



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 05:07 PM UTC

PDB ID : 4KSB / pdb_00004ksb
Title : Structures of P-glycoprotein reveal its conformational flexibility and an epitope on the nucleotide-binding domain
Authors : Ward, A.; Szewczyk, P.; Grimard, V.; Lee, C.-W.; Martinez, L.; Doshi, R.; Caya, A.; Villaluz, M.; Pardon, E.; Cregger, C.; Swartz, D.J.; Falson, P.; Urbatsch, I.; Govaerts, C.; Steyaert, J.; Chang, G.
Deposited on : 2013-05-17
Resolution : 3.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

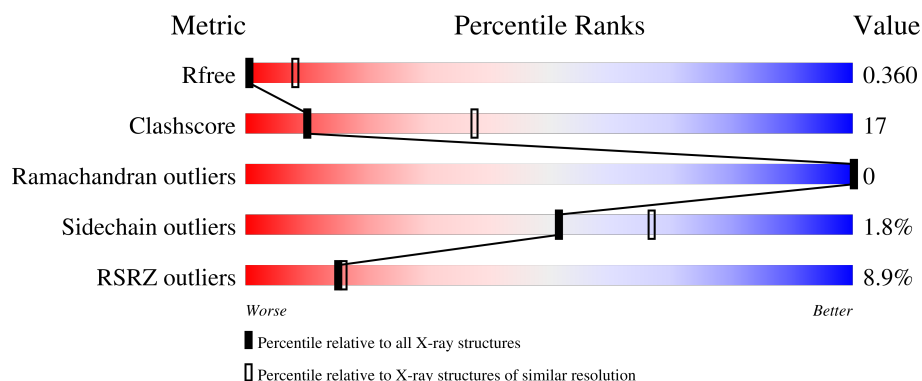
1 Overall quality at a glance

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	8% 59% 32% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9171 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			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	LEU	-	expression tag	UNP P21447
A	1278	GLU	-	expression tag	UNP P21447
A	1279	HIS	-	expression tag	UNP P21447
A	1280	HIS	-	expression tag	UNP P21447
A	1281	HIS	-	expression tag	UNP P21447
A	1282	HIS	-	expression tag	UNP P21447
A	1283	HIS	-	expression tag	UNP P21447
A	1284	HIS	-	expression tag	UNP P21447

LYS ARG SER LEU GLU HIS HIS HIS HIS HIS	A1185	L1186	V1187	R1188	L1193	L1194	L1195	D1196	E1197	S1200	A1201	L1202	D1203	T1204	E1205	S1206	E1207	K1208	V1209	A1213	K1216	A1217	G1220	R1221	V1225	I1226	I1233	Q1234	N1235	A1236	D1237	L1238	I1239	V1240	V1241	G1245	K1246	V1247	Q1259	K1260	G1261	I1262	Y1263	M1266	V1267	S1268	A1271	GLY	ALA		
	E1096	I1097	L1100	N1101	V1102	L1105	R1106	A1107	Q1108	L1109	G1110	Q1114	L1118	F1119	D1120	C1121	I1123	A1124	E1125	N1126	G1130	D1131	N1132	S1137	Y1138	E1139	A1144	I1150	H1151	I1154	D1155	P1158	D1159	K1160	Y1161	G1169	T1170	Q1171	L1172	Q1176	R1179	I1180	A1181	R1184							
	Q1020	K1023	M1026	N1030	V1031	Q1032	F1033	V1037	F1038	N1039	Y1040	P1041	T1042	R1043	P1044	S1045	I1046	P1047	V1048	L1049	Q1050	G1051	L1052	S1053	L1054	E1055	V1056	Q1060	A1063	L1064	V1065	S1068	G1069	C1070	G1071	T1074	V1075	V1076	L1079	E1080	R1081	F1082	Y1083	G1088	S1089	V1090	F1091	L1092	D1093	G1094	
	K1095	E1096	I1097	L1100	N1101	V1102	L1105	R1106	A1107	Q1108	L1109	G1110	Q1114	L1118	F1119	D1120	C1121	I1123	A1124	E1125	N1126	G1130	D1131	N1132	S1137	Y1138	E1139	A1144	I1150	H1151	I1154	D1155	P1158	D1159	K1160	Y1161	G1169	T1170	Q1171	L1172	Q1176	R1179	I1180	A1181	R1184						
	A1185	L1186	V1187	R1188	L1193	L1194	L1195	D1196	E1197	S1200	A1201	L1202	D1203	T1204	E1205	S1206	E1207	K1208	V1209	A1213	K1216	A1217	G1220	R1221	V1225	I1226	I1233	Q1234	N1235	A1236	D1237	L1238	I1239	V1240	V1241	G1245	K1246	V1247	Q1259	K1260	G1261	I1262	Y1263	M1266	V1267	S1268	A1271	GLY	ALA		
	A927	M928	K929	K930	V933	M944	Y949	A950	A951	C952	F953	R954	Y958	T961	Q962	M965	T966	F967	E968	N969	V970	L971	L972	V973	F974	S975	A976	I977	V978	F979	M982	A995	K996	A997	T998	V999	S1000	A1001	S1002	H1003	I1004	I1005	R1006	I1007	I1008	E1009	K1010	T1011	P1012	E1013	I1014
	Q1020	K1023	M1026	N1030	V1031	Q1032	F1033	V1037	F1038	N1039	Y1040	P1041	T1042	R1043	P1044	S1045	I1046	P1047	V1048	L1049	Q1050	G1051	L1052	S1053	L1054	E1055	V1056	Q1060	A1063	L1064	V1065	S1068	G1069	C1070	G1071	T1074	V1075	V1076	L1079	E1080	R1081	F1082	Y1083	G1088	S1089	V1090	F1091	L1092	D1093	G1094	
	K1095	E1096	I1097	L1100	N1101	V1102	L1105	R1106	A1107	Q1108	L1109	G1110	Q1114	L1118	F1119	D1120	C1121	I1123	A1124	E1125	N1126	G1130	D1131	N1132	S1137	Y1138	E1139	A1144	I1150	H1151	I1154	D1155	P1158	D1159	K1160	Y1161	G1169	T1170	Q1171	L1172	Q1176	R1179	I1180	A1181	R1184						
	A1185	L1186	V1187	R1188	L1193	L1194	L1195	D1196	E1197	S1200	A1201	L1202	D1203	T1204	E1205	S1206	E1207	K1208	V1209	A1213	K1216	A1217	G1220	R1221	V1225	I1226	I1233	Q1234	N1235	A1236	D1237	L1238	I1239	V1240	V1241	G1245	K1246	V1247	Q1259	K1260	G1261	I1262	Y1263	M1266	V1267	S1268	A1271	GLY	ALA		
	A927	M928	K929	K930	V933	M944	Y949	A950	A951	C952	F953	R954	Y958	T961	Q962	M965	T966	F967	E968	N969	V970	L971	L972	V973	F974	S975	A976	I977	V978	F979	M982	A995	K996	A997	T998	V999	S1000	A1001	S1002	H1003	I1004	I1005	R1006	I1007	I1008	E1009	K1010	T1011	P1012	E1013	I1014

