



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:44 am BST

PDB ID : 4KSC  
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 : 4.00 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](mailto: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.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

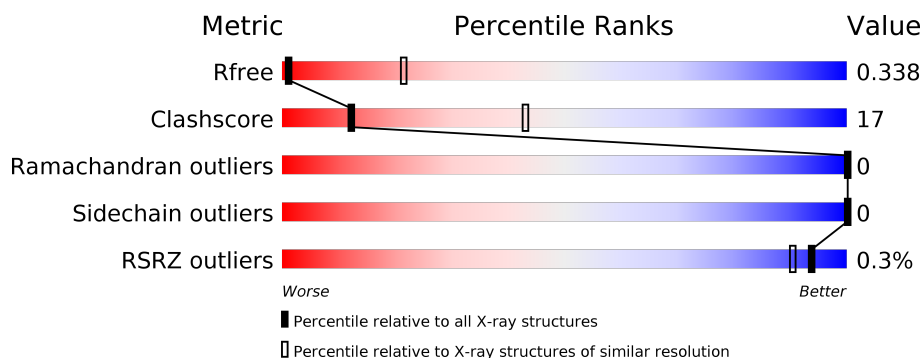
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 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))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

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  $\geq 3$ , 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	<div> <div style="width: 61%; background-color: green;"></div> <div style="width: 31%; background-color: yellow;"></div> <div style="width: 8%; background-color: grey;"></div> </div> <div>61% 31% 8%</div>

## 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



- Molecule 1: Multidrug resistance protein 1A

K930	L829	I711	ALA	V500	L388	L300	T195	M87	MET
V933	A830	F712	CYS	CYS	E389	L301	F196	S88	GLU
F934	V831	C713	LYS	N504	F390		F197	LEU	
	I832	A714	SER	A505		S305			GLU
A943	R833	I715	LYS	Y506	S396	Y306	R206	S92	GLU
M944	Q834	I716	ASP		T397				ASP
	N835	M717	GLU	I509	P398	F310	T211	K96	LEU
	I836		ILE				L212		LYS
Y949	Q721	Q721	ASP	L527	Q404	T314	V213	M99	GLY
G940	F722	F722	ASN			S315	I214		ARG
T941	A723	A723	LEU	Q533	V413	L316	I215	A111	ALA
G952	F724	F724	ASP	R534	K414	F317	A216		ASP
			MET		S415	I318	I217	Y114	LYS
R844			SER	I537	G416		S319		ASN
I845	Q744	Q744	SER	A538		K320	P219	G118	PHE
			SER		V419				SER
I848	F755	F755	LYS		V420	Q326	S224	V121	LYS
T861	L756	L756	ASP	V642	L421	V327		L122	MET
Q962	I757	I757	SER	R543	V422		W228		GLY
	L857	L758	GLY	N544	Q423	V330	A229	A125	
M965		G759	SER	P545	M424	F331	K230		LYS
R969	I860	I760	SER			F332	SER	Q128	LYS
V970	I761	I761	LEU	L549	K429	S333	I231	V129	LYS
P862	S762	S762	ILE			V334			LYS
L863			ARG	E552	T432	L335	S234	S130	LYS
L972	T765	T765	ARG		V433		P235	F131	GLU
V973	F766	F766	ARG	E574		I336	E239	W132	LYS
	F767	F767	SER			G337		C133	LYS
			SER			A338			GLU
F979	L768	L768	THR	T577	Q437		A242	Q139	LYS
	Q769	Q769	ARG	T578	K438	F346	Y243	I140	LYS
M982			LYS	I579	L439				
			SER	V580	V447	R347	G247	F147	ALA
D993	F772	F772	ILE	A582	S448	I348		F148	
			CYS			E349			
	K782	K782	GLY		D453	A350	E252		V33
A997	R783	R783	PRO	N590			M153	M153	S34
T998	L784	L784	HIS		L454			Q154	V35
