



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:35 am BST

PDB ID : 4M1M  
Title : Corrected Structure of Mouse P-glycoprotein  
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Deposited on : 2013-08-03  
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](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

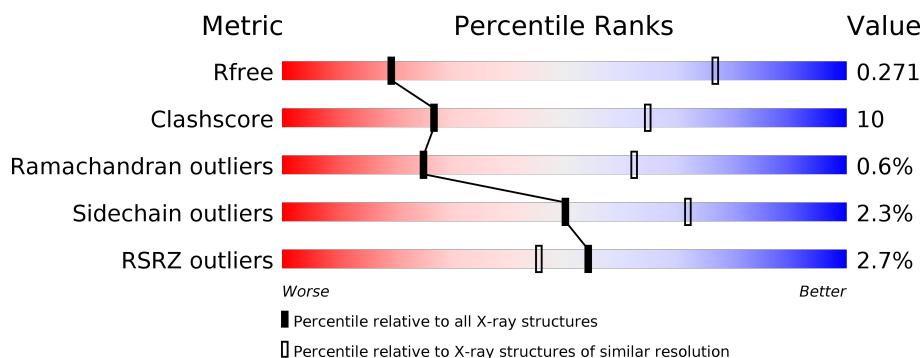
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 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))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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  $\geq 3$ , 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	1282	
1	B	1282	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18378 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	1188	Total	C	N	O	S	0	0	0
			9213	5923	1559	1694	37			
1	B	1180	Total	C	N	O	S	0	0	0
			9152	5887	1550	1678	37			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	83	GLN	ASN	CONFLICT	UNP P21447
A	87	GLN	ASN	CONFLICT	UNP P21447
A	90	GLN	ASN	CONFLICT	UNP P21447
A	952	ALA	CYS	CONFLICT	UNP P21447
A	1277	HIS	-	EXPRESSION TAG	UNP P21447
A	1278	HIS	-	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
B	83	GLN	ASN	CONFLICT	UNP P21447
B	87	GLN	ASN	CONFLICT	UNP P21447
B	90	GLN	ASN	CONFLICT	UNP P21447
B	952	ALA	CYS	CONFLICT	UNP P21447
B	1277	HIS	-	EXPRESSION TAG	UNP P21447
B	1278	HIS	-	EXPRESSION TAG	UNP P21447
B	1279	HIS	-	EXPRESSION TAG	UNP P21447
B	1280	HIS	-	EXPRESSION TAG	UNP P21447
B	1281	HIS	-	EXPRESSION TAG	UNP P21447
B	1282	HIS	-	EXPRESSION TAG	UNP P21447

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total 6	Hg 6	0	0
2	A	7	Total 7	Hg 7	0	0

These plots are drawn for all protein, RNA and DNA 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.

Chain A: 2% 68% 24% 7%

Amino Acid	Segment 1 (2%)	Segment 2 (68%)	Segment 3 (24%)	Segment 4 (7%)
MET				
GLU				
LEU				
GLU				
GLU				
ASP				
LEU				
LVS				
GLY				
ARG				
ALA				
ASP				
LVS				
ASN				
PHE				
SER				
LVS				
MET				
GLY				
LVS				
SER				
LVS				
GLU				
LVS				
GLU				
LVS				
LVS				
K30				
V33				
S34				
V35				
L36				
T37				
M38				
F39				
D46				
M50				
T54				
I58				
I59				
L64				
P65				
L66				
M67				
I70				
A79				
K86				
M107				
T108				
T109				
Y110				
Y113				
I117				
L122				
I123				
V124				
A125				
Y126				
I127				
Q128				
V129				
W132				
A136				
G137				
R138				
Q139				
I140				
I143				
A150				
Q154				
E155				
I156				
G157				
W158				
R170				
D174				
V175				
I178				
G183				
I186				
E200				
E201				
I202				
G203				
R206				
G207				
K208				
K209				
L210				
T211				
L215				
E216				
I217				
S218				
P219				
V220				
I227				
I231				
K238				
E239				
I257				
R258				
T259				
V260				
G264				
G265				
E269				
L277				
E278				
E279				
A280				
K281				
R282				
L283				
K286				
K287				
A288				
I289				
T290				
A291				
I292				
I293				
S294				
V303				
F310				
T314				
S315				
I316				
V317				
V322				
Q326				
V327				
V330				
V334				



