



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 03:06 AM UTC

PDB ID : 3G5U / pdb_00003g5u
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 : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

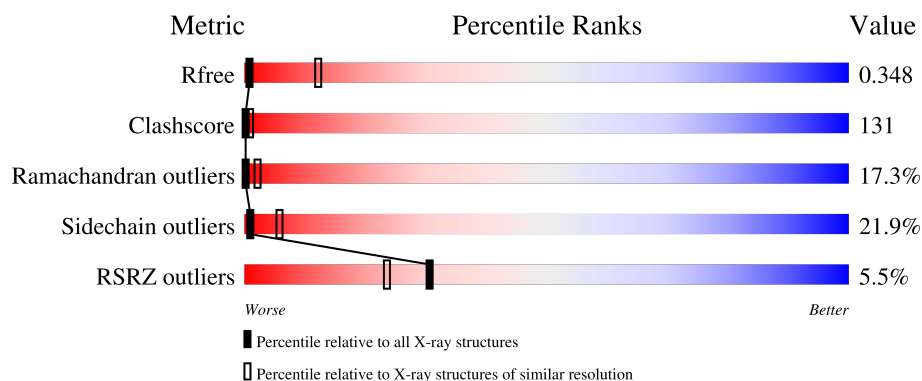
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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 $\leq 5\%$. 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	
1	B	1284	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18352 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
			9170	5895	1552	1686	37			
1	B	1182	Total	C	N	O	S	0	0	0
			9170	5895	1552	1686	37			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	952	ALA	CYS	engineered mutation	UNP Q5I1Y5
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	952	ALA	CYS	engineered mutation	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 MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Hg	0	0
			6	6		

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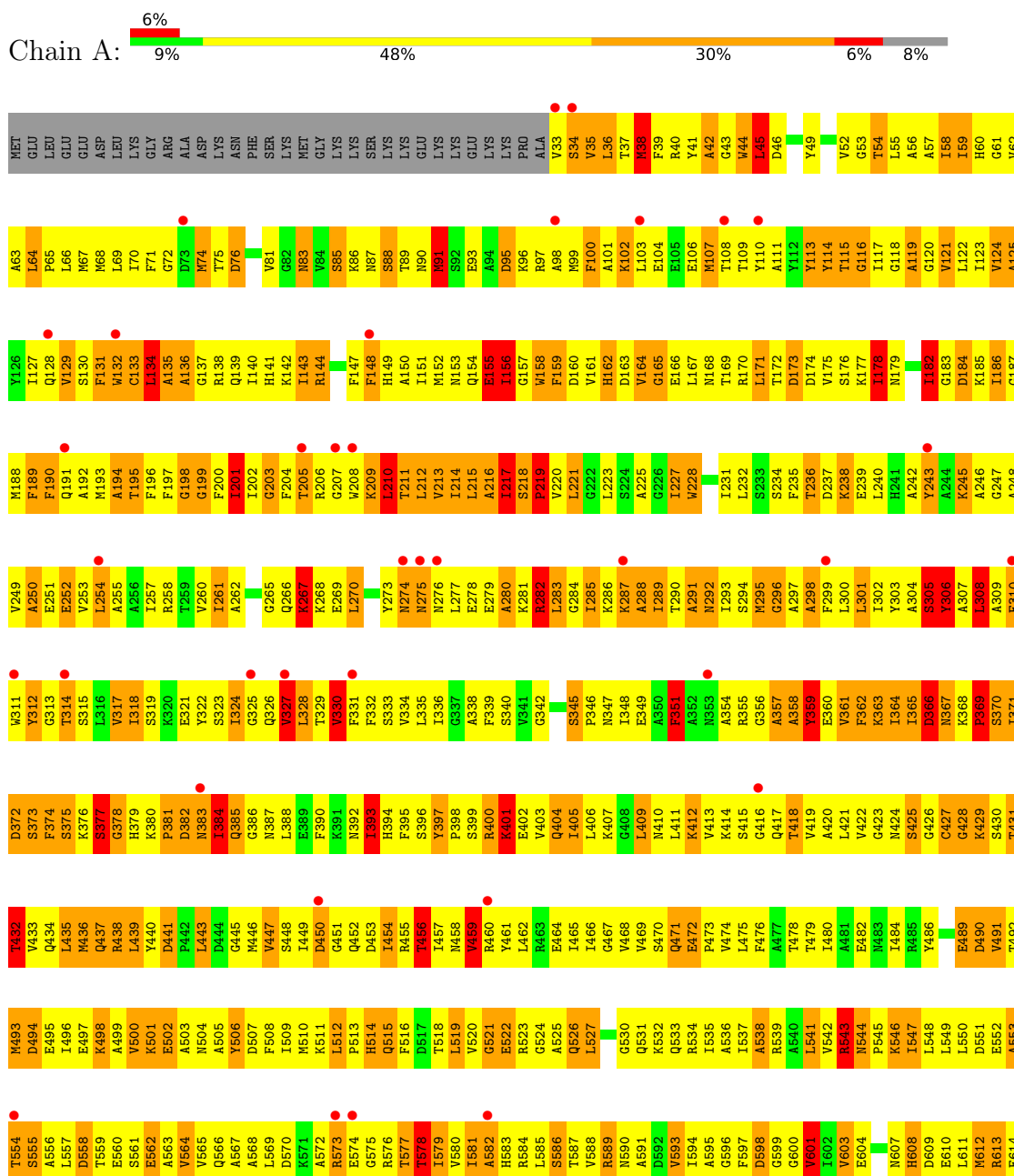
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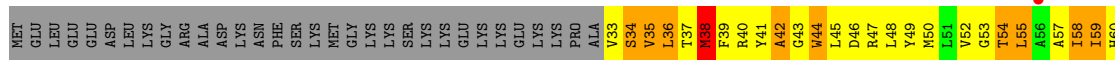
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	Hg	0	0
			6	6		