V999	R785	R785	ASP	G596		R355	A256	E155	M38
S1000	F792	F792	HIS	F597	G356	G356	R258	I156	F39
H1003	V903	V786	GLN	D598	Y461	A357	G157	G157	R40
I1004	V904	V788	ASP		L462	A358	W158	Y41	Y41
I1005	S905	V789	ARG		R463	Y359	K267	K267	L42
			LYS	V603			K268		G43
I1008	K790	K790	LEU	E604	I466	F362	E269	D163	
E1009	S791	S791	SER		G467		L270	W44	G43
E1010	M792	M792	THR	L611	V468	I365	E271	E166	L45
K1010	L793	L793	LYS		V469		R272		D46
T1011	R794	R794	GLY	Y618	S470	K368	L277	R170	R47
P1012	Q795	Q795	ALA		Q471	P369	E278	M179	Y49
	D796	D796	L684	V622		S370		E180	P50
Q1020	V797	V797			E482	I371	L283		V52
			D687	T626	M483	D372	L51	G183	
K1023	F800	F800	ALA		I484	S373	K287	D184	
	D801	D801	GLY	ASN	V486	S375	A288	K185	P65
M1026			L697		K487	K376	I289		
				GLU	R488				

R1229		Y1129	Y1040
T1232		S1137	P1041
T1233		Y1138	T1042
<b>Q1234</b>		<b>E1139</b>	R1043
N1235		E1140	P1044
<b>A1236</b>		<b>I1141</b>	<b>S1045</b>
<b>A1237</b>		V1142	T1046
<b>L1238</b>		R1143	V1048
T1239		<b>A1144</b>	L1049
V1240			Q1050
V1241		H1151	G1051
V1242			L1052
<b>Q1243</b>		<b>I1154</b>	S1053
N1244			L1054
G1245		P1158	K1058
K1246		D1159	G1059
K1260		K1160	Q1060
G1261		Y1161	T1061
T1262			L1062
Y1263		Q1176	A1063
		I1180	
<b>M1266</b>		A1181	S1068
			G1069
<b>A1271</b>		R1184	
GLY		A1185	T1074
ALA		L1186	V1075
LYS		V1187	V1076
ARG		R1188	Q1077
SER			L1078
LEU		H1191	L1079
GLU		L1192	
HIS		L1193	V1090
HIS		L1194	F1091
HIS		L1195	L1092
HIS		D1196	D1093
HIS		E1197	G1094
HIS			K1095
		S1200	E1096
		<b>A1201</b>	<b>I1097</b>
		L1202	
		D1203	L1100
		T1204	
			A1107
		<b>S1206</b>	
		<b>E1207</b>	G1110
		Q1211	Q1114
		E1212	
		A1213	L1118
			F1119
		A1217	D1120
			G1121
		R1221	S1122
		T1222	T1123
			A1124
		T1226	E1125
		A1227	A1126
		<b>E1228</b>	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.65Å 138.29Å 194.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.75 – 4.00 112.75 – 4.00	Depositor EDS
% Data completeness (in resolution range)	86.9 (112.75-4.00) 86.9 (112.75-4.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.24 (at 4.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), CNS	Depositor
R, $R_{free}$	0.316 , 0.338 0.316 , 0.338	Depositor DCC
$R_{free}$ test set	905 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	112.5	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 122.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.28$ , $\langle L^2 \rangle = 0.12$	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 <sup>2</sup> )	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.25	0/9339	0.48	1/12626 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	993	ASP	CB-CG-OD2	5.22	122.99	118.30