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.40Å 138.65Å 185.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.56 – 3.80 92.56 – 3.80	Depositor EDS
% Data completeness (in resolution range)	95.3 (92.56-3.80) 95.3 (92.56-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.90 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), CNS	Depositor
R, R_{free}	0.323 , 0.357 0.326 , 0.360	Depositor DCC
R_{free} test set	1062 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	97.0	Xtriage
Anisotropy	0.442	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 134.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.12$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.72	EDS
Total number of atoms	9171	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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](#)

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	0.35	0/9339	0.85	16/12626 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	689	PRO	N-CA-C	7.88	120.31	110.70
1	A	1071	GLY	N-CA-C	-7.62	103.92	114.67
1	A	367	ASN	CB-CA-C	-6.71	107.03	115.89
1	A	166	GLU	N-CA-C	-6.25	104.36	112.23
1	A	1043	ARG	CA-C-N	-6.13	115.45	121.65
1	A	1043	ARG	C-N-CA	-6.13	115.45	121.65
1	A	740	PRO	CA-C-N	-5.67	114.42	120.03
1	A	740	PRO	C-N-CA	-5.67	114.42	120.03
1	A	515	GLN	CB-CA-C	-5.65	110.04	116.54
1	A	162	HIS	CB-CA-C	-5.54	109.19	115.79
1	A	377	SER	CB-CA-C	-5.45	110.27	116.54
1	A	376	LYS	N-CA-C	5.08	117.14	109.41
1	A	163	ASP	N-CA-C	5.08	119.75	113.50
1	A	1046	ILE	CA-C-N	5.03	125.03	119.90
1	A	1046	ILE	C-N-CA	5.03	125.03	119.90
1	A	427	CYS	CB-CA-C	-5.02	109.81	115.79

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	9171	0	9344	318	0
All	All	9171	0	9344	318	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 17.

