



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 4, 2024 – 11:55 PM EST

PDB ID : 2DR6
Title : Crystal structure of a multidrug transporter reveal a functionally rotating mechanism
Authors : Murakami, S.; Nakashima, R.; Yamashita, E.; Matsumoto, T.
Deposited on : 2006-06-08
Resolution : 3.30 Å(reported)

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

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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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

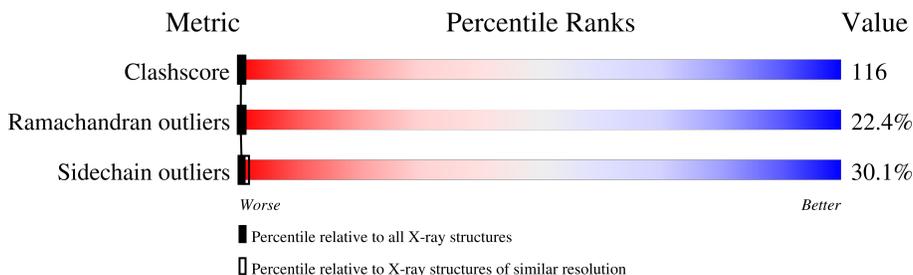
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1053	10% 41% 34% 13% .
1	B	1053	10% 46% 31% 10% .
1	C	1053	9% 39% 34% 15% .

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	DM2	A	2002	X	-	X	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 23361 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.

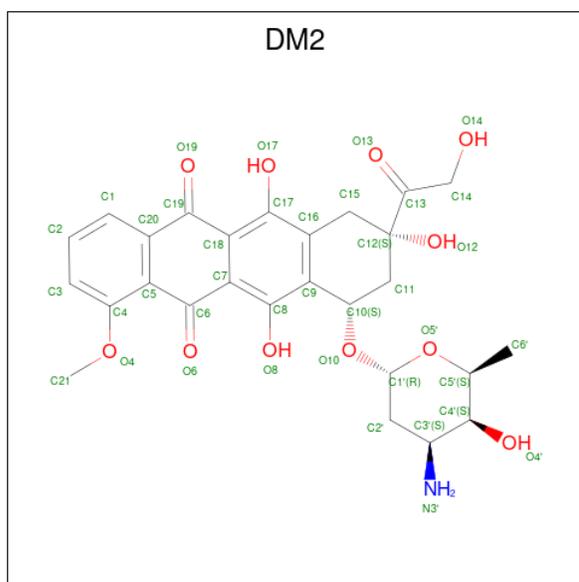
- Molecule 1 is a protein called ACRB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1022	7774	5003	1283	1444	44	0	0	0
1	B	1022	7774	5003	1283	1444	44	0	0	0
1	C	1022	7774	5003	1283	1444	44	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	HIS	-	expression tag	UNP P31224
A	1051	HIS	-	expression tag	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
B	1050	HIS	-	expression tag	UNP P31224
B	1051	HIS	-	expression tag	UNP P31224
B	1052	HIS	-	expression tag	UNP P31224
B	1053	HIS	-	expression tag	UNP P31224
C	1050	HIS	-	expression tag	UNP P31224
C	1051	HIS	-	expression tag	UNP P31224
C	1052	HIS	-	expression tag	UNP P31224
C	1053	HIS	-	expression tag	UNP P31224

- Molecule 2 is DOXORUBICIN (three-letter code: DM2) (formula: C₂₇H₂₉NO₁₁).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	39	27	1	11	0	0