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.54Å 115.43Å 378.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.89 – 3.80 42.33 – 3.79	Depositor EDS
% Data completeness (in resolution range)	95.9 (24.89-3.80) 95.5 (42.33-3.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.19 (at 3.76Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.212 , 0.267 0.223 , 0.271	Depositor DCC
$R_{free}$ test set	4245 reflections (10.21%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	132.2	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 87.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	18378	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	155.0	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.*

<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

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	0.31	0/9382	0.51	0/12684
1	B	0.30	0/9321	0.50	0/12601
All	All	0.31	0/18703	0.51	0/25285

There are no bond length outliers.

There are no bond angle outliers.

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	9213	0	9383	203	0
1	B	9152	0	9333	179	0
2	A	7	0	0	0	0
2	B	6	0	0	0	0
All	All	18378	0	18716	379	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 10.

All (379) 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:281:LYS:HZ2	1:A:782:LYS:HA	1.26	0.98
1:A:559:THR:HG22	1:A:584:ARG:HH12	1.39	0.87
1:B:1021:GLY:HA2	1:B:1101:ASN:HB2	1.60	0.81
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.64	0.80
1:A:1149:ASN:O	1:A:1179:ARG:NH2	2.14	0.79
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.64	0.79
1:B:257:ILE:HG12	1:B:800:PHE:CE2	2.20	0.77
1:A:966:THR:OG1	1:A:967:PHE:N	2.15	0.77
1:B:1022:LEU:HD11	1:B:1100:LEU:HA	1.67	0.75
1:A:257:ILE:HG12	1:A:800:PHE:CE2	2.22	0.75
1:A:792:MET:HE1	1:A:810:LEU:HB3	1.71	0.73
1:A:396:SER:HB3	1:A:404:GLN:HA	1.70	0.72
1:B:784:LEU:HD22	1:B:821:VAL:HG11	1.72	0.72
1:A:281:LYS:NZ	1:A:785:ARG:HD2	2.05	0.71
1:A:122:LEU:HB3	1:A:943:ALA:HB2	1.72	0.71
1:B:257:ILE:HG12	1:B:800:PHE:HE2	1.54	0.70
1:A:281:LYS:NZ	1:A:782:LYS:HA	2.06	0.70
1:A:208:TRP:HE3	1:A:209:LYS:HG2	1.55	0.70
1:A:854:THR:HG23	1:A:977:ILE:HD11	1.74	0.69
1:A:208:TRP:CE3	1:A:209:LYS:HG2	2.28	0.69
1:A:239:GLU:OE1	1:A:287:LYS:NZ	2.20	0.68
1:A:257:ILE:HG12	1:A:800:PHE:HE2	1.57	0.68
1:B:272:ARG:NH2	1:B:1125:GLU:OE2	2.27	0.68
1:B:966:THR:H	1:B:967:PHE:HA	1.59	0.67