All (318) 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:704:TRP:CZ2	1:A:707:PHE:HB2	1.48	1.45
1:A:310:PHE:CD2	1:A:332:PHE:CZ	2.30	1.20
1:A:306:TYR:CE1	1:A:332:PHE:CE2	2.31	1.18
1:A:704:TRP:CZ2	1:A:707:PHE:CB	2.31	1.14
1:A:310:PHE:CE2	1:A:332:PHE:CZ	2.38	1.11
1:A:310:PHE:CD2	1:A:332:PHE:HZ	1.64	1.10
1:A:704:TRP:CE2	1:A:707:PHE:HB2	1.89	1.07
1:A:306:TYR:CE1	1:A:332:PHE:HE2	1.70	1.06
1:A:704:TRP:NE1	1:A:707:PHE:CD2	2.28	1.02
1:A:306:TYR:CE1	1:A:332:PHE:CD2	2.50	0.99
1:A:704:TRP:HZ2	1:A:707:PHE:CB	1.74	0.96
1:A:310:PHE:HD2	1:A:332:PHE:HZ	1.05	0.94
1:A:1020:GLN:HG3	1:A:1100:LEU:HD12	1.60	0.82
1:A:306:TYR:CZ	1:A:332:PHE:HE2	1.97	0.81
1:A:704:TRP:NE1	1:A:707:PHE:HD2	1.79	0.80
1:A:369:PRO:O	1:A:371:ILE:HG23	1.82	0.80
1:A:306:TYR:CZ	1:A:332:PHE:CE2	2.70	0.80
1:A:396:SER:HB2	1:A:404:GLN:HG3	1.62	0.80
1:A:38:MET:HA	1:A:41:TYR:HB3	1.65	0.79
1:A:35:VAL:HB	1:A:355:ARG:HE	1.48	0.78
1:A:416:GLY:H	1:A:577:THR:HG22	1.49	0.77
1:A:326:GLN:O	1:A:330:VAL:HG23	1.84	0.77
1:A:1033:PHE:HB2	1:A:1054:LEU:H	1.52	0.74
1:A:306:TYR:HE1	1:A:332:PHE:CD2	2.03	0.74
1:A:958:TYR:O	1:A:962:GLN:N	2.20	0.74
1:A:328:LEU:O	1:A:332:PHE:HD1	1.70	0.74
1:A:310:PHE:CE2	1:A:332:PHE:CE1	2.75	0.74
1:A:820:GLN:HB3	1:A:997:ALA:HA	1.70	0.73
1:A:704:TRP:HZ2	1:A:707:PHE:HB3	1.54	0.72
1:A:328:LEU:O	1:A:332:PHE:CD1	2.41	0.72
1:A:370:SER:O	1:A:371:ILE:HG12	1.91	0.70
1:A:488:ARG:HE	1:A:542:VAL:HG12	1.56	0.70
1:A:306:TYR:HE1	1:A:332:PHE:HD2	1.36	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:VAL:HA	1:A:330:VAL:HB	1.74	0.69
1:A:1090:VAL:HG13	1:A:1097:ILE:HB	1.73	0.69
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.74	0.69
1:A:263:PHE:HA	1:A:1188:ARG:HH12	1.57	0.69
1:A:306:TYR:CD1	1:A:332:PHE:CE2	2.82	0.68
1:A:243:TYR:O	1:A:247:GLY:N	2.27	0.67
1:A:310:PHE:HE2	1:A:332:PHE:CZ	2.07	0.67
1:A:370:SER:O	1:A:371:ILE:CG1	2.42	0.67
1:A:228:TRP:HZ2	1:A:295:MET:HB2	1.60	0.67
1:A:969:ASN:H	1:A:972:LEU:HD13	1.59	0.67
1:A:131:PHE:HE2	1:A:186:ILE:HB	1.60	0.66
1:A:82:GLY:HA3	1:A:737:ASN:HA	1.77	0.66
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.78	0.65
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.78	0.65
1:A:214:ILE:HG23	1:A:335:LEU:HD21	1.79	0.65
1:A:687:ASP:H	1:A:813:ARG:HH22	1.45	0.65
1:A:81:VAL:HG13	1:A:99:MET:HB3	1.80	0.64
1:A:132:TRP:HB2	1:A:184:ASP:HB3	1.79	0.64
1:A:306:TYR:CD1	1:A:332:PHE:HE2	2.14	0.64
1:A:724:PHE:HB2	1:A:758:LEU:HD11	1.79	0.63
1:A:258:ARG:NH2	1:A:801:ASP:O	2.31	0.63
1:A:486:TYR:HB3	1:A:908:ARG:HD3	1.80	0.63
1:A:463:ARG:O	1:A:543:ARG:NH2	2.32	0.63
1:A:310:PHE:HD2	1:A:332:PHE:CZ	1.91	0.62
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.81	0.62
1:A:901:ARG:O	1:A:904:VAL:HG12	2.00	0.62
1:A:163:ASP:HB3	1:A:166:GLU:HB2	1.81	0.61
1:A:706:TYR:O	1:A:707:PHE:CD2	2.54	0.61
1:A:421:LEU:HB2	1:A:581:ILE:HG13	1.83	0.61