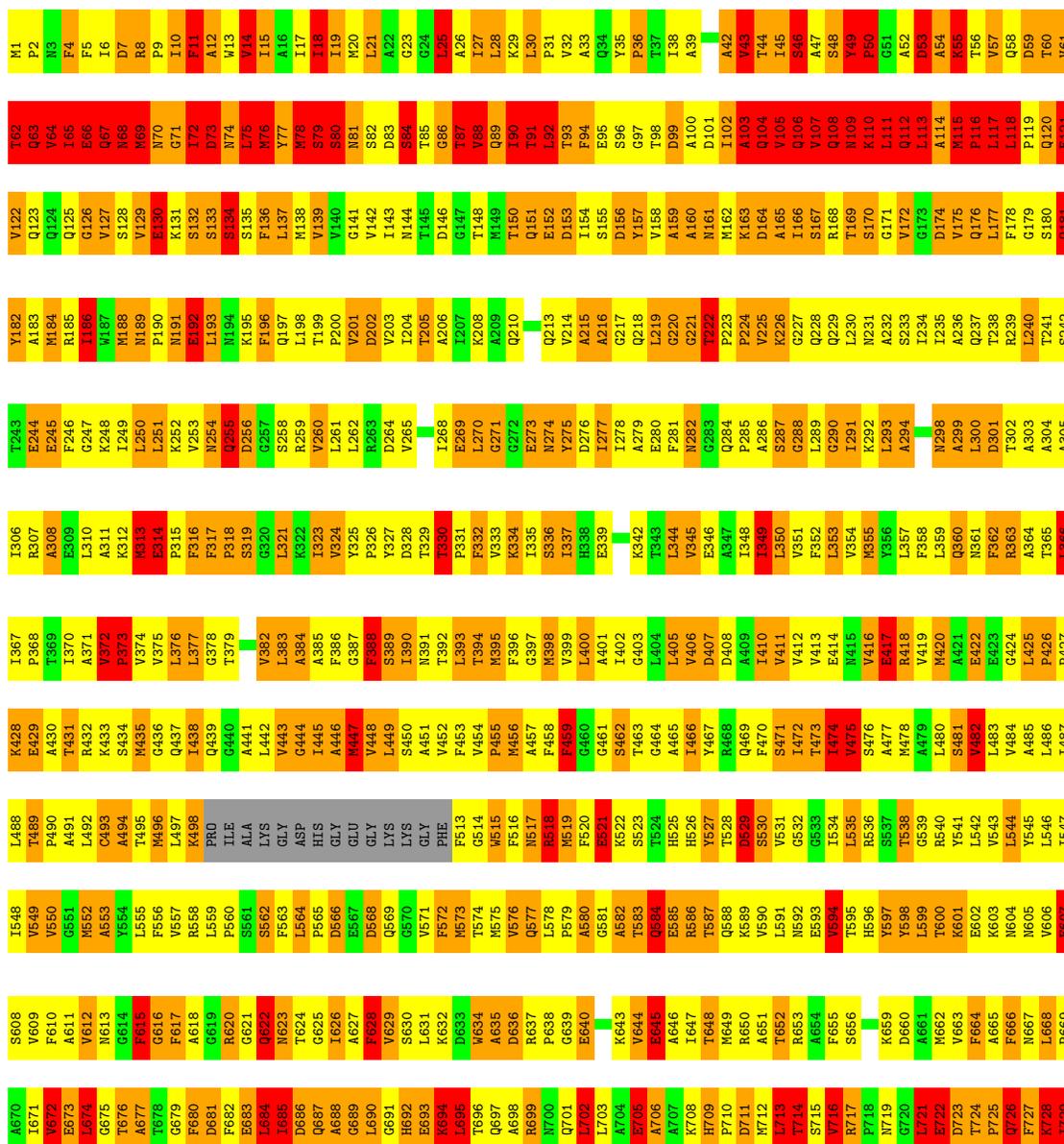
3 Residue-property plots

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

- Molecule 1: ACRB

Chain A: 



