



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 04:05 PM GMT

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 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/ValidationPDFNotes.html>

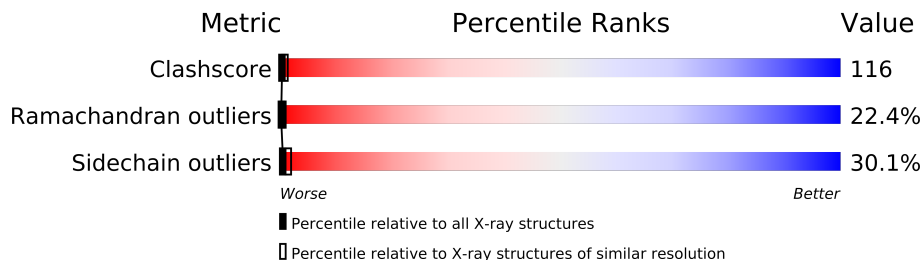
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1053	
1	B	1053	
1	C	1053	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23361 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

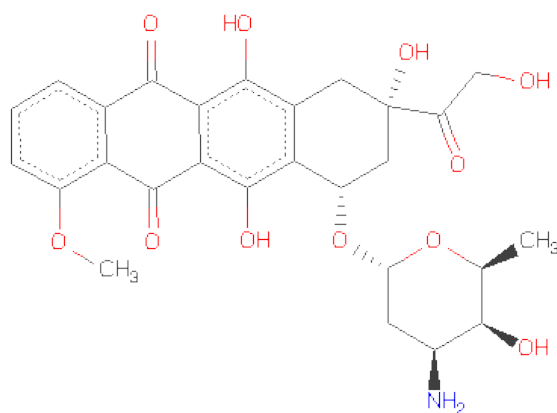
- Molecule 1 is a protein called ACRB.