1:A:300:LEU:HD22	1:A:759:GLY:HA2	1.83	0.61
1:A:493:MET:HA	1:A:496:ILE:HB	1.83	0.61
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.66	0.60
1:A:362:PHE:HA	1:A:365:ILE:HB	1.84	0.60
1:A:756:LEU:HA	1:A:760:ILE:HD13	1.84	0.60
1:A:382:ASP:O	1:A:384:ILE:HG12	2.02	0.59
1:A:193:MET:HA	1:A:196:PHE:HB3	1.84	0.59
1:A:1048:VAL:HG23	1:A:1049:LEU:HD22	1.85	0.59
1:A:92:SER:OG	1:A:96:LYS:NZ	2.35	0.59
1:A:267:LYS:HA	1:A:270:LEU:HD22	1.84	0.58
1:A:484:ILE:HG21	1:A:496:ILE:HG13	1.85	0.58
1:A:156:ILE:HG12	1:A:439:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:GLU:HB2	1:A:448:SER:HB3	1.86	0.58
1:A:153:ASN:ND2	1:A:368:LYS:HB3	2.19	0.58
1:A:481:ALA:HB2	1:A:516:PHE:HB3	1.86	0.57
1:A:270:LEU:HG	1:A:790:LYS:HD2	1.85	0.57
1:A:787:MET:HE2	1:A:1008:ILE:HD11	1.86	0.56
1:A:1023:LYS:N	1:A:1026:MET:SD	2.76	0.56
1:A:374:PHE:HD1	1:A:376:LYS:H	1.53	0.56
1:A:714:ALA:HB1	1:A:833:PHE:HB2	1.87	0.56
1:A:421:LEU:HD22	1:A:581:ILE:HD11	1.86	0.56
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.39	0.56
1:A:132:TRP:HE3	1:A:184:ASP:H	1.53	0.56
1:A:527:LEU:H	1:A:527:LEU:HD23	1.71	0.55
1:A:131:PHE:CE2	1:A:186:ILE:HB	2.41	0.55
1:A:796:ASP:OD1	1:A:796:ASP:N	2.36	0.55
1:A:1014:ILE:HB	1:A:1102:VAL:HG11	1.89	0.54
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.88	0.54
1:A:453:ASP:OD1	1:A:454:ILE:N	2.41	0.54
1:A:845:ILE:HG23	1:A:972:LEU:HD23	1.90	0.54
1:A:796:ASP:HA	1:A:800:PHE:HD2	1.73	0.54
1:A:1110:GLY:HA3	1:A:1193:LEU:HA	1.89	0.54
1:A:44:TRP:HD1	1:A:45:LEU:HD12	1.72	0.54
1:A:310:PHE:CD2	1:A:332:PHE:CE1	2.92	0.54
1:A:1014:ILE:HD12	1:A:1102:VAL:HG21	1.89	0.54
1:A:1118:LEU:HD21	1:A:1180:ILE:HD12	1.90	0.54
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.90	0.54
1:A:798:SER:OG	1:A:1041:PRO:HG2	2.07	0.53
1:A:970:VAL:HG23	1:A:971:LEU:HD22	1.89	0.53
1:A:1023:LYS:HB2	1:A:1026:MET:HG3	1.89	0.53
1:A:961:THR:HA	1:A:965:MET:HB2	1.90	0.53
1:A:1114:GLN:HG2	1:A:1197:GLU:HB2	1.90	0.53
1:A:463:ARG:HH12	1:A:903:VAL:HG22	1.73	0.53
1:A:1010:LYS:HG2	1:A:1011:THR:H	1.73	0.53
1:A:1122:SER:HB3	1:A:1125:GLU:HG2	1.89	0.53
1:A:1040:TYR:O	1:A:1042:THR:N	2.39	0.53
1:A:1037:VAL:HG12	1:A:1050:GLN:HA	1.91	0.53
1:A:1123:ILE:HD11	1:A:1161:TYR:HA	1.91	0.53
1:A:469:VAL:HG13	1:A:533:GLN:NE2	2.24	0.52
1:A:1038:PHE:HD2	1:A:1049:LEU:HD23	1.74	0.52
1:A:437:GLN:HB2	1:A:439:LEU:HD23	1.90	0.52
1:A:845:ILE:O	1:A:848:ILE:HG12	2.10	0.52
1:A:923:PRO:O	1:A:927:ALA:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.91	0.52
1:A:715:ILE:HD12	1:A:836:ILE:HG13	1.93	0.51
1:A:1079:LEU:HD23	1:A:1194:LEU:HD11	1.92	0.51
1:A:786:TYR:O	1:A:790:LYS:HG2	2.09	0.51
1:A:419:VAL:HG13	1:A:579:ILE:HG13	1.92	0.51
1:A:346:PRO:O	1:A:350:ALA:N	2.39	0.51
1:A:856:LEU:O	1:A:860:ILE:HG12	2.11	0.51
1:A:390:PHE:CD1	1:A:447:VAL:HG23	2.45	0.51
1:A:193:MET:O	1:A:197:PHE:N	2.42	0.51
1:A:1235:ASN:OD1	1:A:1235:ASN:N	2.43	0.51