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	314	0
All	All	9171	0	9344	314	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 (314) 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	1.40	1.53
1:A:704:TRP:CZ2	1:A:707:PHE:CB	2.25	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:CE1	1:A:332:PHE:CE2	2.35	1.14
1:A:310:PHE:CE1	1:A:332:PHE:HE2	1.66	1.11
1:A:704:TRP:HZ2	1:A:707:PHE:CB	1.62	1.09
1:A:306:TYR:CE1	1:A:332:PHE:CE1	2.41	1.09
1:A:704:TRP:CE2	1:A:707:PHE:HB2	1.90	1.05
1:A:704:TRP:NE1	1:A:707:PHE:CD2	2.23	1.04
1:A:306:TYR:CD1	1:A:332:PHE:CE1	2.51	0.99
1:A:705:PRO:O	1:A:706:TYR:CD1	2.17	0.97
1:A:306:TYR:CD1	1:A:332:PHE:HE1	1.82	0.95
1:A:704:TRP:HZ2	1:A:707:PHE:HB2	1.12	0.93
1:A:704:TRP:NE1	1:A:707:PHE:HD2	1.69	0.86
1:A:416:GLY:H	1:A:577:THR:HG22	1.39	0.85
1:A:1033:PHE:HB2	1:A:1054:LEU:H	1.45	0.81
1:A:724:PHE:HB2	1:A:758:LEU:HD11	1.61	0.80
1:A:326:GLN:O	1:A:330:VAL:HG23	1.83	0.78
1:A:389:GLU:HB2	1:A:448:SER:HB3	1.64	0.78
1:A:38:MET:HA	1:A:41:TYR:HB3	1.66	0.78
1:A:310:PHE:HE1	1:A:332:PHE:CE2	2.02	0.76
1:A:369:PRO:O	1:A:371:ILE:HG23	1.86	0.76
1:A:1241:VAL:HG21	1:A:1263:TYR:HB2	1.67	0.75
1:A:228:TRP:HZ2	1:A:295:MET:HB2	1.52	0.75
1:A:704:TRP:HZ2	1:A:707:PHE:HB3	1.49	0.75
1:A:820:GLN:HB3	1:A:997:ALA:HA	1.69	0.75
1:A:153:ASN:ND2	1:A:368:LYS:HB3	2.03	0.73
1:A:1020:GLN:HG3	1:A:1100:LEU:HD12	1.72	0.72
1:A:132:TRP:HB2	1:A:184:ASP:HB3	1.72	0.71
1:A:132:TRP:HD1	1:A:133:CYS:HG	1.39	0.70
1:A:306:TYR:HD1	1:A:332:PHE:HE1	1.38	0.70
1:A:35:VAL:HB	1:A:355:ARG:HE	1.57	0.69
1:A:310:PHE:CZ	1:A:332:PHE:CE2	2.80	0.69
1:A:306:TYR:CE1	1:A:332:PHE:CZ	2.80	0.69
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.26	0.69
1:A:370:SER:O	1:A:371:ILE:HG12	1.93	0.68
1:A:1151:HIS:HA	1:A:1154:ILE:HB	1.77	0.67
1:A:125:ALA:HA	1:A:128:GLN:HE21	1.56	0.67
1:A:1090:VAL:HG13	1:A:1097:ILE:HB	1.75	0.67
1:A:327:VAL:HA	1:A:330:VAL:HB	1.77	0.67
1:A:488:ARG:HE	1:A:542:VAL:HG12	1.59	0.67
1:A:370:SER:O	1:A:371:ILE:CG1	2.43	0.66
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.77	0.66
1:A:306:TYR:HE1	1:A:332:PHE:CE1	2.06	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:OE2	1:A:782:LYS:NZ	2.28	0.65
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.77	0.65
1:A:396:SER:HB2	1:A:404:GLN:HG3	1.78	0.65