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

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

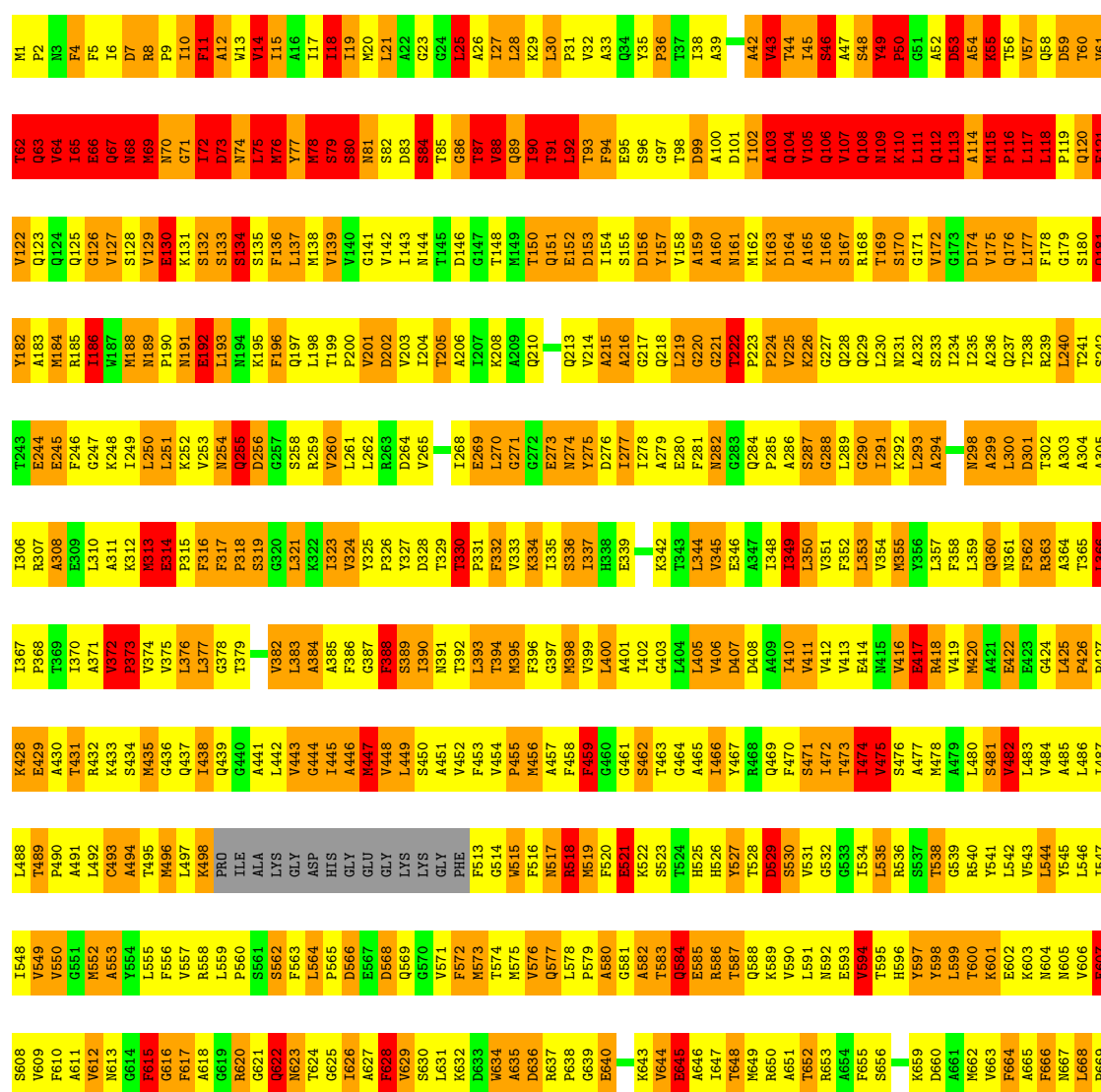
3 Residue-property plots

These plots are drawn for all protein, RNA 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.

Note EDS was not executed.

• Molecule 1: ACRB

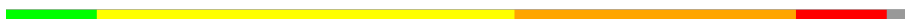
Chain A:



L488	L489	E429	K428	P368	A308	F246	R185	Q124	T62	M1	L972	A912	L851	V791	D730	A670
T489	P490	E430	E429	T369	E309	G247	I186	Q125	Q63	P2	R973	L913	P852	R792	I731	I671
A491	T431	A430	T431	I370	L310	K248	M187	Q126	V64	N3	P974	L914	R853	R792	D732	V672
L492	R432	R432	R432	A371	A311	T249	M188	V127	I65	F4	P975	A915	G854	A794	Q733	E673
C493	R433	R433	R433	V372	K312	L250	M189	V128	E66	F5	N976	A916	R855	D795	Q734	L674
A494	S434	S434	S434	P373	M313	L251	P190	V129	Q67	I6	N977	T917	G856	T796	K735	L675
T495	M436	M436	M436	V374	E314	K252	M191	E130	N68	D7	T978	F918	R857	Q797	A736	T676
M496	G436	G436	G436	V375	F316	V253	E192	K131	M69	R8	S979	G920	D858	R798	Q737	A677
M496	L376	L376	L376	V376	F316	M254	L193	S132	N70	P9	P982	G920	R859	R799	A738	T678
L497	Q377	Q377	Q377	V377	F317	S133	M194	S133	G71	I10	P982	L921	T860	P800	L739	G679
K498	L438	L438	L438	Q378	P318	D256	K195	S133	I72	F11	R983	T922	G861	R901	G740	F680
PR0	Q439	Q439	Q439	G379	S319	G257	F196	F136	D73	A12	L984	N923	M862	S802	T741	D681
ALA	G440	G440	G440	F380	G320	S258	Q197	L137	N74	M13	G985	D924	S863	S803	S742	F682
LYS	L441	L441	L441	A381	L321	R259	L198	M138	L75	V14	V986	V925	Y864	F804	I743	E683
GLY	L442	L442	L442	V382	K322	V260	T199	V139	R76	I15	P987	V926	Q865	S905	N744	L684
ASP	V443	V443	V443	L261	K323	L261	P200	V140	Y77	A16	P988	F927	E866	S906	N745	L685
GLY	G444	G444	G444	L262	V324	L262	V201	V141	M78	I17	L989	Q928	R867	S907	I746	D686
HIS	I445	I445	I445	L263	R263	G142	D202	V142	N81	I18	V990	V929	L868	R908	N747	Q687
GLY	L446	L446	L446	R264	V203	I143	V203	I143	S82	I19	P991	G930	S869	V803	T748	A688
GLU	M447	M447	M447	V265	L204	M144	T204	M144	S82	M20	S992	L931	G870	E810	T749	G689
GLY	V448	V448	V448	D328	T205	N145	T205	L145	D83	L21	S993	L932	N871	Y811	L750	L690
LYS	L449	L449	L449	A206	A206	G147	A206	G147	G86	G24	G994	T933	Q872	G812	G751	G691
LYS	S450	S450	S450	L207	L207	T148	L207	T148	T87	L25	A995	T934	A873	S813	A752	H692
GLY	A451	A451	A451	K208	K208	M149	V88	M149	V88	A26	G996	T935	P874	P814	A753	E693
PHE	V452	V452	V452	A209	A209	T150	V88	T150	Q89	L27	A999	L937	S875	R815	A754	K694
F513	F513	F513	F513	L393	V333	G272	Q210	T150	Q89	L27	A999	L937	L876	R816	G755	L695
G514	G514	G514	G514	T394	K334	E273	N211	Q151	T91	K29	Q1000	S938	R877	R817	G756	T696
M515	M515	M515	M515	M395	T335	M274	A212	E152	T91	A939	M1001	S938	A878	R818	S757	Q697
F516	F516	F516	F516	F396	S336	L275	Q213	E153	L92	L30	A1002	L930	R879	Y819	A768	A698
M517	M517	M517	M517	G397	I337	D276	Q213	I154	T93	P31	V1003	N941	S880	N820	V759	R699
R518	R518	R518	R518	G397	I337	D276	Q213	S155	F94	V32	G1004	A942	L881	G821	N760	Q701
R519	R519	R519	R519	M398	H338	I277	A216	S156	E96	A33	T1005	T943	I882	L822	D761	T701
F520	F520	F520	F520	V399	E339	I278	Q217	D156	S96	L28	Q1006	L944	R883	L823	F762	L702
E521	E521	E521	E521	L400	V340	A279	G218	Y157	Q97	Y35	M1007	T945	L886	N825	F762	L702
K522	K522	K522	K522	A401	V341	E280	L219	V158	G97	T37	P1008	V946	S924	N826	D764	A704
S523	S523	S523	S523	L402	K342	F281	G221	A159	T98	T37	G1009	V946	C887	E826	A705	E705
G524	G524	G524	G524	G403	T343	G283	T222	A160	D99	I38	G1010	F948	L888	T827	R767	A706
T524	T524	T524	T524	L404	L344	G283	T222	N161	A100	A39	M1011	A949	A889	L828	V768	A707
H525	H525	H525	H525	L405	V345	Q284	P223	M162	D101	P40	V1012	A950	A890	L829	K769	K708
H526	H526	H526	H526	V406	E346	S287	P224	K163	I102	P41	V1013	D951	L891	Q830	K770	H709
Y527	Y527	Y527	Y527	D407	A347	S287	P224	D164	A103	A42	A1014	L952	Y892	A831	V771	P710
T528	T528	T528	T528	D408	I348	G288	K226	A165	Q104	A42	A1015	L953	E893	A832	Y772	D711
D529	D529	D529	D529	A409	I349	L289	G227	I166	Q105	V43	T1015	N953	S894	A833	V773	M712
S530	S530	S530	S530	L410	L350	G290	Q228	S167	Q106	T44	V1016	D954	S894	P833	M774	L713
V531	V531	V531	V531	V411	V351	I291	Q228	R168	V107	I45	L1017	K955	W895	G834	M774	L713
G532	G532	G532	G532	V412	F352	K292	L230	T169	Q108	S46	L1018	E956	S896	K835	S775	T714
G533	G533	G533	G533	V413	L353	L293	N231	S170	K109	A47	I1019	G957	I897	S836	E776	T714
F534	F534	F534	F534	E414	V354	A294	A232	G171	K110	S48	F1020	G958	P898	T837	A777	V716
L535	L535	L535	L535	M415	M355	T295	S233	V172	L111	Y49	F1021	G959	F899	G838	K778	R717
H536	H536	H536	H536	V416	V356	G296	L234	G173	Q112	P50	V1022	L960	S900	E839	Y779	P718
S537	S537	S537	S537	E417	L357	A297	T235	D174	L113	G51	P1023	P961	V901	R840	R780	N719
T538	T538	T538	T538	R418	F358	M288	A236	V175	A114	A82	P1024	E962	M902	H841	M761	G720
G539	G539	G539	G539	V419	L359	A299	Q237	Q176	M115	D63	V1025	A963	L903	E942	L782	L721
R540	R540	R540	R540	M420	Q360	L300	T238	L177	P116	A54	F1026	T964	V904	L843	P783	E722
Y541	Y541	Y541	Y541	A421	N361	D301	R239	F178	L117	K55	V1027	T964	V905	M844	D784	E723
L542	L542	L542	L542	E422	F362	T302	L240	G179	L118	T56	V1028	D966	P906	E845	D785	T724
V543	V543	V543	V543	E423	R363	A303	T241	S190	P119	V57	V1029	A967	L907	Q846	I786	T725
L544	L544	L544	L544	E424	A364	A304	S242	Q181	Q120	Q58	R1030	V963	G908	L847	G787	Q726
Y545	Y545	Y545	Y545	L425	T365	A305	T243	Y182	E121	D69	R1031	V969	V909	A948	D788	F727
L546	L546	L546	L546	P426	L366	I121	E244	A183	V122	T60	R1032	N970	S849	R789	F728	L729
I547	I547	I547	I547	P427	L367	R307	E245	M184	Q123	V61	F1033	R971	G911	K850	Y790	I729