1:A:471:GLN:N	1:A:471:GLN:OE1	2.43	0.51
1:A:1176:GLN:OE1	1:A:1176:GLN:N	2.39	0.51
1:A:356:GLY:HA2	1:A:359:TYR:CE2	2.46	0.51
1:A:438:ARG:CZ	1:A:455:ARG:HA	2.41	0.50
1:A:370:SER:C	1:A:371:ILE:HG12	2.36	0.50
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	1.92	0.50
1:A:334:VAL:O	1:A:338:ALA:N	2.45	0.50
1:A:486:TYR:HB3	1:A:908:ARG:HH21	1.76	0.50
1:A:824:ALA:HB2	1:A:997:ALA:HB1	1.93	0.50
1:A:421:LEU:HB2	1:A:581:ILE:CG1	2.42	0.50
1:A:949:TYR:HD1	1:A:953:PHE:HE2	1.59	0.50
1:A:1039:ASN:HD22	1:A:1047:PRO:HG3	1.77	0.50
1:A:44:TRP:CD1	1:A:45:LEU:HD12	2.47	0.50
1:A:235:PHE:HB3	1:A:287:LYS:HE2	1.93	0.50
1:A:1202:LEU:HB3	1:A:1207:GLU:HG2	1.94	0.49
1:A:722:PRO:HG2	1:A:841:THR:HB	1.94	0.49
1:A:310:PHE:O	1:A:314:THR:N	2.37	0.49
1:A:1049:LEU:HD12	1:A:1052:LEU:HD22	1.94	0.49
1:A:219:PRO:O	1:A:223:LEU:N	2.45	0.49
1:A:83:ASN:HA	1:A:738:GLY:O	2.13	0.49
1:A:711:ILE:HD11	1:A:832:ILE:HG21	1.94	0.49
1:A:846:SER:HB3	1:A:854:THR:HG23	1.94	0.49
1:A:999:VAL:HG12	1:A:1003:HIS:NE2	2.28	0.49
1:A:1039:ASN:ND2	1:A:1045:SER:OG	2.45	0.49
1:A:192:ALA:O	1:A:195:THR:OG1	2.27	0.49
1:A:478:THR:OG1	1:A:483:ASN:OD1	2.31	0.49
1:A:843:ILE:O	1:A:847:LEU:N	2.45	0.49
1:A:603:VAL:HG23	1:A:604:GLU:H	1.77	0.49
1:A:211:THR:HG23	1:A:331:PHE:HE2	1.78	0.49
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.76	0.49
1:A:550:LEU:HD23	1:A:569:LEU:HD13	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ILE:HG22	1:A:384:ILE:O	2.13	0.48
1:A:1043:ARG:HB3	1:A:1044:PRO:HD3	1.96	0.48
1:A:1049:LEU:HD21	1:A:1074:THR:OG1	2.13	0.48
1:A:1071:GLY:HA2	1:A:1074:THR:OG1	2.14	0.48
1:A:132:TRP:HD1	1:A:133:CYS:SG	2.37	0.48
1:A:864:ILE:HG22	1:A:944:MET:HB3	1.95	0.48
1:A:318:ILE:HD13	1:A:744:GLN:HA	1.94	0.48
1:A:1181:ALA:HA	1:A:1184:ARG:HE	1.78	0.48
1:A:999:VAL:HG12	1:A:1003:HIS:HE2	1.78	0.48
1:A:433:VAL:CG2	1:A:581:ILE:HD13	2.43	0.48
1:A:463:ARG:NH1	1:A:903:VAL:O	2.46	0.48
1:A:686:GLU:HB3	1:A:813:ARG:HH22	1.79	0.48
1:A:1002:SER:O	1:A:1006:ARG:NE	2.42	0.48
1:A:155:GLU:OE1	1:A:373:SER:OG	2.29	0.47
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.78	0.47
1:A:466:ILE:HG23	1:A:549:LEU:HD13	1.95	0.47
1:A:696:ILE:HG13	1:A:697:LEU:H	1.78	0.47
1:A:773:PHE:HB3	1:A:829:LEU:HD22	1.97	0.47
1:A:906:LEU:HG	1:A:909:GLU:HG3	1.96	0.47
1:A:148:PHE:HB3	1:A:913:GLU:OE2	2.15	0.47
1:A:499:ALA:HA	1:A:541:LEU:HD23	1.97	0.47
1:A:856:LEU:HD21	1:A:951:ALA:HB1	1.97	0.47
1:A:886:LEU:O	1:A:890:GLY:N	2.45	0.47
1:A:257:ILE:HG12	1:A:800:PHE:CD1	2.50	0.47
1:A:979:PHE:HA	1:A:982:MET:HG2	1.97	0.47
1:A:861:VAL:HB	1:A:862:PRO:HD3	1.97	0.46
1:A:1155:ASP:O	1:A:1160:LYS:NZ	2.48	0.46
1:A:1213:ALA:O	1:A:1217:ALA:N	2.48	0.46
1:A:65:PRO:O	1:A:69:LEU:N	2.49	0.46
1:A:327:VAL:O	1:A:331:PHE:N	2.36	0.46
1:A:700:ASN:O	1:A:704:TRP:N	2.48	0.46
1:A:703:GLU:O	1:A:705:PRO:HD3	2.15	0.46
1:A:715:ILE:HD11	1:A:832:ILE:HG22	1.97	0.46