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.79	0.65
1:A:153:ASN:HD22	1:A:368:LYS:HB3	1.62	0.64
1:A:163:ASP:HB3	1:A:166:GLU:HB2	1.80	0.64
1:A:463:ARG:NH1	1:A:903:VAL:O	2.31	0.64
1:A:463:ARG:HH12	1:A:903:VAL:HG22	1.63	0.64
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.80	0.64
1:A:706:TYR:O	1:A:707:PHE:CD2	2.51	0.64
1:A:756:LEU:HA	1:A:760:ILE:HD13	1.80	0.63
1:A:92:SER:OG	1:A:96:LYS:NZ	2.31	0.63
1:A:258:ARG:NH2	1:A:801:ASP:O	2.32	0.62
1:A:362:PHE:HA	1:A:365:ILE:HB	1.81	0.62
1:A:484:ILE:HG21	1:A:496:ILE:HG13	1.79	0.62
1:A:901:ARG:O	1:A:904:VAL:HG12	1.99	0.62
1:A:958:TYR:O	1:A:962:GLN:N	2.32	0.62
1:A:463:ARG:O	1:A:543:ARG:NH2	2.33	0.62
1:A:466:ILE:HG23	1:A:549:LEU:HD13	1.82	0.61
1:A:242:ALA:HB2	1:A:283:LEU:HD12	1.83	0.61
1:A:856:LEU:HD21	1:A:951:ALA:HB1	1.82	0.60
1:A:132:TRP:HE3	1:A:184:ASP:H	1.50	0.60
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.83	0.60
1:A:306:TYR:CD1	1:A:332:PHE:CZ	2.89	0.60
1:A:1191:HIS:HA	1:A:1221:ARG:HD2	1.84	0.59
1:A:267:LYS:HA	1:A:270:LEU:HD22	1.84	0.59
1:A:1010:LYS:HD2	1:A:1012:PRO:HA	1.83	0.59
1:A:1038:PHE:HD2	1:A:1049:LEU:HD23	1.68	0.59
1:A:715:ILE:HD11	1:A:832:ILE:HG22	1.83	0.59
1:A:1114:GLN:HG2	1:A:1197:GLU:HB2	1.84	0.59
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.67	0.59
1:A:310:PHE:O	1:A:314:THR:N	2.30	0.59
1:A:1197:GLU:HB3	1:A:1200:SER:HB2	1.84	0.58
1:A:421:LEU:HB2	1:A:581:ILE:HG13	1.85	0.58
1:A:1048:VAL:HG23	1:A:1049:LEU:HD22	1.85	0.58
1:A:153:ASN:ND2	1:A:368:LYS:CB	2.66	0.58
1:A:796:ASP:N	1:A:796:ASP:OD1	2.37	0.58
1:A:1110:GLY:HA3	1:A:1193:LEU:HA	1.84	0.58
1:A:155:GLU:OE1	1:A:373:SER:OG	2.21	0.58
1:A:382:ASP:O	1:A:384:ILE:HG12	2.03	0.58
1:A:469:VAL:HG13	1:A:533:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HB3	1:A:782:LYS:HG2	1.86	0.57
1:A:714:ALA:HB1	1:A:833:PHE:HB2	1.86	0.57
1:A:471:GLN:N	1:A:471:GLN:OE1	2.37	0.57
1:A:429:LYS:HB3	1:A:581:ILE:HG12	1.87	0.56
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.37	0.56
1:A:44:TRP:HD1	1:A:45:LEU:HD12	1.70	0.56
1:A:486:TYR:HB3	1:A:908:ARG:HD3	1.87	0.56
1:A:214:ILE:HG23	1:A:335:LEU:HD21	1.87	0.55
1:A:270:LEU:HG	1:A:790:LYS:HD2	1.87	0.55
1:A:424:ASN:H	1:A:598:ASP:HA	1.72	0.55
1:A:81:VAL:HG13	1:A:99:MET:HB3	1.88	0.55
1:A:687:ASP:HA	1:A:1003:HIS:CE1	2.43	0.54
1:A:41:TYR:O	1:A:139:GLN:NE2	2.33	0.54
1:A:552:GLU:HG2	1:A:582:ALA:HA	1.90	0.54
1:A:374:PHE:HD1	1:A:376:LYS:H	1.55	0.54
1:A:453:ASP:OD1	1:A:454:ILE:N	2.41	0.54
1:A:224:SER:HB3	1:A:301:LEU:HD12	1.89	0.53