1:A:281:LYS:HZ3	1:A:785:ARG:HD2	1.60	0.66
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.76	0.66
1:A:384:ILE:HD11	1:A:546:LYS:HB2	1.78	0.66
1:B:484:ILE:HG21	1:B:496:ILE:HG23	1.77	0.66
1:B:160:ASP:OD1	1:B:901:ARG:NH2	2.29	0.66
1:B:396:SER:OG	1:B:403:VAL:O	2.14	0.65
1:A:34:SER:OG	1:A:37:THR:OG1	2.13	0.65
1:B:94:ALA:HB1	1:B:97:ARG:HE	1.62	0.64
1:B:122:LEU:HB3	1:B:943:ALA:HB2	1.78	0.63
1:A:388:LEU:HB2	1:A:413:VAL:HB	1.81	0.63
1:B:282:ARG:HH22	1:B:779:ILE:HA	1.65	0.62
1:A:371:ILE:O	1:A:373:SER:HB3	2.00	0.62
1:A:206:ARG:HE	1:A:206:ARG:HA	1.65	0.61
1:A:794:ARG:HG2	1:A:1012:PRO:HG3	1.82	0.61
1:B:102:LYS:HE3	1:B:106:GLU:OE2	2.00	0.61
1:A:780:LEU:O	1:A:784:LEU:HB2	1.99	0.61
1:A:513:PRO:HB2	1:A:514:HIS:CD2	2.35	0.61
1:A:70:ILE:HD13	1:A:113:TYR:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1033:PHE:HD1	1:B:1036:VAL:HG21	1.67	0.59
1:A:419:VAL:HG22	1:A:593:VAL:HB	1.85	0.59
1:A:784:LEU:HD22	1:A:821:VAL:HG11	1.84	0.59
1:A:1112:VAL:HB	1:A:1195:LEU:HD23	1.84	0.59
1:A:554:THR:HB	1:A:562:GLU:HG3	1.84	0.58
1:A:337:GLY:O	1:A:340:SER:OG	2.21	0.58
1:A:833:PHE:HA	1:A:836:ILE:HG22	1.84	0.58
1:A:1110:GLY:O	1:A:1194:LEU:N	2.33	0.58
1:A:840:GLY:O	1:A:843:ILE:HG22	2.04	0.57
1:A:612:MET:HE1	1:A:622:VAL:HG11	1.86	0.57
1:A:1199:THR:OG1	1:A:1229:ARG:NH2	2.37	0.57
1:A:1036:VAL:H	1:A:1088:GLY:HA3	1.70	0.57
1:B:378:GLY:H	1:B:458:ASN:HB2	1.69	0.57
1:A:1021:GLY:HA3	1:A:1101:ASN:HB2	1.88	0.56
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.38	0.56
1:B:1149:ASN:O	1:B:1179:ARG:NH2	2.38	0.56
1:B:65:PRO:HB2	1:B:202:ILE:HD12	1.87	0.56
1:A:510:MET:SD	1:A:515:GLN:NE2	2.79	0.56
1:B:1096:GLU:OE1	1:B:1098:LYS:N	2.32	0.56
1:B:1065:VAL:HG23	1:B:1241:VAL:HA	1.87	0.56
1:A:123:ILE:O	1:A:127:ILE:HG12	2.05	0.56
1:B:1072:LYS:HD3	1:B:1226:ILE:HG23	1.88	0.56
1:A:1079:LEU:HG	1:A:1109:LEU:HD21	1.89	0.55
1:A:215:LEU:O	1:A:218:SER:OG	2.23	0.55
1:A:281:LYS:HZ2	1:A:782:LYS:CA	2.11	0.55
1:B:510:MET:SD	1:B:515:GLN:NE2	2.80	0.55
1:A:1096:GLU:OE1	1:A:1098:LYS:N	2.36	0.55
1:A:310:PHE:CD2	1:A:755:PHE:HE2	2.24	0.55
1:B:32:ALA:H	1:B:356:GLY:HA2	1.71	0.55
1:A:893:ALA:O	1:A:897:ILE:HG12	2.06	0.55
1:B:289:ILE:HD13	1:B:771:PHE:HE1	1.72	0.55
1:B:292:ASN:ND2	1:B:766:PHE:O	2.41	0.54
1:A:200:PHE:HE2	1:A:215:LEU:HD12	1.72	0.54
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.88	0.54
1:B:554:THR:HB	1:B:562:GLU:HG3	1.89	0.54