1:A:1241:VAL:HG21	1:A:1263:TYR:HB2	1.98	0.46
1:A:923:PRO:HA	1:A:926:ASN:HB3	1.98	0.46
1:A:132:TRP:HA	1:A:183:GLY:HA2	1.98	0.46
1:A:846:SER:HA	1:A:849:TYR:CE2	2.51	0.46
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.80	0.46
1:A:464:GLU:HA	1:A:543:ARG:HE	1.81	0.46
1:A:1107:ALA:O	1:A:1188:ARG:HD3	2.16	0.46
1:A:105:GLU:O	1:A:109:THR:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:MET:HB3	1:A:1008:ILE:HD11	1.97	0.46
1:A:1158:PRO:C	1:A:1160:LYS:H	2.24	0.46
1:A:429:LYS:O	1:A:432:THR:OG1	2.25	0.46
1:A:603:VAL:HG23	1:A:604:GLU:N	2.30	0.46
1:A:184:ASP:O	1:A:188:MET:N	2.36	0.45
1:A:1093:ASP:HB3	1:A:1095:LYS:HD3	1.96	0.45
1:A:33:VAL:HG23	1:A:34:SER:H	1.80	0.45
1:A:1100:LEU:HD23	1:A:1105:LEU:HB2	1.98	0.45
1:A:454:ILE:HD11	1:A:462:LEU:HD21	1.97	0.45
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.41	0.45
1:A:359:TYR:HA	1:A:362:PHE:HB2	1.99	0.45
1:A:1053:SER:O	1:A:1054:LEU:HD13	2.17	0.45
1:A:71:PHE:CE2	1:A:329:THR:HG21	2.51	0.45
1:A:158:TRP:HB2	1:A:164:VAL:HG12	1.99	0.45
1:A:333:SER:O	1:A:337:GLY:N	2.43	0.45
1:A:797:VAL:O	1:A:797:VAL:HG13	2.16	0.45
1:A:1197:GLU:HB3	1:A:1200:SER:HB2	1.99	0.45
1:A:486:TYR:CG	1:A:908:ARG:HD3	2.51	0.45
1:A:125:ALA:HA	1:A:128:GLN:HE21	1.82	0.45
1:A:295:MET:HG2	1:A:766:PHE:CZ	2.52	0.45
1:A:529:GLY:HA2	1:A:532:LYS:HD3	1.99	0.45
1:A:784:LEU:O	1:A:788:VAL:HG23	2.17	0.45
1:A:806:THR:HG23	1:A:809:ALA:H	1.82	0.45
1:A:1011:THR:HG23	1:A:1011:THR:O	2.15	0.45
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.51	0.44
1:A:461:TYR:O	1:A:465:ILE:HG12	2.17	0.44
1:A:704:TRP:CD1	1:A:707:PHE:CD2	3.03	0.44
1:A:534:ARG:HA	1:A:537:ILE:HD12	1.99	0.44
1:A:930:LYS:HA	1:A:933:VAL:HB	1.99	0.44
1:A:842:GLY:O	1:A:846:SER:N	2.40	0.44
1:A:196:PHE:O	1:A:200:PHE:HD1	2.01	0.44
1:A:429:LYS:HE2	1:A:429:LYS:HB2	1.77	0.44
1:A:1000:SER:HA	1:A:1003:HIS:CD2	2.53	0.44
1:A:289:ILE:O	1:A:293:ILE:HG13	2.17	0.44
1:A:590:ASN:OD1	1:A:590:ASN:N	2.42	0.44
1:A:622:VAL:O	1:A:626:THR:N	2.51	0.44
1:A:892:ILE:O	1:A:916:TYR:OH	2.32	0.44
1:A:1123:ILE:HA	1:A:1126:ASN:HB2	1.98	0.44
1:A:727:ILE:O	1:A:731:VAL:HG23	2.18	0.43
1:A:958:TYR:N	1:A:961:THR:HB	2.33	0.43
1:A:1150:ILE:HD13	1:A:1179:ARG:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:THR:O	1:A:332:PHE:HB2	2.18	0.43
1:A:1120:ASP:OD1	1:A:1120:ASP:N	2.45	0.43
1:A:711:ILE:O	1:A:715:ILE:HG12	2.18	0.43
1:A:93:GLU:OE1	1:A:93:GLU:N	2.51	0.43
1:A:133:CYS:O	1:A:137:GLY:N	2.36	0.43
1:A:486:TYR:O	1:A:908:ARG:NH2	2.52	0.43
1:A:721:GLN:HB3	1:A:722:PRO:HD3	1.99	0.43
1:A:156:ILE:H	1:A:156:ILE:HD12	1.83	0.43
1:A:775:LYS:HA	1:A:778:GLU:HB3	2.01	0.43
1:A:125:ALA:O	1:A:129:VAL:HG23	2.18	0.43
1:A:704:TRP:CE2	1:A:707:PHE:CB	2.81	0.43
1:A:1139:GLU:CD	1:A:1139:GLU:H	2.27	0.43
1:A:327:VAL:HB	1:A:331:PHE:CE1	2.54	0.43
1:A:414:LYS:H	1:A:414:LYS:HD2	1.84	0.43