1:A:1000:SER:HA	1:A:1003:HIS:CD2	2.43	0.53
1:A:156:ILE:HG12	1:A:439:LEU:O	2.07	0.53
1:A:300:LEU:HD22	1:A:759:GLY:HA2	1.88	0.53
1:A:334:VAL:O	1:A:338:ALA:N	2.40	0.53
1:A:705:PRO:O	1:A:706:TYR:CG	2.61	0.53
1:A:969:ASN:H	1:A:972:LEU:HD13	1.74	0.53
1:A:969:ASN:O	1:A:973:VAL:HG23	2.08	0.53
1:A:1040:TYR:O	1:A:1042:THR:N	2.36	0.53
1:A:1107:ALA:O	1:A:1188:ARG:HD3	2.09	0.53
1:A:1126:ASN:HA	1:A:1129:TYR:CE1	2.44	0.53
1:A:122:LEU:HD13	1:A:943:ALA:HB2	1.91	0.53
1:A:722:PRO:HG2	1:A:841:THR:HB	1.91	0.53
1:A:970:VAL:HG23	1:A:971:LEU:HD22	1.91	0.53
1:A:267:LYS:HA	1:A:270:LEU:HB2	1.91	0.52
1:A:147:PHE:CD1	1:A:365:ILE:HG23	2.43	0.52
1:A:1039:ASN:HD22	1:A:1047:PRO:HG3	1.74	0.52
1:A:786:TYR:HE1	1:A:790:LYS:HZ2	1.58	0.52
1:A:44:TRP:CD1	1:A:45:LEU:HD12	2.45	0.52
1:A:493:MET:HA	1:A:496:ILE:HB	1.92	0.52
1:A:1010:LYS:HG2	1:A:1011:THR:H	1.75	0.51
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.36	0.51
1:A:243:TYR:O	1:A:247:GLY:N	2.36	0.51
1:A:923:PRO:O	1:A:927:ALA:N	2.40	0.51
1:A:824:ALA:HB2	1:A:997:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TRP:HE3	1:A:184:ASP:N	2.09	0.51
1:A:50:MET:HG3	1:A:131:PHE:CE1	2.45	0.51
1:A:864:ILE:HG22	1:A:944:MET:HB3	1.93	0.51
1:A:886:LEU:O	1:A:890:GLY:N	2.39	0.51
1:A:1235:ASN:OD1	1:A:1235:ASN:N	2.43	0.51
1:A:423:GLY:HA3	1:A:429:LYS:HD2	1.93	0.51
1:A:856:LEU:O	1:A:860:ILE:HG12	2.11	0.51
1:A:949:TYR:HD1	1:A:953:PHE:HE2	1.59	0.51
1:A:390:PHE:CD1	1:A:447:VAL:HG23	2.46	0.51
1:A:543:ARG:NH2	1:A:905:SER:HA	2.26	0.51
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.92	0.51
1:A:193:MET:O	1:A:197:PHE:N	2.43	0.51
1:A:1050:GLN:H	1:A:1245:GLY:HA3	1.76	0.50
1:A:527:LEU:HD23	1:A:527:LEU:H	1.75	0.50
1:A:796:ASP:HA	1:A:800:PHE:HD2	1.77	0.50
1:A:252:GLU:O	1:A:256:ALA:N	2.44	0.50
1:A:715:ILE:HD12	1:A:836:ILE:HG13	1.93	0.50
1:A:603:VAL:HG23	1:A:604:GLU:H	1.76	0.50
1:A:979:PHE:HA	1:A:982:MET:HG2	1.93	0.50
1:A:1043:ARG:HB3	1:A:1044:PRO:HD3	1.94	0.50
1:A:184:ASP:O	1:A:188:MET:N	2.33	0.50
1:A:257:ILE:HG12	1:A:800:PHE:CD1	2.47	0.50
1:A:359:TYR:HA	1:A:362:PHE:HB2	1.94	0.50
1:A:845:ILE:HG23	1:A:972:LEU:HD23	1.94	0.50
1:A:384:ILE:O	1:A:384:ILE:HG22	2.12	0.49
1:A:786:TYR:O	1:A:790:LYS:HG2	2.12	0.49
1:A:1211:GLN:NE2	1:A:1232:THR:HB	2.27	0.49
1:A:696:ILE:HG13	1:A:697:LEU:H	1.76	0.49
1:A:711:ILE:HD11	1:A:832:ILE:HG21	1.95	0.49
1:A:421:LEU:HB2	1:A:581:ILE:CG1	2.41	0.49
1:A:611:LEU:HD23	1:A:618:TYR:CG	2.48	0.49
1:A:148:PHE:HB3	1:A:913:GLU:OE2	2.13	0.49