V609	E673	E734	A794	G854	L914	P974	K1036
F610	L674	K735	D795	V855	A915	I975	ASN
A611	G675	A736	G796	G856	A916	L976	GLU
V612	T676	Q737	Q797	V857	T917	M977	ASP
	A677	A738	N798	D858	F918	T978	ILE
F615	T678	L739	V799	V859	R919	S979	GLU
G616	G679	G740	P800	T860	G920	L980	HIS
F617	F680	V741	F801	G861	L921	A981	SER
A618	F681	S742	S802	V862	T922	F982	HIS
G619	F682	I743	A803	S863	R923	I983	HIS
R620	E683	N744	F804	V864	D924	L984	THR
		I745	F805	S865	R925	I985	VAL
G621	L684	D746	D806	V866	V926	G986	ASP
Q622	L685	I747	S807	V867	F927	M987	HIS
M623	D686	N747	R808	L868	Q928	P988	HIS
	Q687	T748	R809	V869	V929	L989	HIS
I626	A688	T749	A810	G870	I930	V990	HIS
A628	G689	L750	E811	N871	L931	I991	HIS
F628	L690	G751	Y812	R872	L932	S992	HIS
V629	G691	A752	G813	A873	T933	T993	HIS
		A753	S813	R874	I934	G994	HIS
K632	E693	W754	P814	S875	T935	A995	HIS
	K694	G755	R815	V876	G936	G996	HIS
V634	L695	L756	L816	R877	G937	S997	HIS
	T696	S757	E817	V878	L937	G998	HIS
	G697	V758	R818	A879	S938	G999	HIS
R637	Q698	V759	Y819	L880	A939	Q1000	HIS
P638	A699	N760	N820	V881	R940	I1001	HIS
G639	K699	D761	G821	S880	N941	L1002	HIS
E640	L700	L762	L822	L881	L942	A1003	HIS
E641	Q701	F762	R823	I882	I943	L1004	HIS
N642	L702	I763	P823	V883	L944	G1005	HIS
K643	L703	D764	S824	V884	I945	T1006	HIS
	K644	A704	M825	F885	L946	G1007	HIS
	E645	E705	E826	L886	V947	V1008	HIS
	E646	A706	L827	V887	F948	M1009	HIS
	A647	A707	L828	L888	A949	G1010	HIS
	T648	K708	G829	A889	K950	L1011	HIS
	M649	K709	Q830	A890	D951	V1012	HIS
	R650	P710	A831	A891	L952	L1013	HIS
	A651	D711	A832	E892	M953	P1014	HIS
	T652	W712	P833	V893	D954	A1015	HIS
	L653	L713	G834	S894	K955	Q1016	HIS
	A654	T714	K835	V895	L956	V1017	HIS
	F655	S715	S836	I897	G957	L1018	HIS
	S656	A776	T837	V897	K958	I1019	HIS
	Q657	K778	G838	F898	L959	F1020	HIS
	P658	Y779	E839	S900	L960	A47	HIS
	L659	R780	A840	V901	I961	S48	HIS
	D660	M781	M841	M902	E962	Y49	HIS
	G661	L782	E842	L903	A963	P50	HIS
	A662	L721	L843	V904	T964	G51	HIS
	M663	E722	M844	V905	L965	A52	HIS
	V664	D723	E845	P906	D966	D53	HIS
	T724	I724	E846	L907	A967	A54	HIS
	A665	G727	L847	G908	V968	K55	HIS
	F666	K728	A848	V909	I969	L118	HIS
	N667	D729	S849	W909	R969	P119	HIS
	L668	I729	K850	I910	M970	V57	HIS
	P669	D730	L851	G911	R971	Q58	HIS
	A670	I731	R952	L972	L972	D59	HIS
	L671	D732	R953	A912	R1032	E121	HIS
	V672	Q733	T853	L913	R973	S242	HIS