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Multidrug resistance protein 1a





A917	L857	F735	ASP	K615	T554	T492	T432	1371	G247	G187	A125	G61
Q918	L858	T736	ARG	G616	S555	M493	V433	D372	A248	M188	T126	V62
S919	A859	N737	LYS	A556	A557	E494	Q434	F373	F189	F189	Q127	A63
L920	T860	G738	LEU	Y617	L557	D495	Q435	F374	A250	F190	Q128	L64
Q921	T861	G739	SER	Y618	D558	E496	N436	S375	E251	Q191	S129	P65
L922	P862	P740	THR	K620	T559	E497	Q437	K376	E252	A192	S130	L66
P923	T863	P741	LYS	L621	E560	K498	R438	S377	V253	M193	F131	M67
Y924	T864	E742	GLU	V622	S561	A499	L439	G378	L254	M194	A194	M68
R925	A865	T743	ALA	M623	E562	V500	Y440	H379	A255	T195	C132	L69
N926	T866	Q746	L684	Q625	E563	E501	D441	K380	F196	F196	A134	L70
A927	T867	Q747	D685	Q626	V564	E502	P442	K381	I257	F197	A135	F71
N928	G868	N747	E686	Q627	A565	K501	D443	S319	G198	G198	A136	G72
K929	T869	S748	D687	ALA	Q566	A503	L443	S320	T259	G199	G137	D73
K930	T870	N749	V688	GLY	A567	A504	D444	E321	V260	F200	R138	M74
A931	E871	L750	ASN	GLY	A568	A505	G445	Y322	I261	I201	Q139	T75
H932	T872	F751	P689	ASN	L569	Y506	N446	Y323	I262	A262	I140	D76
F933	T873	S752	GLU	GLU	D570	D507	N447	S324	I140	G203	H141	S77
F934	K874	L753	I691	IIE	K571	F508	S448	L388	F263	F204	K142	F78
G935	L875	L754	S992	GLU	T577	I509	I449	E389	G264	F205	K143	S79
T936	S876	F755	F693	LEU	A572	M510	D450	F390	G265	T206	I144	V81
T937	T877	F756	M694	GLY	R573	K511	G451	V327	Q266	G207	R144	G82
F938	T878	L757	R695	ASN	E574	L512	Q452	L328	K267	G208	F147	N83
S939	A878	I758	L696	GLU	G575	P513	D453	T329	K268	K209	F148	N84
F940	A879	L758	L697	ALA	R576	H514	L454	F331	E269	F149	H149	S85
T941	L880	G759	K698	CYS	T578	Q515	R455	F332	L270	L210	H150	K86
T942	K881	I760	L699	LYS	T579	F516	T456	F333	E271	T211	T151	N87
Q943	D882	I761	N700	SER	I579	D517	I457	S333	N274	L212	M152	S88
A944	K883	S762	S701	LYS	V580	T518	N458	V334	E279	S218	M153	T89
N945	T884	F763	T702	ASP	L581	L519	P459	S340	A280	G219	V161	N90
Y946	E885	G764	E703	GLU	A582	V520	R460	V341	K281	V220	D160	A98
Y947	L886	I765	W704	IIE	H633	G521	Y461	G342	L283	G222	G162	M99
F947	T887	F766	P705	ASP	R584	E522	L462	A338	G284	L223	D163	F100
S948	R828	F767	Y706	ASN	L585	R523	R463	F339	I285	S224	A101	A101
Y949	L829	L768	F707	LEU	S886	G524	E464	S340	K286	A225	V164	K102
A950	A830	Q769	W708	LEU	T587	A525	L465	S340	K287	G226	G165	L103
