



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:51 AM GMT

PDB ID : 3G60
Title : Structure of P-glycoprotein Reveals a Molecular Basis for Poly-Specific Drug Binding
Authors : Aller, S.G.; Yu, J.; Ward, A.; Weng, Y.; Chittaboina, S.; Zhuo, R.; Harrell, P.M.; Trinh, Y.T.; Zhang, Q.; Urbatsch, I.L.; Chang, G.
Deposited on : 2009-02-05
Resolution : 4.40 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
<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

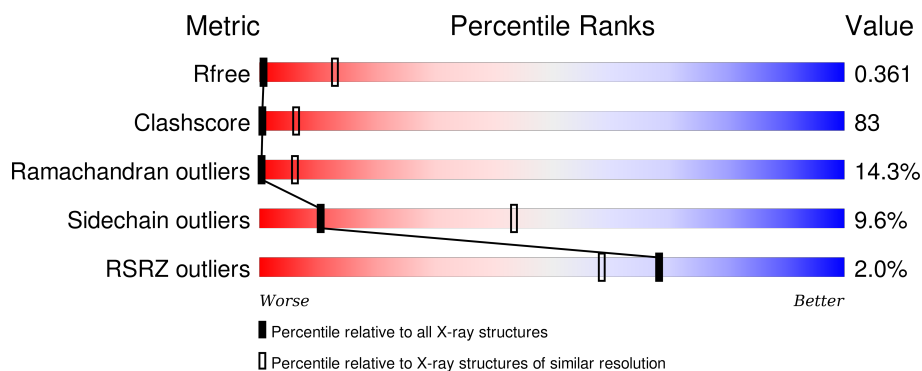
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1067 (5.20-3.60)
Clashscore	102246	1175 (5.20-3.60)
Ramachandran outliers	100387	1114 (5.20-3.60)
Sidechain outliers	100360	1096 (5.20-3.60)
RSRZ outliers	91569	1071 (5.20-3.60)

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	1284	 2% 16% 59% 15% • 8%
1	B	1284	 2% 16% 59% 16% • 8%

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	0JZ	A	6001	-	-	-	X
2	0JZ	B	6002	-	-	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18414 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.

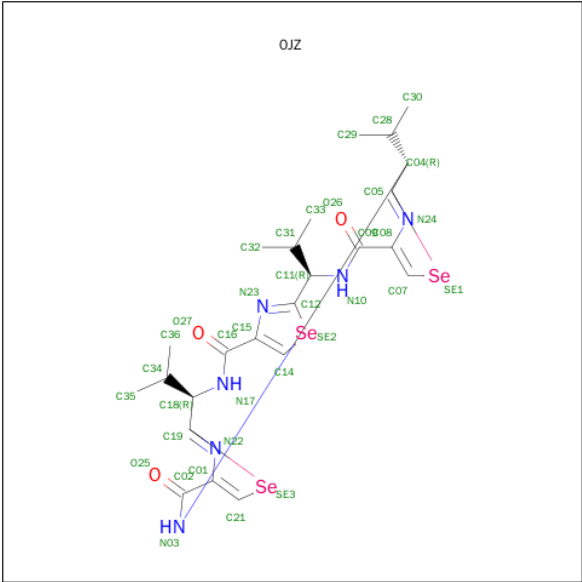
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			
1	B	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			