• Molecule 1: ACRB



M1	V61	Q123	A183	T243	A305	T365	P426
P2	T62	Q124	M184	E244	I306	L366	P427
N3	Q63	Q125	R185	F245	R307	I367	K428
F4	V64	G126	I186	E246	A308	P368	E429
I5	L65	V127	W187	G247	E309	A369	A430
I6	E66	S128	M188	K248	L310	T431	T431
D7	Q67	V129	N189	T249	A311	V372	R432
R8	M68	E130	P190	L250	K312	P373	K433
P9	Q69	I131	N191	L251	M313	S374	S434
I10	S70	S132	E192	K252	E314	V375	M435
F11	I72	S133	L193	V253	P315	L376	C436
A12	D73	G134	N194	N254	F316	L377	Q437
A13	M74	S135	K195	Q255	F317	F378	I438
V14	L75	F136	F196	D256	P318	T379	Q439
I15	M76	L137	Q197	G257	S319	F380	G440
A16	Y77	M138	L198	S258	A320	A381	A441
I17	M78	V139	T199	R259	L321	V382	G442
I18	S79	Q140	P200	V260	K322	R383	G443
I19	S80	G141	V201	L261	I323	A384	I445
K20	R81	V142	D202	L262	V324	A385	A446
L21	S82	W143	V203	R263	F325	F386	M447
G22	D83	M144	I204	D264	P326	V387	V448
G23	S84	T145	T205	V265	Y327	F388	L449
G24	T85	D146	A206	A266	D328	S389	S450
L25	G86	G147	L207	K267	T329	I390	A451
A26	T87	T148	K208	L268	T330	N391	V452
L27	Q88	M149	A209	E269	F331	T392	F453
L28	R89	T150	L270	R270	L332	L393	V454
L29	N90	Q151	G271	C271	V333	M394	P455
K30	I90	E152	N212	G272	A334	M395	M456
L31	T91	L153	A213	C273	I335	F396	A457
P32	R92	D154	Q214	N274	S336	G397	F458
V33	F94	I155	A215	Y275	I337	M398	V459
A33	Q94	D156	A216	D276	V338	V399	G460
G34	V95	V157	G217	L277	E339	L400	G461
Y35	F96	V158	Q218	L278	V340	A401	S462
P36	R98	A159	L219	A279	V341	I402	T463
T37	A100	A160	G220	E280	K342	G403	G464
L38	D101	M161	G221	Q281	T343	L404	A465
A39	I102	M162	T222	Q282	L344	L405	I466
P40	P41	A103	P223	P283	V406	D407	V467
A42	A42	D164	P224	A286	D408	A408	R468
V43	V43	V105	V225	S287	D409	A409	Q469
T44	T44	Q106	K226	C288	I410	I410	F470
I45	V107	S167	G227	L289	V411	V411	S471
A46	Q108	R168	Q228	G290	L412	V412	I472
A47	M109	T169	Q229	I291	V351	V413	T473
A48	S48	K110	L230	K292	L414	E414	I474
Y49	L11	G171	N231	S293	M415	M415	V475
P50	Q112	V172	A232	A294	V354	V416	S476
G51	L113	G173	S233	T295	M355	V417	A477
A52	A114	D174	I234	G296	E417	E417	M478
D53	M115	P175	I235	A297	R418	R418	A479
A54	P116	Q176	A236	N298	L419	L419	L480
K55	L117	L177	Q237	A300	M420	M420	S481
T56	L118	F178	T238	L300	Q360	Q360	V482
V57	P119	G179	R239	D301	N361	N361	L483
Q58	Q120	S180	L240	T302	E423	E423	V484
D59	E121	Q181	T241	A303	G424	G424	A485
T60	V122	Y182	S242	A304	L425	L425	L486

