781~(92%)	65~(8%)	13 40
1	В	847/852~(99%)	789~(93%)	58 (7%)	16 45
1	С	843/852~(99%)	774 (92%)	69~(8%)	11 37
1	D	846/852~(99%)	789~(93%)	57 (7%)	16 46
1	Ε	845/852~(99%)	775~(92%)	70 (8%)	11 36
1	F	845/852~(99%)	789~(93%)	56 (7%)	16 46
All	All	5072/5112~(99%)	4697 (93%)	375 (7%)	13 42

 $5~{\rm of}~375$ residues with a non-rotameric side chain are listed below:

Mol	Chain	\mathbf{Res}	Type
1	D	738	ILE
1	Е	575	MET
1	D	926	LEU
1	Е	177	LEU
1	Е	690	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
1	Е	67	GLN
1	F	755	ASN
1	Е	605	ASN
1	F	682	GLN
1	Е	569	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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).

Mal	Turne	Chain	Dec	Tink	В	ond leng	gths	B	ond ang	les
MIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LMT	F	2000	-	36,36,36	1.85	8 (22%)	47,47,47	1.14	4 (8%)
2	LMT	В	2000	-	36,36,36	1.81	12 (33%)	47,47,47	1.50	8 (17%)
2	LMT	Е	1101	-	36,36,36	1.83	10 (27%)	47,47,47	1.92	9 (19%)
2	LMT	D	2000	-	36,36,36	1.87	9 (25%)	47,47,47	1.70	8 (17%)
2	LMT	А	1101	-	36,36,36	1.80	11 (30%)	47,47,47	1.37	6 (12%)
2	LMT	С	1101	-	36,36,36	1.85	10 (27%)	47,47,47	1.40	<mark>6 (12%)</mark>

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	LMT	F	2000	-	-	15/21/61/61	0/2/2/2
2	LMT	В	2000	-	-	13/21/61/61	0/2/2/2
2	LMT	Е	1101	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	D	2000	-	1/1/10/10	12/21/61/61	0/2/2/2
2	LMT	А	1101	-	-	8/21/61/61	0/2/2/2
2	LMT	С	1101	-	-	12/21/61/61	0/2/2/2



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Е	1101	LMT	O1'-C1'	4.20	1.47	1.40
2	С	1101	LMT	O5'-C5'	4.10	1.54	1.44
2	F	2000	LMT	O5'-C1'	4.07	1.52	1.41
2	В	2000	LMT	O5'-C5'	3.97	1.54	1.44
2	F	2000	LMT	O5'-C5'	3.97	1.54	1.44

The worst 5 of 60 bond length outliers are listed below:

The worst 5 of 41 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	Е	1101	LMT	O1B-C4'-C5'	-5.21	95.18	109.45
2	D	2000	LMT	O1'-C1'-C2'	5.11	116.28	108.30
2	С	1101	LMT	O1'-C1'-C2'	4.87	115.91	108.30
2	Е	1101	LMT	C4B-C3B-C2B	4.82	119.23	110.82
2	Е	1101	LMT	C3B-C4B-C5B	4.70	118.63	110.24

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	2000	LMT	C3B
2	Е	1101	LMT	C2B

5 of 72 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	С	1101	LMT	C2'-C1'-O1'-C1
2	С	1101	LMT	O5'-C1'-O1'-C1
2	Е	1101	LMT	C2-C1-O1'-C1'
2	F	2000	LMT	C2'-C1'-O1'-C1
2	Е	1101	LMT	C4B-C5B-C6B-O6B

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2000	LMT	1	0
2	В	2000	LMT	3	0
2	Е	1101	LMT	8	0
2	D	2000	LMT	3	0
2	А	1101	LMT	4	0
2	С	1101	LMT	1	0



The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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 sufficient the outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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, 95^{th} 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	А	1038/1044~(99%)	0.42	127 (12%) 4 5	27, 75, 109, 132	0
1	В	1039/1044~(99%)	0.37	102 (9%) 7 9	18, 68, 104, 130	0
1	С	1035/1044~(99%)	0.49	125 (12%) 4 5	17, 69, 104, 126	0
1	D	1038/1044~(99%)	0.59	162 (15%) 2 2	16, 90, 130, 173	0
1	Ε	1037/1044~(99%)	0.69	180 (17%) 1 1	40, 91, 115, 134	0
1	F	1037/1044~(99%)	0.73	177 (17%) 1 2	24, 84, 118, 142	0
All	All	6224/6264~(99%)	0.55	873 (14%) 2 3	16, 80, 115, 173	0

The worst 5 of 873 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Е	128	SER	16.7
1	Е	314	GLU	14.0
1	Ε	315	PRO	12.2
1	F	714	ASN	11.8
1	F	442	LEU	11.2

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 monosaccharides 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, 95^{th} 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	$B-factors(Å^2)$	Q<0.9
2	LMT	В	2000	35/35	0.73	0.43	31,50,60,69	0
2	LMT	Е	1101	35/35	0.78	0.42	41,74,104,107	0
2	LMT	D	2000	35/35	0.82	0.34	21,41,56,63	0
2	LMT	С	1101	35/35	0.82	0.33	12,41,56,72	0
2	LMT	F	2000	35/35	0.82	0.39	40,64,89,94	0
2	LMT	А	1101	35/35	0.86	0.32	31,41,90,99	0
3	NI	Е	1102	1/1	0.96	0.15	170,170,170,170	0
3	NI	А	1102	1/1	0.97	0.19	154,154,154,154	0
3	NI	C	1102	1/1	0.98	0.09	41,41,41,41	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.















6.5 Other polymers (i)

There are no such residues in this entry.