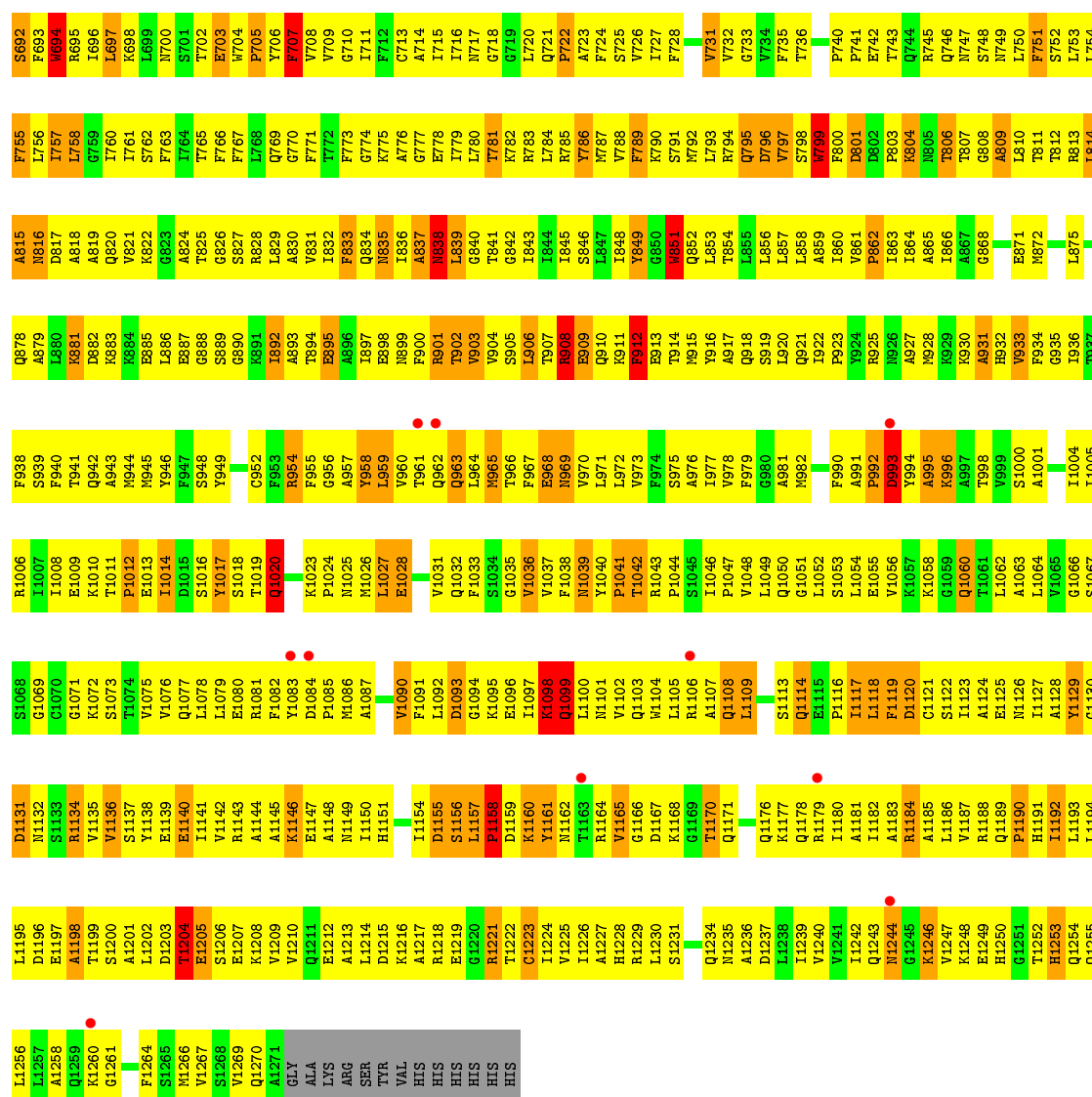
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TYR	-	EXPRESSION TAG	UNP Q5I1Y5
A	1278	VAL	-	EXPRESSION TAG	UNP Q5I1Y5
A	1279	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
A	1280	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
A	1281	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
A	1282	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
A	1283	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
A	1284	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1277	TYR	-	EXPRESSION TAG	UNP Q5I1Y5
B	1278	VAL	-	EXPRESSION TAG	UNP Q5I1Y5
B	1279	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1280	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1281	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1282	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1283	HIS	-	EXPRESSION TAG	UNP Q5I1Y5
B	1284	HIS	-	EXPRESSION TAG	UNP Q5I1Y5

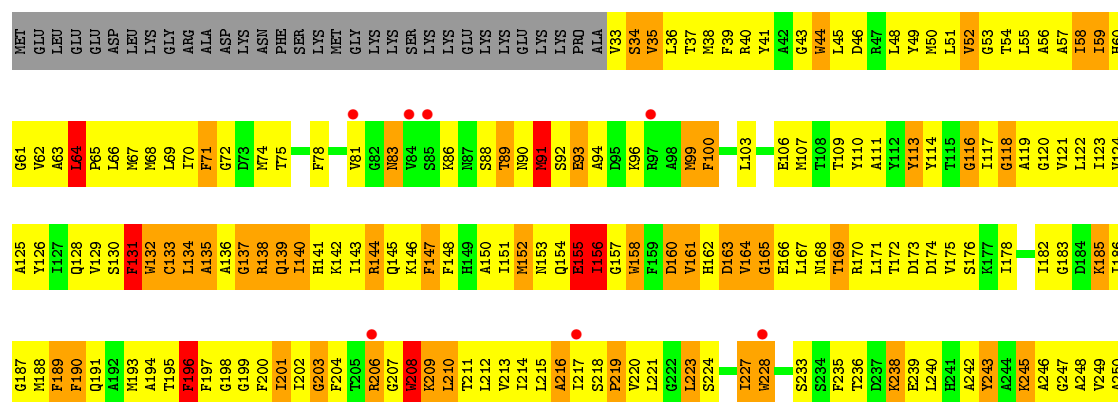
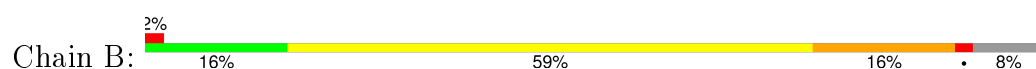
- Molecule 2 is (4R,11R,18R)-4,11,18-TRI(PROPAN-2-YL)-6,13,20-TRISELENA-3,10,17,22,23,24-HEXAAZATETRACYCLO[17.2.1.1 5,8 .1 12,15]TETRACOSA-1(21),5(24),7,12(23),14,19(22)-HEXAENE-2,9,16-TRIONE (three-letter code: 0JZ) (formula: C₂₄H₃₀N₆O₃Se₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		