1:B:500:VAL:HG11	1:B:509:ILE:HD12	1.90	0.54
1:A:453:ASP:OD1	1:A:454:ILE:N	2.41	0.53
1:B:393:ILE:H	1:B:445:GLY:HA3	1.73	0.53
1:A:1230:LEU:HD23	1:A:1233:ILE:HD12	1.89	0.53
1:A:846:SER:HB2	1:A:973:VAL:HG13	1.90	0.53
1:B:206:ARG:O	1:B:326:GLN:NE2	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:475:LEU:HD12	1:B:532:LYS:HG2	1.90	0.53
1:A:373:SER:HB2	1:A:459:VAL:HG11	1.90	0.53
1:B:1033:PHE:CD1	1:B:1036:VAL:HG21	2.43	0.53
1:B:289:ILE:O	1:B:293:ILE:HG12	2.08	0.53
1:A:393:ILE:HB	1:A:409:LEU:HB3	1.89	0.53
1:A:485:ARG:NH2	1:B:914:THR:OG1	2.42	0.53
1:A:175:VAL:HA	1:A:178:ILE:HG22	1.91	0.53
1:B:206:ARG:HG3	1:B:326:GLN:HG3	1.90	0.53
1:A:1020:GLN:HG2	1:A:1021:GLY:N	2.23	0.53
1:A:1049:LEU:HD13	1:A:1052:LEU:HD21	1.91	0.53
1:A:66:LEU:HD23	1:A:202:ILE:HD11	1.90	0.53
1:A:1234:GLN:HG2	1:A:1253:HIS:CE1	2.44	0.53
1:A:496:ILE:O	1:A:500:VAL:HG23	2.09	0.53
1:A:607:ASN:HB3	1:A:610:GLU:OE2	2.08	0.52
1:B:711:ILE:O	1:B:715:ILE:HG13	2.09	0.52
1:B:1136:VAL:HG22	1:B:1137:SER:H	1.75	0.52
1:B:907:THR:O	1:B:908:ARG:NE	2.42	0.52
1:A:316:LEU:HD23	1:A:322:TYR:CD1	2.44	0.52
1:A:728:PHE:CE1	1:A:971:LEU:HD21	2.44	0.52
1:B:695:ARG:HA	1:B:698:LYS:NZ	2.25	0.52
1:B:792:MET:HE1	1:B:810:LEU:HB3	1.92	0.52
1:A:925:ARG:HA	1:B:514:HIS:HD2	1.74	0.52
1:A:46:ASP:OD1	1:A:138:ARG:NH1	2.43	0.52
1:A:360:GLU:O	1:A:364:ILE:HG12	2.10	0.51
1:A:1120:ASP:HB3	1:A:1168:LYS:HD3	1.92	0.51
1:A:33:VAL:HG12	1:A:37:THR:HB	1.91	0.51
1:B:460:ARG:HG3	1:B:907:THR:HG21	1.92	0.51
1:B:317:VAL:HG23	1:B:323:SER:HA	1.92	0.51
1:B:507:ASP:OD1	1:B:508:PHE:N	2.44	0.51
1:B:300:LEU:HD11	1:B:760:ILE:HD13	1.92	0.51
1:B:520:VAL:HG22	1:B:521:GLY:H	1.75	0.51
1:A:831:VAL:HG13	1:A:987:VAL:HG12	1.93	0.51
1:A:937:THR:O	1:A:941:THR:HG23	2.11	0.51
1:B:1230:LEU:HD23	1:B:1233:ILE:HD12	1.92	0.51
1:B:965:MET:HB3	1:B:966:THR:OG1	2.11	0.51
1:A:1033:PHE:HD1	1:A:1036:VAL:HG11	1.76	0.51
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.43	0.50
1:A:170:ARG:HG3	1:A:174:ASP:HB2	1.93	0.50
1:A:175:VAL:O	1:A:178:ILE:HG22	2.11	0.50
1:A:382:ASP:OD1	1:A:382:ASP:N	2.43	0.50
1:B:723:ALA:O	1:B:727:ILE:HG12	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:ILE:O	1:B:500:VAL:HG23	2.11	0.50
1:B:849:TYR:HB3	1:B:969:ASN:HB3	1.92	0.50
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.92	0.50
1:A:756:LEU:O	1:A:760:ILE:HG12	2.12	0.50
1:B:379:HIS:H	1:B:457:ILE:HA	1.77	0.50