1:A:253:VAL:O	1:A:257:ILE:N	2.52	0.42
1:A:373:SER:OG	1:A:374:PHE:N	2.52	0.42
1:A:976:ALA:HA	1:A:979:PHE:CD2	2.53	0.42
1:A:252:GLU:O	1:A:256:ALA:N	2.50	0.42
1:A:543:ARG:NH2	1:A:905:SER:HA	2.34	0.42
1:A:969:ASN:O	1:A:973:VAL:HG23	2.19	0.42
1:A:217:ILE:HG21	1:A:305:SER:HB2	2.00	0.42
1:A:704:TRP:CD1	1:A:707:PHE:HD2	2.35	0.42
1:A:1005:ILE:O	1:A:1009:GLU:HG2	2.20	0.42
1:A:1010:LYS:HD2	1:A:1012:PRO:HA	2.00	0.42
1:A:1137:SER:OG	1:A:1139:GLU:OE2	2.36	0.42
1:A:43:GLY:HA3	1:A:46:ASP:HB2	2.02	0.42
1:A:381:PRO:HG2	1:A:461:TYR:CE2	2.54	0.42
1:A:698:LYS:O	1:A:702:THR:OG1	2.26	0.42
1:A:744:GLN:O	1:A:748:SER:OG	2.30	0.42
1:A:828:ARG:O	1:A:832:ILE:HG12	2.19	0.42
1:A:1216:LYS:HA	1:A:1216:LYS:HD3	1.84	0.42
1:A:366:ASP:CG	1:A:367:ASN:H	2.28	0.42
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.50	0.42
1:A:922:ILE:HB	1:A:923:PRO:HD3	2.00	0.42
1:A:1220:GLY:O	1:A:1221:ARG:NH1	2.48	0.42
1:A:370:SER:OG	1:A:371:ILE:N	2.53	0.42
1:A:824:ALA:O	1:A:828:ARG:HG2	2.20	0.42
1:A:140:ILE:HG13	1:A:179:ASN:ND2	2.34	0.42
1:A:268:LYS:O	1:A:272:ARG:HG3	2.20	0.42
1:A:332:PHE:O	1:A:335:LEU:HB2	2.20	0.42
1:A:370:SER:C	1:A:371:ILE:CG1	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LYS:HA	1:A:270:LEU:HB2	2.01	0.42
1:A:361:VAL:O	1:A:365:ILE:HG13	2.20	0.42
1:A:156:ILE:HG22	1:A:160:ASP:OD1	2.20	0.42
1:A:171:LEU:O	1:A:175:VAL:HG13	2.20	0.42
1:A:427:CYS:C	1:A:429:LYS:H	2.28	0.41
1:A:486:TYR:CB	1:A:908:ARG:HD3	2.47	0.41
1:A:33:VAL:HG23	1:A:34:SER:N	2.35	0.41
1:A:107:MET:HE1	1:A:954:ARG:HG2	2.02	0.41
1:A:1202:LEU:HD23	1:A:1207:GLU:HA	2.01	0.41
1:A:761:ILE:O	1:A:765:THR:HG22	2.20	0.41
1:A:975:SER:O	1:A:978:VAL:HG12	2.21	0.41
1:A:109:THR:HB	1:A:113:TYR:CZ	2.55	0.41
1:A:132:TRP:HE3	1:A:184:ASP:N	2.16	0.41
1:A:848:ILE:HD11	1:A:972:LEU:HD21	2.03	0.41
1:A:924:TYR:O	1:A:928:MET:HG3	2.20	0.41
1:A:1005:ILE:O	1:A:1008:ILE:HG22	2.20	0.41
1:A:88:SER:OG	1:A:89:THR:N	2.52	0.41
1:A:724:PHE:HB2	1:A:758:LEU:HD21	2.03	0.41
1:A:1060:GLN:HB2	1:A:1237:ASP:CG	2.44	0.41
1:A:1233:ILE:HD12	1:A:1233:ILE:HA	1.91	0.41
1:A:1259:GLN:HG3	1:A:1260:LYS:H	1.85	0.41
1:A:1080:GLU:OE2	1:A:1109:LEU:HD13	2.21	0.41
1:A:180:GLU:O	1:A:185:LYS:HG3	2.21	0.41
1:A:552:GLU:OE2	1:A:583:HIS:NE2	2.49	0.41
1:A:83:ASN:O	1:A:87:ASN:HB2	2.20	0.41
1:A:1026:MET:HA	1:A:1093:ASP:CG	2.46	0.41
1:A:374:PHE:HD1	1:A:376:LYS:N	2.17	0.40
1:A:533:GLN:O	1:A:537:ILE:HG13	2.21	0.40
1:A:722:PRO:O	1:A:726:VAL:N	2.51	0.40
1:A:377:SER:O	1:A:458:ASN:ND2	2.53	0.40
1:A:686:GLU:HB3	1:A:813:ARG:NH2	2.35	0.40
1:A:704:TRP:NE1	1:A:707:PHE:HB2	2.32	0.40
1:A:1262:ILE:O	1:A:1266:MET:HG2	2.21	0.40
1:A:214:ILE:HG23	1:A:335:LEU:CD2	2.51	0.40
1:A:358:ALA:O	1:A:362:PHE:HB2	2.21	0.40
1:A:1068:SER:OG	1:A:1069:GLY:N	2.54	0.40
1:A:249:VAL:HG13	1:A:272:ARG:HH21	1.87	0.40
1:A:486:TYR:HB3	1:A:908:ARG:NH2	2.36	0.40
1:A:768:LEU:O	1:A:772:THR:HG23	2.21	0.40