• Molecule 1: Multidrug resistance protein 1a



Q1189	N1126	A1063	P934	G868	G808	S748	B686	T626	D558	E497	Q434	F374	G313	E251
P1190	I1127	L1064	G935	E871	A809	N749	D697	ALA	T559	K498	L435	S375	T314	E252
H1191	A1011	G1065	I936	M872	L810	L750	P689	GLY	B560	K498	M436	S376	S315	E253
I1192	Y1129	G1066	T937	M872	T811	F751	P689	ASN	S561	V500	Q437	S377	L316	L254
L1193	H1037	S1067	P938	L875	T812	S752	P690	GLU	E562	E502	R438	G378	V317	A255
L1194	D1131	S1068	S939	L875	R813	L753	A691	ILE	E563	E502	L439	H379	I318	A256
L1195	N1132	G1069	P940	L875	L814	L754	S692	GLU	V564	A503	Y440	K380	K319	L257
L1196	S1133	C1070	T941	Q878	A815	L755	P693	LEU	V565	M504	Y440	K381	K320	A258
E1197	H1134	G1071	Q942	A879	N816	L756	P694	GLY	Q566	A505	L443	P382	E321	T259
A1198	V1135	K1072	Q943	L880	D817	L757	H695	ASN	A567	Y506	D444	N383	Y322	V260
T1199	E1136	S1073	M944	K881	A818	L758	L696	GLU	A568	D507	G445	L384	S323	
S1200	S1137	T1074	M945	D882	A819	G759	L697	ALA	L569	F508	M446	Q385	I324	F263
A1201	Y1138	Y1075	Y946	K883	Q820	L760	L697	CYS	D570	I509	V447	G386	G325	
L1202	T1011	P1012	F947	K884	V821	L761	M700	LYS	M510	M510	S446	N387	Q326	Q266
D1203	E1013	E1013	S948	E885	K822	S762	S701	SER	R573	K511	L449	L388	V327	K267
T1204	L1014	L1014	Y949	L886	G823	F763	T702	LYS	B574	L512	D450	L328	E321	K268
E1205	D1015	D1015	Y949	E887	A824	L765	E703	ASP	G575	P613	F390	E269	S329	E269
S1206	P1016	P1016	C952	E888	T825	T765	H704	GLU	H576	H514	D453	V330	V330	L270
E1207	P1017	R1081	P953	S889	G826	F766	P705	ILE	T577	Q515	L454	N392	F331	E271
A1208	T1019	F1082	R954	L892	S827	F767	T706	ASP	T579	T518	R455	N393	F332	R272
K1208	Q1020	G1083	P955	A893	R828	L768	F707	ASN	L579	L519	T456	H394	S333	Y273
V1209	G1021	D1084	G956	T894	L829	Q769	V708	LEU	V580	V520	I457	F395	V334	N274
Q1210	L1022	P1085	A957	T894	A830	G770	V709	ASP	L581	V520	M458	S396	L335	N275
E1212	K1023	M086	Y958	E895	V831	F771	G710	MET	A582	G521	V459	Y397	I336	N276
A1213	L959	A1087	L959	A896	I832	T772	I711	SER	H583	E522	R460	P398	G337	L277
L1214	V960		V960	L897	F833	F773	F712	SER	H584	R523	Y461	S399		E278
D1215	L1027	F1090	T961	E898	Q834	G774	G713	LYS	L585	G524	L462	R400	S340	
K1216	F1091	F1091	Q962	N899	N835	K775	A714	ASP	A525	A525	R463	K401	V341	E279
D1155	L1092	L1092	L963	F900	I836	A776	I715	SER	V588	Q526	E464	E402	G342	K281
R1218	D1093	D1093	Q964	R901	A837	G777	I716	GLY	H589	L527	I465	V403	Q343	R282