V1029	R969	A848	D768	K728	S608	I548	L487
R1030	I910	S849	W789	T729	V609	V549	L488
R1031	G911	R850	Y790	D730	F610	V550	L489
S1034	A912	L851	Y791	I731	A611	G551	P490
R1035	R913	R852	R792	D732	V612	M552	A491
K1036	L914	T853	A793	Q733	N613	A492	L492
ASN	A915	G854	A794	E734	F614	C493	C493
GLU	A916	W855	D795	K735	G616	L555	A494
ASP	T917	G856	Y796	A736	F617	F556	I495
GLU	F918	W857	K797	Q737	A618	V557	M496
ILE	R919	D858	W798	A738	G619	V558	L497
GLU	G920	W859	V799	L739	R620	L559	K498
HIS	L921	T860	P800	G740	G621	P560	PRD
SER	T922	G861	F801	W741	S621	S561	ILE
HIS	N923	R862	S802	S742	Q622	S562	ALA
THR	D924	S863	A803	T743	N623	F563	LYS
VAL	Y925	Y864	F804	N744	T624	L564	GLY
ASP	Y926	Q865	S805	D745	G625	P565	ASP
HIS	F927	E866	S806	I746	I626	D566	HIS
HIS	Q928	R867	S807	N747	A627	E567	GLY
HIS	Y929	L868	R808	T748	F628	D568	GLU
HIS	G930	S869	W809	L749	V629	Q569	GLY
HIS	L931	G870	E810	L750	S630	G570	LYS
HIS	L932	N871	Y811	G751	L631	V571	LYS
HIS	T933	O872	G812	A752	K632	F572	GLY
G994	T934	A873	S813	A753	D633	M573	PHE
A995	I935	F874	R814	W754	W634	T574	F513
G996	G936	S875	R815	G755	A635	M575	G514
S997	L937	L876	E816	G756	D636	V576	W515
G998	S938	Y877	E817	S757	Q637	Q577	F516
A999	A939	G878	R818	Y758	P638	L578	N517
Q1000	K940	S880	Y819	W759	G639	P579	R518
M1001	N941	L881	M820	N760	E640	A580	M519
A1002	A942	T882	G821	Q701	E641	G581	F520
G1003	T943	W883	L822	L702	N642	A582	E521
T1004	L944	W884	P823	L703	K643	T583	T524
T1005	T945	F885	S824	A704	V644	Q584	HE25
G1006	V946	L886	M825	E705	E645	E585	HE26
V1007	E947	C887	E826	A706	A646	E586	Y527
M1008	F948	L888	R827	A707	T647	T587	Y528
G1009	A949	A889	L828	K708	T648	Q588	D529
G1010	K950	A890	G829	H709	M649	K589	S530
M1011	D951	L891	Q830	P710	R650	V590	W531
L952	N952	Y892	A831	D711	A651	L591	G532
M953	M953	E893	A832	M712	T652	M592	G533
D954	D954	S894	P833	L713	R653	G593	I534
K955	K955	W895	G834	T714	A654	V594	L535
E956	E956	S896	K835	S775	F655	T595	R536
G957	G957	I897	S836	E776	S656	H596	S537
K958	K958	P898	T837	A777	Q657	Y597	T538
G959	G959	F899	C838	K778	L658	Y598	G539
F1020	F1020	S900	W839	Y779	K659	L599	R540
F1021	I961	Y901	A840	R780	D660	T600	Y541
F1022	E962	H902	M841	L721	A661	K601	L542
P1023	A963	L903	E842	L782	H662	E602	V543
T1024	T964	Y904	L843	D723	V663	K603	L544
F1025	L965	V905	M844	T724	F664	M604	Y545
F1026	D966	P906	E845	P725	A665	M605	L546
F1027	A967	L907	D846	T786	F666	V606	L547
V1028	Y968	G908	L847	G787	N667	I547	

4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	227.05Å 134.56Å 161.70Å 90.00° 98.08° 90.00°	Depositor
Resolution (Å)	10.00 – 3.30	Depositor
% Data completeness (in resolution range)	94.2 (10.00-3.30)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.298 , 0.359	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

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: DM2

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	2.18	252/7920 (3.2%)	1.95	258/10756 (2.4%)
1	B	1.57	63/7920 (0.8%)	1.59	113/10756 (1.1%)
1	C	2.04	222/7920 (2.8%)	1.89	245/10756 (2.3%)
All	All	1.95	537/23760 (2.3%)	1.82	616/32268 (1.9%)

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	1	31
1	B	0	11
1	C	0	19
All	All	1	61