1:A:1023:LYS:HB2	1:A:1026:MET:HG3	1.95	0.49
1:A:132:TRP:HD1	1:A:133:CYS:SG	2.34	0.49
1:A:715:ILE:HG23	1:A:836:ILE:HG13	1.94	0.49
1:A:381:PRO:HG2	1:A:461:TYR:CE2	2.48	0.48
1:A:140:ILE:HG13	1:A:179:ASN:ND2	2.28	0.48
1:A:590:ASN:OD1	1:A:590:ASN:N	2.39	0.48
1:A:356:GLY:HA2	1:A:359:TYR:CE2	2.48	0.48
1:A:180:GLU:O	1:A:185:LYS:HG3	2.14	0.48
1:A:1123:ILE:HD11	1:A:1161:TYR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:784:LEU:HD12	1:A:1004:ILE:HD13	1.96	0.48
1:A:1060:GLN:HB2	1:A:1237:ASP:CG	2.34	0.48
1:A:346:PRO:O	1:A:350:ALA:N	2.43	0.47
1:A:923:PRO:HA	1:A:926:ASN:HB3	1.95	0.47
1:A:414:LYS:HD2	1:A:414:LYS:H	1.79	0.47
1:A:132:TRP:CE3	1:A:183:GLY:HA3	2.50	0.47
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.79	0.47
1:A:845:ILE:O	1:A:848:ILE:HG12	2.14	0.47
1:A:930:LYS:HA	1:A:933:VAL:HB	1.96	0.47
1:A:1000:SER:HA	1:A:1003:HIS:HD2	1.79	0.47
1:A:153:ASN:HD21	1:A:368:LYS:HD2	1.78	0.47
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.96	0.47
1:A:421:LEU:HD22	1:A:581:ILE:HD11	1.94	0.47
1:A:65:PRO:O	1:A:69:LEU:N	2.48	0.47
1:A:1207:GLU:CD	1:A:1229:ARG:HH12	2.18	0.47
1:A:1122:SER:HB3	1:A:1125:GLU:HG2	1.96	0.47
1:A:1118:LEU:HD21	1:A:1180:ILE:HD12	1.96	0.47
1:A:132:TRP:HB2	1:A:184:ASP:CB	2.43	0.47
1:A:769:GLN:HG3	1:A:773:PHE:HE2	1.80	0.47
1:A:158:TRP:HE1	1:A:900:PHE:HB3	1.78	0.47
1:A:211:THR:HG23	1:A:331:PHE:HE2	1.80	0.47
1:A:419:VAL:HG13	1:A:579:ILE:HG13	1.97	0.47
1:A:622:VAL:O	1:A:626:THR:N	2.48	0.47
1:A:861:VAL:HB	1:A:862:PRO:HD3	1.97	0.47
1:A:533:GLN:O	1:A:537:ILE:HG13	2.15	0.46
1:A:603:VAL:HG23	1:A:604:GLU:N	2.30	0.46
1:A:1197:GLU:HA	1:A:1227:ALA:HA	1.98	0.46
1:A:268:LYS:O	1:A:272:ARG:HG3	2.15	0.46
1:A:370:SER:C	1:A:371:ILE:HG12	2.35	0.46
1:A:1202:LEU:HD23	1:A:1207:GLU:HA	1.97	0.46
1:A:758:LEU:O	1:A:762:SER:N	2.42	0.46
1:A:1137:SER:HB3	1:A:1140:GLU:HB3	1.98	0.46
1:A:1211:GLN:HG3	1:A:1232:THR:HG21	1.97	0.46
1:A:1079:LEU:HD23	1:A:1194:LEU:HD11	1.97	0.46
1:A:893:ALA:HA	1:A:916:TYR:CZ	2.51	0.46
1:A:231:ILE:HG23	1:A:235:PHE:CD2	2.50	0.46
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.46	0.46
1:A:797:VAL:HG13	1:A:797:VAL:O	2.16	0.46
1:A:1262:ILE:O	1:A:1266:MET:HG2	2.16	0.45
1:A:437:GLN:HB2	1:A:439:LEU:HD23	1.97	0.45
1:A:1005:ILE:O	1:A:1009:GLU:HG2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:VAL:HG12	1:A:1003:HIS:HE2	1.81	0.45
1:A:1011:THR:HG23	1:A:1011:THR:O	2.16	0.45
1:A:1196:ASP:HA	1:A:1226:ILE:HG12	1.97	0.45
1:A:33:VAL:HG23	1:A:34:SER:H	1.81	0.45