E1219	G1094	G1094	M965	T902	N838	E778	N717	SER		S528	I466	Q404	A344	L283
G1220	K1095	K1095	T966	V903	L839	I779	G718	SER	V593	G529	Q467	I405	S345	G284
R1221	E1096	E1096	P967	P904	G940	L780	G719	LEU	L594	G530	V468	L406	P346	L285
T1222	N968	N1097	E968	S905	T841	T781	Q721	ILE	F597	K532	V469	K407	N347	K286
C1223	V1037	V1037	N969	L906	G842	K782	Q721	ARG		F597	S470	G408	I348	K287
I1224	F1038	F1038	V970	T907	I943	R783	P722	ARG	D598	Q533	Q471	L409	E349	A288
V1225	N1039	L1100	L971	R908	I844	L784	A723	ARG	G599	R534	R472	N410	P351	L289
I1226	Y1040	Y1040	L972	E909	I845	R785	F724	SER	H600	I535	P473	L411	P351	T290
A1227	P1041	P1041	V973	Q910	S846	K786	S725	THR	V601	A536		K412	A352	A291
H1228	T1042	T1042	F974	K911	L847	M787	V726	ARG	L602	I537	F476	V413	N353	N292
R1229	R1043	R1043	S975	F912	I848	V788	I727	LYS	B603	A538	T478	K414	A354	L293
L1230	P1044	P1044	A976	E913	Y949	F789	F728	SER	B504	R539	T479	S415	R355	S294
S1231	S1045	R1106	I977	T914	G850	K790		ILE		A540	T479	G416	G356	K295
	I1046	A1107	V978	M915	K851	S791	V731	CYS	H608	L541	L480	G417	A357	G296
Q1234	P1047	Q1108	F979	Y916	Q852	N792	V732	GLY		V542	L481	T418	A358	A297
M1235	L1048	L1109	G980	A917	L853	L793	G733	PRO	L611	R543	E482	V419	Y359	A298
A1236	L1049	L1049	A981	Q918	T854	R794	V734	HIS	M612	N544	N483	A420	E360	F299
D1237	M982		M982	S919	L855	Q795	F735	ASP	H613	P545	L484	L421	V361	L300
L1238	Q1050	G1051	Q921	L920	L856	D796	T736	GLU	B614	K346	R485	V422	F362	L301
I1239	L1062	L1062	Q921	L857	L857	V797	V737	ASP	H615	I547	Y486	G423	K363	L302
V1240	S1053	S1053	P923	L858	L858	S798	G738	ARG	G616	L548	Q487	M424	I364	V303
I1241	L1054	L1054	P923	A859	F799	S798	G739	ARG	L617	L549	R488	S425	I365	A304
A1181	E1055	E1055	A991	I860	V861	F800	P740	LEU	V618	L550	E489	G426	N367	S305
Q1243	V1056	V1056	P992	D801	V861	D801	P741	SER	F619	D551	D490	C427	K367	V306
A1183	K1057	K1057	D993	M928	P862	D802	E742	THR	G620	E552	V491	G428	K368	A307
G1245	Y994	Y994	Y994	K929	I863	P803	T743	LYS	L621	A553	T492	K423	P369	L308
K1246	A995	A995	A995	K930	I864	K804	Q744	GLU	V622	T554	K483	K423	S370	A309
V1247	K996	K996	A997	A931	I865	M805	R745	ALA	H623	A556	D494	T431	I371	F311
K1248	T1061	T1061	H932	H932	I866	T806	Q746	ALA	T624	S555	E495	T432	D372	N311
E1249	L1062	E1125	T998	V933	A867	T807	N747	D685	H625	L557	I496	V433	S373	Y312