A951	K891	G770	W709	MET	V588	Q526	I466	L405	A288	I227	E166	A98
A952	T892	F771	G710	SER	R589	L527	Q467	G342	I289	W228	L167	E104
F953	F833	T772	I711	SER	N590	S528	V468	F351	T290	A229	M168	M107
R954	Q834	F773	F712	LYS	A591	G529	V469	A354	A291	K230	T169	T108
F955	N835	G774	G713	ASP	D592	G530	S470	R355	N292	I231	R170	T109
G956	T836	K775	A714	SER	V593	Q531	Q471	G356	I293	L232	L171	Y110
A957	A837	A776	I715	GLY	L594	K532	E472	A357	S294	S233	T172	A111
Y958	N838	G777	I716	SER	A595	Q533	P473	A358	M295	S234	D173	Y112
L959	L839	E778	N717	SER	G596	B534	V474	Y359	G296	F235	D174	Y113
F960	G840	I779	G718	LEU	F597	B534	L475	E360	A297	T236	V175	Y114
T961	T841	L780	G719	IIE	D598	T537	F476	V361	A298	D237	S176	T115
Q962	G842	T781	L720	ARG	G599	A538	A477	F362	E298	K238	K177	G116
Q963	T843	K782	Q721	ARG	G600	L541	T478	G357	I294	E239	T178	I117
L964	T844	R783	P722	ARG	V601	L542	T479	A358	M295	L240	N179	G118
S965	T845	L784	A723	SER	I602	V542	I480	Y359	G296	F235	D174	I119
T966	S846	R785	F724	THR	V603	R543	A481	E360	A297	T236	V175	Y114
F967	L847	Y786	S725	ARG	E604	N544	E482	V361	A298	D237	S176	T115
R968	T848	M787	W726	LYS	G607	P545	N483	F362	E298	K238	K177	G116
E969	Y849	V788	F728	SER	N607	K546	L484	G362	L300	E239	I178	I117
Q970	G850	F789	T727	IIE	H608	L547	R485	I364	L301	L240	N179	G118
L971	K911	K790	S729	CYS	D609	L548	Y486	I365	I302	H241	G182	A119
N972	T852	S791	K730	GLY	E610	L549	Q487	D366	A242	Y243	G183	V121
E913	L853	M792	V731	PRO	L611	L550	R488	N367	A304	Y243	D184	L122
T914	T854	L793	H1S	HIS	M612	D551	E489	K368	S305	A244	L122	L122
L855	T794	R794	G733	ASP	R613	E552	D490	P369	S306	K245	L123	L123
S975	Y916	Q795	V734	GLN	E614	A553	V491	S370	A307	A246	I186	V124



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.80 19.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (19.98-3.80) 95.3 (19.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.19 (at 3.76Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.306 , 0.347 0.309 , 0.348	Depositor DCC
R_{free} test set	4245 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å ²)	132.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 108.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	18352	wwPDB-VP
Average B, all atoms (Å ²)	136.0	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: HG