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	1178/1284 (92%)	1074 (91%)	104 (9%)	0	100	100

There are no Ramachandran outliers to report.

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%)	958 (98%)	18 (2%)	51	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	58	ILE
1	A	64	LEU
1	A	409	LEU
1	A	509	ILE
1	A	581	ILE
1	A	593	VAL
1	A	601	VAL
1	A	696	ILE
1	A	796	ASP
1	A	847	LEU
1	A	961	THR
1	A	1056	VAL

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Mol	Chain	Res	Type
1	A	1064	LEU
1	A	1065	VAL
1	A	1225	VAL
1	A	1235	ASN
1	A	1247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	153	ASN
1	A	179	ASN
1	A	274	ASN
1	A	326	GLN
1	A	749	ASN
1	A	820	GLN
1	A	835	ASN
1	A	899	ASN
1	A	942	GLN
1	A	969	ASN
1	A	1003	HIS
1	A	1114	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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

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%)	0.77	105 (8%)	15 16	40, 103, 150, 183	0

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	852	GLN	11.8
1	A	574	GLU	5.6
1	A	306	TYR	5.0
1	A	329	THR	4.6
1	A	974	PHE	4.4
1	A	598	ASP	3.9
1	A	1033	PHE	3.8
1	A	336	ILE	3.7
1	A	704	TRP	3.6
1	A	1132	ASN	3.6
1	A	386	GLY	3.6
1	A	828	ARG	3.6
1	A	970	VAL	3.5
1	A	1055	GLU	3.5
1	A	213	VAL	3.5
1	A	162	HIS	3.5
1	A	579	ILE	3.4
1	A	1125	GLU	3.4
1	A	316	LEU	3.3
1	A	747	ASN	3.1
1	A	1169	GLY	3.0
1	A	549	LEU	3.0
1	A	167	LEU	2.9
1	A	299	PHE	2.9
1	A	1083	TYR	2.9
1	A	837	ALA	2.9
1	A	327	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLN	2.8
1	A	240	LEU	2.8
1	A	577	THR	2.8
1	A	335	LEU	2.8
1	A	548	LEU	2.8
1	A	35	VAL	2.8
1	A	303	TYR	2.8
1	A	547	ILE	2.7
1	A	170	ARG	2.7
1	A	171	LEU	2.7
1	A	576	ARG	2.7
1	A	1171	GLN	2.7
1	A	850	GLY	2.7
1	A	848	ILE	2.7
1	A	272	ARG	2.6
1	A	707	PHE	2.6
1	A	312	TYR	2.6
1	A	688	VAL	2.6
1	A	691	ALA	2.6
1	A	332	PHE	2.5
1	A	1088	GLY	2.5
1	A	742	GLU	2.5
1	A	1172	LEU	2.5
1	A	1082	PHE	2.5
1	A	328	LEU	2.5
1	A	268	LYS	2.5
1	A	709	VAL	2.5
1	A	1080	GLU	2.5
1	A	302	ILE	2.5
1	A	853	LEU	2.5
1	A	732	VAL	2.5
1	A	977	ILE	2.4
1	A	851	TRP	2.4
1	A	68	MET	2.4
1	A	366	ASP	2.4
1	A	116	GLY	2.4
1	A	580	VAL	2.4
1	A	1054	LEU	2.4
1	A	1130	GLY	2.4
1	A	502	GLU	2.4
1	A	63	ALA	2.4
1	A	573	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	900	PHE	2.3
1	A	575	GLY	2.3
1	A	842	GLY	2.3
1	A	163	ASP	2.3
1	A	581	ILE	2.3
1	A	266	GLN	2.3
1	A	529	GLY	2.3
1	A	908	ARG	2.3
1	A	706	TYR	2.2
1	A	416	GLY	2.2
1	A	1030	ASN	2.2
1	A	166	GLU	2.2
1	A	1268	SER	2.2
1	A	265	GLY	2.2
1	A	101	ALA	2.1
1	A	1131	ASP	2.1
1	A	570	ASP	2.1
1	A	916	TYR	2.1
1	A	784	LEU	2.1
1	A	966	THR	2.1
1	A	1240	VAL	2.1
1	A	801	ASP	2.1
1	A	467	GLY	2.1
1	A	293	ILE	2.1
1	A	969	ASN	2.1
1	A	81	VAL	2.1
1	A	165	GLY	2.1
1	A	135	ALA	2.1
1	A	995	ALA	2.1
1	A	221	LEU	2.1
1	A	1044	PRO	2.0
1	A	1262	ILE	2.0
1	A	968	GLU	2.0
1	A	71	PHE	2.0
1	A	36	LEU	2.0
1	A	703	GLU	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.