1:A:429:LYS:HB2	1:A:429:LYS:HE2	1.79	0.45
1:A:496:ILE:O	1:A:500:VAL:HG22	2.16	0.45
1:A:316:LEU:HD22	1:A:320:LYS:HD2	1.97	0.45
1:A:703:GLU:O	1:A:705:PRO:HD3	2.17	0.45
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.98	0.45
1:A:454:ILE:HD11	1:A:462:LEU:HD21	1.98	0.45
1:A:711:ILE:O	1:A:715:ILE:HG12	2.16	0.45
1:A:1181:ALA:HA	1:A:1184:ARG:HE	1.81	0.45
1:A:153:ASN:HD21	1:A:368:LYS:CD	2.30	0.45
1:A:1039:ASN:ND2	1:A:1047:PRO:HG3	2.31	0.45
1:A:1039:ASN:ND2	1:A:1045:SER:OG	2.48	0.44
1:A:39:PHE:CE1	1:A:355:ARG:HA	2.52	0.44
1:A:1074:THR:O	1:A:1078:LEU:HG	2.18	0.44
1:A:422:VAL:HG23	1:A:596:GLY:HA2	1.98	0.44
1:A:1093:ASP:HB3	1:A:1095:LYS:HD3	2.00	0.44
1:A:1068:SER:OG	1:A:1069:GLY:N	2.51	0.44
1:A:788:VAL:O	1:A:792:MET:N	2.47	0.44
1:A:999:VAL:HG12	1:A:1003:HIS:NE2	2.32	0.44
1:A:235:PHE:HB3	1:A:287:LYS:HE2	1.99	0.44
1:A:1037:VAL:HG12	1:A:1050:GLN:HA	2.00	0.44
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.18	0.44
1:A:787:MET:HB3	1:A:1008:ILE:HD11	1.99	0.43
1:A:1052:LEU:HD13	1:A:1242:ILE:HD13	2.00	0.43
1:A:1233:ILE:HA	1:A:1233:ILE:HD12	1.90	0.43
1:A:333:SER:O	1:A:337:GLY:N	2.44	0.43
1:A:1063:ALA:HB3	1:A:1239:ILE:HG13	1.99	0.43
1:A:482:GLU:HA	1:A:485:ARG:HB3	2.00	0.43
1:A:687:ASP:H	1:A:813:ARG:HH22	1.66	0.43
1:A:48:LEU:O	1:A:52:VAL:HG23	2.19	0.43
1:A:714:ALA:O	1:A:833:PHE:HD1	2.01	0.43
1:A:1213:ALA:O	1:A:1217:ALA:N	2.51	0.43
1:A:289:ILE:O	1:A:293:ILE:HG13	2.19	0.43
1:A:721:GLN:HB3	1:A:722:PRO:HD3	1.99	0.43
1:A:83:ASN:O	1:A:87:ASN:HB2	2.19	0.43
1:A:1039:ASN:HB2	1:A:1047:PRO:HB3	2.00	0.43
1:A:1207:GLU:OE2	1:A:1229:ARG:NH2	2.38	0.43
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TYR:CD1	1:A:509:ILE:HD11	2.54	0.43
1:A:538:ALA:O	1:A:542:VAL:HG23	2.18	0.43
1:A:857:LEU:HD12	1:A:973:VAL:HG13	2.00	0.43
1:A:1260:LYS:HB3	1:A:1260:LYS:HE3	1.79	0.42
1:A:1196:ASP:OD1	1:A:1226:ILE:HD11	2.19	0.42
1:A:327:VAL:HB	1:A:331:PHE:CE1	2.54	0.42
1:A:358:ALA:O	1:A:362:PHE:HB2	2.19	0.42
1:A:831:VAL:HA	1:A:834:GLN:HE21	1.83	0.42
1:A:713:CYS:SG	1:A:768:LEU:HB3	2.60	0.42
1:A:961:THR:HA	1:A:965:MET:HB2	2.00	0.42
1:A:1049:LEU:HD21	1:A:1074:THR:OG1	2.20	0.42
1:A:504:ASN:ND2	1:A:534:ARG:HD3	2.35	0.42
1:A:1049:LEU:HD12	1:A:1052:LEU:HD22	2.00	0.42
1:A:1053:SER:O	1:A:1054:LEU:HD13	2.19	0.42
1:A:1120:ASP:N	1:A:1120:ASP:OD1	2.47	0.42
1:A:213:VAL:O	1:A:217:ILE:HG23	2.19	0.42
1:A:43:GLY:CA	1:A:46:ASP:HB2	2.49	0.42
1:A:717:ASN:HB2	1:A:765:THR:OG1	2.19	0.42
1:A:1138:TYR:O	1:A:1142:VAL:HG23	2.19	0.42