H1250	G1251	T1252	H1253	Q1254	Q1255	L1256	L1257	A1258	Q1259	K1260	G1261	F1264	S1265	M1266	V1267	S1268	V1269	Q1270	A1271	GLY	ALA	LYS	ARG	SER	TYR	VAL	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.63Å 115.09Å 374.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 4.40 49.02 – 4.31	Depositor EDS
% Data completeness (in resolution range)	94.7 (19.99-4.40) 93.3 (49.02-4.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 4.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.314 , 0.365 0.316 , 0.361	Depositor DCC
R_{free} test set	2562 reflections (10.02%)	DCC
Wilson B-factor (Å ²)	201.9	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 103.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 28597 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	18414	wwPDB-VP
Average B, all atoms (Å ²)	198.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 0JZ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	1/9339 (0.0%)	0.70	13/12626 (0.1%)
1	B	0.41	0/9339	0.68	8/12626 (0.1%)
All	All	0.41	1/18678 (0.0%)	0.69	21/25252 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	851	TRP	CB-CG	5.17	1.59	1.50

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	CYS	N-CA-C	9.35	136.24	111.00
1	A	1098	LYS	N-CA-C	-7.80	89.94	111.00
1	A	164	VAL	N-CA-C	-7.79	89.98	111.00
1	A	267	LYS	N-CA-C	7.23	130.52	111.00
1	A	165	GLY	N-CA-C	-7.16	95.21	113.10

There are no chirality outliers.

There are no planarity outliers.

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	9171	0	9344	1558	0
1	B	9171	0	9344	1534	0
2	A	36	0	27	12	0
2	B	36	0	27	10	0
All	All	18414	0	18742	3089	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 83.

The worst 5 of 3089 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:B:797:VAL:O	1:B:801:ASP:HB2	1.45	1.15
1:A:523:ARG:HD3	1:A:524:GLY:H	0.99	1.13
1:B:523:ARG:HD3	1:B:524:GLY:H	0.98	1.12
1:B:858:LEU:O	1:B:862:PRO:HD2	1.51	1.11
1:B:1204:THR:O	1:B:1206:SER:N	1.83	1.10

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	1178/1284 (92%)	704 (60%)	302 (26%)	172 (15%)	0	6
1	B	1178/1284 (92%)	707 (60%)	305 (26%)	166 (14%)	0	6
All	All	2356/2568 (92%)	1411 (60%)	607 (26%)	338 (14%)	0	6

5 of 338 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER

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Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	89	THR
1	A	133	CYS

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	976/1065 (92%)	884 (91%)	92 (9%)	11	45
1	B	976/1065 (92%)	880 (90%)	96 (10%)	10	42
All	All	1952/2130 (92%)	1764 (90%)	188 (10%)	10	43

5 of 188 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1140	GLU
1	B	158	TRP
1	B	1010	LYS
1	A	1192	ILE
1	B	91	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1149	ASN
1	B	154	GLN
1	B	1108	GLN
1	A	1191	HIS
1	B	60	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	0JZ	A	6001	-	27,39,39	1.87	6 (22%)	24,57,57	2.48	9 (37%)
2	0JZ	B	6002	-	27,39,39	1.54	4 (14%)	24,57,57	1.89	6 (25%)

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	0JZ	A	6001	-	-	0/24/48/48	0/0/4/4
2	0JZ	B	6002	-	-	0/24/48/48	0/0/4/4

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6002	0JZ	C15-C16	-2.62	1.44	1.50
2	A	6001	0JZ	C34-C18	2.03	1.60	1.54
2	B	6002	0JZ	C16-N17	2.44	1.39	1.34
2	A	6001	0JZ	C18-N17	2.85	1.52	1.46
2	A	6001	0JZ	C19-C18	2.97	1.54	1.51

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	6001	0JZ	C29-C28-C04	2.06	113.18	111.30
2	A	6001	0JZ	C15-C16-N17	2.18	119.96	115.10
2	B	6002	0JZ	C01-C02-N03	2.33	120.29	115.10
2	B	6002	0JZ	C18-N17-C16	2.71	126.58	122.02
2	A	6001	0JZ	C33-C31-C11	2.91	113.96	111.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	0JZ	12	0
2	B	6002	0JZ	10	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	1182/1284 (92%)	-0.07	22 (1%) 70 61	118, 194, 243, 306	0
1	B	1182/1284 (92%)	-0.09	25 (2%) 67 57	123, 200, 243, 301	0
All	All	2364/2568 (92%)	-0.08	47 (1%) 68 58	118, 197, 244, 306	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	963	GLN	5.1
1	B	1199	THR	4.8
1	A	1084	ASP	4.2
1	B	228	TRP	4.1
1	A	574	GLU	4.0

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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	OJZ	A	6001	36/36	0.64	0.43	2.00	196,196,196,196	0
2	OJZ	B	6002	36/36	0.63	0.41	0.80	196,196,196,196	0

6.5 Other polymers [i](#)

There are no such residues in this entry.