• Molecule 1: ACRB

Chain B:





V1029	R1030	R1031	S1034	R1035	K1036	ASN	GLU	GLU	ILE	ASP	GLU	THR	VAL	ASP	HIS	HIS	HIS	HIS	HIS
R969	M970	R971	L972	R973	P974	I975	L976	M977	T978	S979	R980	A981	L982	F983	L984	G985	V986	M987	P988
I989	G990	A991	L992	R993	T994	S995	M996	L997	F998	G999	H1000	A1001	L1002	G1003	T1004	L1005	G1006	V1007	M1008
I1009	F1010	A1011	L1012	R1013	T1014	S1015	M1016	L1017	A1018	F1019	G1020	H1021	L1022	P1023	T1024	F1025	F1026	F1027	V1028
I903	I910	G911	A912	L913	R914	A915	A916	T917	F918	R919	G920	L921	T922	N923	D924	G925	Y926	F927	Q928
S929	I930	A931	L932	R933	T934	S935	M936	L937	F938	G939	H940	A941	L942	G943	T944	L945	Y946	E947	F948
R949	G950	A951	L952	R953	D954	K955	S956	G957	K958	G959	L960	F961	E962	A963	T964	F965	P966	F967	V968
R969	T970	A971	L972	R973	T974	S975	M976	L977	F978	G979	H980	A981	L982	R983	G984	V985	P986	F987	G988
D788	W789	Y790	F791	R792	A793	A794	D795	D796	W797	R798	F799	R800	F801	S802	A803	F804	S805	S806	S807
K728	I729	D730	L731	R732	K733	F734	K735	A736	W737	R738	L739	G740	F801	S802	A803	F804	S805	S806	S807
L668	P669	A670	L671	R672	S673	L674	G675	T676	A677	R678	G679	F680	D681	F682	E683	L684	L685	D686	Q687
S608	V609	F610	A611	R612	N613	G614	F615	G616	F617	A618	G619	R620	G621	S622	N623	L624	G625	L626	A627
I548	V549	Y550	G551	R552	L553	R554	L555	F556	V557	R558	L559	P560	S561	S562	F563	L564	P565	D566	E567
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
P426	P427	K428	E429	A430	T431	R432	K433	K434	M435	L436	Q437	T438	Q439	G440	A441	G444	T445	L446	M447
L447	V448	L449	L450	L451	L452	F453	F454	P455	M456	N457	R458	F459	F460	G461	S462	T463	G464	A465	Y466
L467	R468	D469	S470	V471	G472	S473	L474	R475	S476	T477	S478	L479	G480	L481	L482	L483	Y484	L485	L486
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H499	L499	L499
L487	L488	T489	P490	A491	L492	C493	A494	L495	M496	L497	K498	P499	I499	A499	L499	G499	H49		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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.	Xtriage
Total number of atoms	23361	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	Mainchain,Peptide
1	A	65	ILE	Peptide
1	A	68	ASN	Sidechain
1	A	69	MET	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 116.

The worst 5 of 5470 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:118:LEU:CG	1:A:118:LEU:CD2	1.75	1.64
1:C:60:THR:CG2	1:C:60:THR:CB	1.75	1.62

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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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 ⓘ

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	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	833/859 (97%)	594 (71%)	239 (29%)	0	2
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	398	MET
1	B	782	LEU
1	C	774	MET
1	B	437	GLN
1	B	601	LYS

Some 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	361	ASN
1	B	700	ASN
1	C	692	HIS
1	B	415	ASN
1	B	584	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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	-	43,43,43	3.96	23 (53%)	67,67,67	3.75	37 (55%)

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	0/14/60/60	0/1/5/5

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2002	DM2	C2-C3	-9.87	1.16	1.39
2	A	2002	DM2	C1-C20	9.71	1.56	1.39
2	A	2002	DM2	C5-C4	8.86	1.55	1.40
2	A	2002	DM2	C20-C5	7.92	1.53	1.41
2	A	2002	DM2	C3-C4	-7.19	1.24	1.39

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2002	DM2	C3-C2-C1	11.49	137.98	120.25
2	A	2002	DM2	C2-C1-C20	-8.63	102.65	119.84
2	A	2002	DM2	C2-C3-C4	8.51	135.83	119.75
2	A	2002	DM2	C3-C4-C5	-8.03	105.31	120.34
2	A	2002	DM2	C6'-C5'-C4'	7.54	125.31	113.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2002	DM2	C4'

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.