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	0.77	12/9338 (0.1%)	1.36	157/12625 (1.2%)
1	B	0.71	3/9338 (0.0%)	1.34	168/12625 (1.3%)
All	All	0.74	15/18676 (0.1%)	1.35	325/25250 (1.3%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	995	ALA	C-O	-7.57	1.17	1.24
1	A	1206	SER	CA-C	-7.47	1.44	1.53
1	A	600	GLY	CA-C	7.47	1.62	1.51
1	A	852	GLN	CA-C	6.94	1.62	1.52
1	A	209	LYS	CA-C	6.74	1.61	1.52

The worst 5 of 325 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	693	PHE	N-CA-C	17.64	132.54	111.02
1	B	292	ASN	N-CA-C	-17.62	92.15	111.36
1	A	292	ASN	N-CA-C	-16.14	91.84	111.69
1	A	573	ARG	N-CA-C	15.15	127.88	111.36
1	B	1020	GLN	N-CA-C	13.67	131.80	111.02

There are no chirality outliers.

There are no planarity outliers.

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	9170	0	9338	2487	1
1	B	9170	0	9337	2367	1
2	A	6	0	0	0	0
2	B	6	0	0	0	0
All	All	18352	0	18675	4841	1

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 131.

The worst 5 of 4841 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:830:ALA:HB2	1:B:990:PHE:CE2	1.25	1.61
1:B:830:ALA:CB	1:B:990:PHE:CE2	2.06	1.36
1:B:830:ALA:CB	1:B:990:PHE:HE2	1.38	1.36
1:B:263:PHE:HE2	1:B:266:GLN:NE2	1.32	1.27
1:A:856:LEU:HD13	1:A:955:PHE:CD1	1.70	1.25

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:GLN:CG	1:B:450:ASP:OD1[1_455]	2.03	0.17

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%)	678 (58%)	299 (25%)	201 (17%)	0 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1178/1284 (92%)	676 (57%)	295 (25%)	207 (18%)	0	2
All	All	2356/2568 (92%)	1354 (58%)	594 (25%)	408 (17%)	0	2

5 of 408 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	SER
1	A	115	THR
1	A	135	ALA
1	A	156	ILE
1	A	164	VAL

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	975/1064 (92%)	757 (78%)	218 (22%)	1	5
1	B	975/1064 (92%)	766 (79%)	209 (21%)	1	6
All	All	1950/2128 (92%)	1523 (78%)	427 (22%)	1	6

5 of 427 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	129	VAL
1	B	412	LYS
1	B	1090	VAL
1	B	158	TRP
1	B	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	383	ASN
1	B	838	ASN

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Mol	Chain	Res	Type
1	B	387	ASN
1	B	625	GLN
1	B	932	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.39	73 (6%) 26 22	36, 127, 195, 207	0
1	B	1182/1284 (92%)	0.35	56 (4%) 36 27	47, 141, 200, 207	0
All	All	2364/2568 (92%)	0.37	129 (5%) 30 23	36, 135, 198, 207	0

The worst 5 of 129 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	299	PHE	7.3
1	B	205	THR	6.5
1	A	1017	TYR	6.4
1	A	207	GLY	5.2
1	A	191	GLN	4.8

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	HG	A	1286	1/1	0.60	0.30	166,166,166,166	1
2	HG	B	1286	1/1	0.80	0.25	109,109,109,109	1
2	HG	A	1290	1/1	0.92	0.06	147,147,147,147	0
2	HG	B	1288	1/1	0.92	0.17	147,147,147,147	0
2	HG	B	1287	1/1	0.94	0.05	147,147,147,147	0
2	HG	A	1288	1/1	0.96	0.07	147,147,147,147	0
2	HG	B	1285	1/1	0.97	0.04	147,147,147,147	0
2	HG	A	1285	1/1	0.97	0.04	147,147,147,147	0
2	HG	A	1289	1/1	0.98	0.06	147,147,147,147	0
2	HG	A	1287	1/1	0.98	0.04	147,147,147,147	0
2	HG	B	1289	1/1	0.98	0.06	147,147,147,147	0
2	HG	B	1290	1/1	0.99	0.03	147,147,147,147	0

6.5 Other polymers [i](#)

There are no such residues in this entry.