1:B:94:ALA:HB1	1:B:97:ARG:NE	2.27	0.50
1:A:238:LYS:HG2	1:A:283:LEU:HD11	1.93	0.49
1:B:1110:GLY:HA3	1:B:1193:LEU:HD23	1.94	0.49
1:A:1150:ILE:HG22	1:A:1179:ARG:HB3	1.94	0.49
1:A:538:ALA:O	1:A:542:VAL:HG23	2.12	0.49
1:B:808:GLY:HA2	1:B:811:THR:HG22	1.94	0.49
1:A:1241:VAL:HB	1:A:1249:GLU:HB2	1.93	0.49
1:A:723:ALA:O	1:A:727:ILE:HG12	2.13	0.49
1:B:312:TYR:O	1:B:315:SER:OG	2.21	0.49
1:A:260:VAL:O	1:A:264:GLY:N	2.45	0.49
1:A:424:ASN:H	1:A:429:LYS:HZ1	1.60	0.49
1:B:281:LYS:HD2	1:B:781:THR:HB	1.92	0.49
1:B:879:ALA:O	1:B:883:LYS:HG2	2.12	0.49
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.94	0.49
1:A:227:ILE:O	1:A:231:ILE:HG13	2.13	0.49
1:A:604:GLU:OE2	1:A:616:GLY:HA3	2.12	0.49
1:A:981:ALA:O	1:A:984:VAL:HG22	2.13	0.49
1:B:784:LEU:HD21	1:B:1004:ILE:HG21	1.95	0.49
1:A:794:ARG:NH1	1:A:1015:ASP:OD2	2.46	0.48
1:A:617:ILE:HD12	1:A:617:ILE:H	1.77	0.48
1:A:920:LEU:O	1:A:923:PRO:HD2	2.13	0.48
1:A:79:ALA:HB2	1:A:736:THR:HG22	1.95	0.48
1:B:278:GLU:HG3	1:B:282:ARG:HD2	1.95	0.48
1:B:257:ILE:HD12	1:B:260:VAL:HB	1.95	0.48
1:A:388:LEU:HD11	1:A:547:ILE:HD13	1.95	0.48
1:B:966:THR:OG1	1:B:969:ASN:HB2	2.14	0.48
1:B:1078:LEU:HD22	1:B:1085:PRO:HD3	1.95	0.48
1:B:291:ALA:O	1:B:294:SER:OG	2.22	0.48
1:B:388:LEU:HD13	1:B:577:THR:HG21	1.96	0.48
1:A:1178:GLN:O	1:A:1182:ILE:HG12	2.13	0.48
1:B:61:GLY:HA3	1:B:194:ALA:HB3	1.96	0.48
1:B:1022:LEU:HD11	1:B:1100:LEU:HD23	1.95	0.48
1:B:299:PHE:HA	1:B:302:ILE:HG12	1.95	0.48
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.96	0.48
1:B:1061:THR:HG21	1:B:1218:ARG:HD3	1.95	0.48
1:B:277:LEU:C	1:B:279:GLU:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1045:SER:OG	1:B:1046:ILE:N	2.47	0.47
1:B:217:ILE:O	1:B:220:VAL:HG12	2.13	0.47
1:B:453:ASP:OD1	1:B:454:ILE:N	2.47	0.47
1:A:158:TRP:HZ2	1:A:364:ILE:HD12	1.79	0.47
1:B:855:LEU:HA	1:B:858:LEU:HG	1.95	0.47
1:B:90:GLN:HG2	1:B:91:MET:H	1.79	0.47
1:B:385:GLN:HB2	1:B:450:ASP:OD2	2.13	0.47
1:B:835:ASN:CG	1:B:984:VAL:HG13	2.35	0.47
1:A:1158:PRO:HA	1:A:1159:ASP:HA	1.62	0.47
1:B:1035:GLY:N	1:B:1053:SER:OG	2.40	0.47
1:B:960:VAL:HG21	1:B:967:PHE:HB2	1.96	0.47
1:B:1175:GLY:HA2	1:B:1202:LEU:HD11	1.95	0.47
1:B:533:GLN:O	1:B:537:ILE:HG13	2.13	0.47
1:B:585:LEU:HD11	1:B:621:LEU:HB3	1.97	0.47
1:B:376:LYS:HA	1:B:377:SER:HA	1.63	0.47
1:A:129:VAL:HG13	1:A:935:GLY:HA2	1.97	0.47
1:B:689:PRO:HG3	1:B:1003:HIS:CD2	2.50	0.47
1:B:174:ASP:O	1:B:178:ILE:HG13	2.14	0.47