1:A:1260:LYS:HG2	1:A:1261:GLY:N	2.34	0.42
1:A:192:ALA:O	1:A:195:THR:OG1	2.28	0.42
1:A:193:MET:HA	1:A:196:PHE:HB3	2.01	0.42
1:A:33:VAL:HG23	1:A:34:SER:N	2.34	0.42
1:A:118:GLY:HA2	1:A:121:VAL:HG22	2.00	0.42
1:A:218:SER:HB3	1:A:219:PRO:HD3	2.02	0.42
1:A:370:SER:OG	1:A:371:ILE:N	2.53	0.42
1:A:132:TRP:HA	1:A:183:GLY:HA2	2.01	0.42
1:A:296:GLY:O	1:A:300:LEU:HG	2.20	0.42
1:A:534:ARG:HA	1:A:537:ILE:HD12	2.02	0.42
1:A:755:PHE:O	1:A:759:GLY:N	2.52	0.42
1:A:88:SER:OG	1:A:89:THR:N	2.50	0.41
1:A:1196:ASP:CG	1:A:1226:ILE:HD11	2.40	0.41
1:A:881:LYS:O	1:A:885:GLU:HG3	2.20	0.41
1:A:1158:PRO:C	1:A:1160:LYS:H	2.24	0.41
1:A:1244:ASN:O	1:A:1246:LYS:HD2	2.21	0.41
1:A:217:ILE:HG21	1:A:305:SER:HB2	2.01	0.41
1:A:912:PHE:HA	1:A:912:PHE:HD1	1.75	0.41
1:A:206:ARG:HB3	1:A:327:VAL:HG11	2.03	0.41
1:A:1123:ILE:HA	1:A:1126:ASN:HB2	2.03	0.41
1:A:790:LYS:O	1:A:794:ARG:NE	2.51	0.41
1:A:1005:ILE:O	1:A:1008:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:LYS:HA	1:A:1222:THR:OG1	2.20	0.41
1:A:318:ILE:HD13	1:A:744:GLN:HA	2.02	0.41
1:A:784:LEU:O	1:A:788:VAL:HG23	2.20	0.41
1:A:910:GLN:O	1:A:914:THR:N	2.53	0.41
1:A:1054:LEU:HD11	1:A:1240:VAL:HG11	2.02	0.41
1:A:773:PHE:HB3	1:A:829:LEU:HD22	2.01	0.41
1:A:370:SER:O	1:A:371:ILE:HG13	2.20	0.41
1:A:390:PHE:HE2	1:A:432:THR:HB	1.86	0.41
1:A:840:GLY:O	1:A:844:ILE:HG12	2.21	0.41
1:A:916:TYR:O	1:A:920:LEU:N	2.39	0.41
1:A:230:LYS:O	1:A:234:SER:OG	2.35	0.41
1:A:295:MET:HG2	1:A:766:PHE:CZ	2.56	0.41
1:A:768:LEU:O	1:A:772:THR:HG23	2.21	0.41
1:A:467:GLY:HA3	1:A:545:PRO:HG3	2.03	0.40
1:A:214:ILE:O	1:A:217:ILE:HG12	2.21	0.40
1:A:397:TYR:CG	1:A:398:PRO:HD2	2.56	0.40
1:A:930:LYS:HD2	1:A:934:PHE:CE1	2.57	0.40
1:A:129:VAL:O	1:A:132:TRP:HB3	2.21	0.40
1:A:189:PHE:CZ	1:A:348:ILE:HD11	2.56	0.40
1:A:1061:THR:N	1:A:1237:ASP:OD1	2.42	0.40
1:A:216:ALA:O	1:A:219:PRO:HD2	2.22	0.40
1:A:269:GLU:OE1	1:A:272:ARG:NH2	2.54	0.40
1:A:704:TRP:CD1	1:A:707:PHE:CD2	3.06	0.40
1:A:848:ILE:HD11	1:A:972:LEU:HD21	2.03	0.40
1:A:900:PHE:O	1:A:903:VAL:HG12	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%)	1073 (91%)	105 (9%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	976/1065 (92%)	976 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	153	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1182/1284 (92%)	-0.15	4 (0%) 94 90	32, 95, 153, 200	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	828	ARG	3.4
1	A	574	GLU	3.1
1	A	170	ARG	2.3
1	A	705	PRO	2.2

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.