The worst 5 of 537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	VAL	CA-CB	33.72	2.25	1.54
1	A	818	ARG	CZ-NH1	27.46	1.68	1.33
1	A	66	GLU	N-CA	21.61	1.89	1.46
1	A	66	GLU	CD-OE1	18.81	1.46	1.25
1	A	68	ASN	CA-CB	18.59	2.01	1.53

The worst 5 of 616 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	818	ARG	NE-CZ-NH2	-48.52	96.04	120.30
1	C	767	ARG	NE-CZ-NH1	-25.67	107.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	LEU	CB-CG-CD1	-25.55	67.57	111.00
1	C	164	ASP	CB-CG-OD2	-20.31	100.02	118.30
1	A	99	ASP	CB-CG-OD1	-17.20	102.82	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	61	VAL	CA

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	62	THR	Peptide
1	A	64	VAL	Peptide,Mainchain
1	A	65	ILE	Peptide
1	A	68	ASN	Sidechain
1	A	69	MET	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	A	7774	0	7928	1898	0
1	B	7774	0	7931	1841	0
1	C	7774	0	7930	1919	0
2	A	39	0	27	23	0
All	All	23361	0	23816	5470	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 116.

The worst 5 of 5470 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:118:LEU:CD2	1:A:118:LEU:CG	1.75	1.64
1:C:60:THR:CB	1:C:60:THR:CG2	1.75	1.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:CA	1:C:88:VAL:CB	1.80	1.59
1:C:767:ARG:CB	1:C:767:ARG:CG	1.78	1.59
1:C:65:ILE:CB	1:C:65:ILE:CG2	1.77	1.59

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	1018/1053 (97%)	530 (52%)	251 (25%)	237 (23%)	0	0
1	B	1018/1053 (97%)	558 (55%)	238 (23%)	222 (22%)	0	0
1	C	1018/1053 (97%)	565 (56%)	229 (22%)	224 (22%)	0	0
All	All	3054/3159 (97%)	1653 (54%)	718 (24%)	683 (22%)	0	0

5 of 683 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ILE
1	A	54	ALA
1	A	63	GLN
1	A	64	VAL
1	A	66	GLU

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	833/859 (97%)	592 (71%)	241 (29%)	0	1
1	B	833/859 (97%)	594 (71%)	239 (29%)	0	1
1	C	833/859 (97%)	560 (67%)	273 (33%)	0	1
All	All	2499/2577 (97%)	1746 (70%)	753 (30%)	0	1

5 of 753 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	962	GLU
1	C	280	GLU
1	B	1016	VAL
1	B	960	LEU
1	C	124	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	700	ASN
1	C	74	ASN
1	C	830	GLN
1	B	733	GLN
1	B	871	ASN

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](#)

1 ligand is 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	DM2	A	2002	-	41,43,43	4.31	24 (58%)	55,67,67	4.17	34 (61%)

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	DM2	A	2002	-	1/1/9/9	4/13/60/60	0/5/5/5

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	DM2	C2-C3	-10.86	1.16	1.38
2	A	2002	DM2	C1-C20	10.33	1.56	1.39
2	A	2002	DM2	C5-C4	8.54	1.55	1.40
2	A	2002	DM2	C20-C5	8.38	1.53	1.41
2	A	2002	DM2	C8-C9	7.95	1.54	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	DM2	C3-C2-C1	12.49	137.98	120.25
2	A	2002	DM2	C2-C1-C20	-9.08	102.65	119.81
2	A	2002	DM2	C2-C3-C4	8.77	135.83	119.71
2	A	2002	DM2	O4-C4-C5	7.48	126.27	115.85
2	A	2002	DM2	C3-C4-C5	-7.32	105.31	120.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	DM2	C4'

All (4) torsion outliers are listed below:

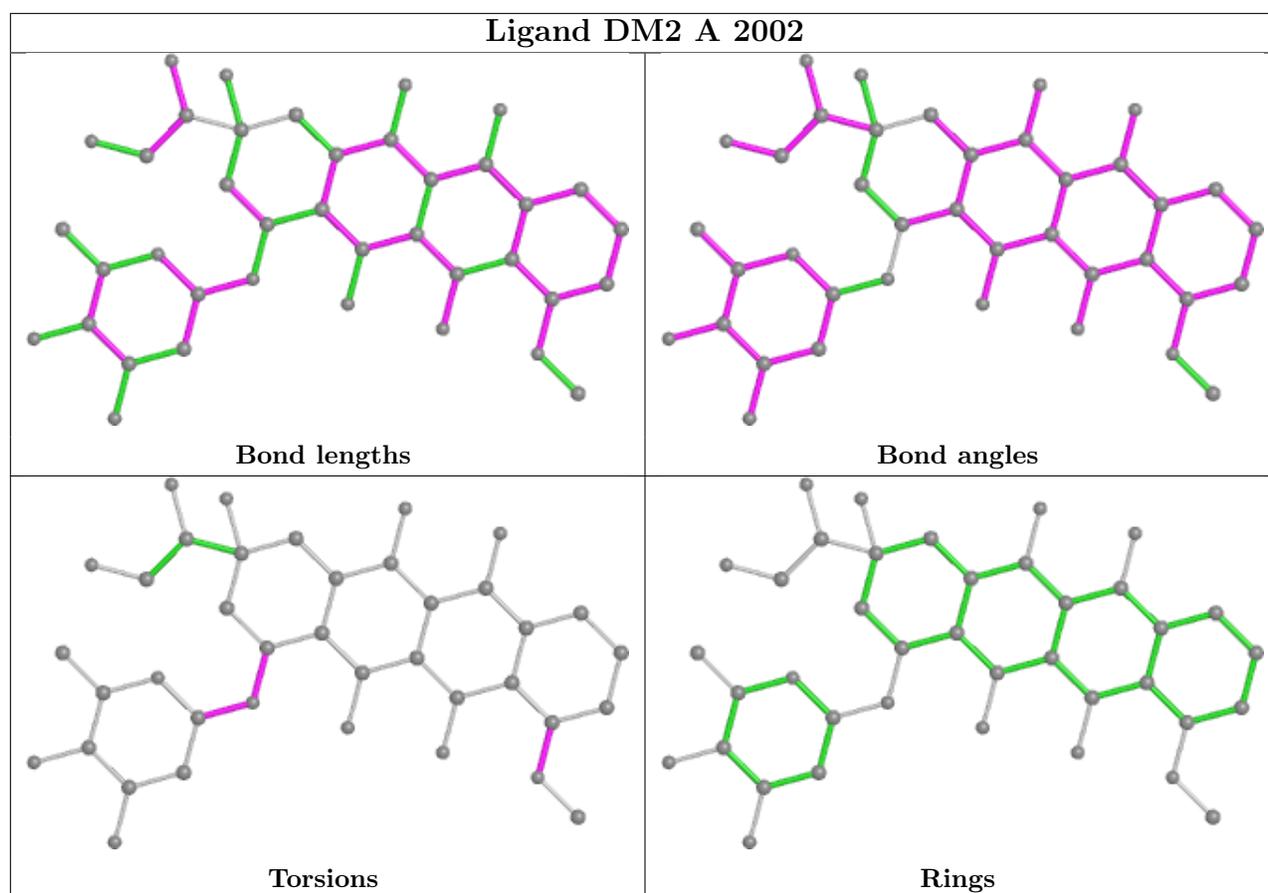
Mol	Chain	Res	Type	Atoms
2	A	2002	DM2	C2'-C1'-O10-C10
2	A	2002	DM2	O5'-C1'-O10-C10
2	A	2002	DM2	C5-C4-O4-C21
2	A	2002	DM2	C11-C10-O10-C1'

There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2002	DM2	23	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.



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](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.