1:B:780:LEU:O	1:B:784:LEU:HB2	2.15	0.47
1:A:86:LYS:HZ2	1:A:739:GLY:HA2	1.80	0.46
1:B:1183:ALA:O	1:B:1187:VAL:HG23	2.15	0.46
1:B:714:ALA:HB1	1:B:834:GLN:HG3	1.97	0.46
1:A:562:GLU:OE1	1:A:584:ARG:NH1	2.48	0.46
1:A:1024:PRO:HD2	1:A:1104:TRP:CZ2	2.51	0.46
1:A:702:THR:OG1	1:A:783:ARG:NH2	2.48	0.46
1:B:538:ALA:O	1:B:542:VAL:HG23	2.15	0.46
1:B:263:PHE:CZ	1:B:1184:ARG:HD3	2.51	0.46
1:B:122:LEU:HD12	1:B:123:ILE:N	2.30	0.46
1:A:481:ALA:O	1:A:485:ARG:HG2	2.16	0.46
1:A:488:ARG:HA	1:A:908:ARG:HH11	1.80	0.46
1:B:140:ILE:HD13	1:B:140:ILE:HA	1.84	0.46
1:B:163:ASP:HB3	1:B:166:GLU:HG2	1.97	0.46
1:B:125:ALA:O	1:B:129:VAL:HG12	2.16	0.46
1:A:1183:ALA:O	1:A:1187:VAL:HG23	2.15	0.46
1:A:730:LYS:HB3	1:A:751:PHE:CE2	2.50	0.46
1:A:1159:ASP:OD1	1:A:1159:ASP:N	2.43	0.45
1:A:64:LEU:HD12	1:A:336:ILE:HG21	1.98	0.45
1:A:852:GLN:CD	1:A:852:GLN:H	2.20	0.45
1:A:265:GLY:O	1:A:269:GLU:HG2	2.16	0.45
1:A:957:ALA:HA	1:A:960:VAL:HG12	1.97	0.45
1:B:727:ILE:HD12	1:B:754:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:736:THR:HG21	1:B:967:PHE:HE2	1.80	0.45
1:A:314:THR:HA	1:A:317:VAL:HG12	1.97	0.45
1:A:827:SER:O	1:A:831:VAL:HG23	2.17	0.45
1:B:1151:HIS:ND1	1:B:1154:ILE:HD11	2.31	0.45
1:B:1165:VAL:HA	1:B:1166:GLY:HA2	1.79	0.45
1:A:50:MET:HE1	1:A:139:GLN:HE22	1.81	0.45
1:B:728:PHE:CE2	1:B:971:LEU:HD21	2.52	0.45
1:A:286:LYS:O	1:A:290:THR:HG23	2.16	0.45
1:A:257:ILE:HD12	1:A:260:VAL:HB	1.99	0.45
1:A:471:GLN:HB3	1:A:552:GLU:HB2	1.98	0.45
1:A:478:THR:HB	1:A:482:GLU:HB2	1.98	0.45
1:B:307:ALA:HA	1:B:755:PHE:CE1	2.51	0.45
1:B:38:MET:HA	1:B:362:PHE:HE2	1.81	0.45
1:B:404:GLN:HB3	1:B:407:LYS:NZ	2.32	0.45
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.98	0.45
1:A:217:ILE:O	1:A:220:VAL:HG12	2.17	0.45
1:B:500:VAL:HG21	1:B:516:PHE:HE1	1.82	0.45
1:B:607:ASN:HB3	1:B:610:GLU:OE1	2.16	0.45
1:B:908:ARG:HE	1:B:908:ARG:HA	1.83	0.44
1:A:1061:THR:HG21	1:A:1218:ARG:HD3	1.98	0.44
1:A:784:LEU:HD21	1:A:1004:ILE:HG21	1.99	0.44
1:B:617:ILE:H	1:B:617:ILE:HD12	1.82	0.44
1:A:1165:VAL:HA	1:A:1166:GLY:HA2	1.71	0.44
1:A:689:PRO:HG3	1:A:1003:HIS:CD2	2.52	0.44
1:A:741:PRO:HA	1:A:744:GLN:HG3	1.98	0.44
1:B:407:LYS:O	1:B:601:VAL:HG22	2.17	0.44
1:B:882:ASP:HA	1:B:885:GLU:HG2	2.00	0.44
1:A:65:PRO:HB2	1:A:202:ILE:HD12	1.99	0.44
1:A:38:MET:SD	1:A:355:ARG:HG2	2.58	0.44
1:A:975:SER:O	1:A:979:PHE:HB2	2.18	0.44
1:B:265:GLY:O	1:B:269:GLU:HG2	2.18	0.44
1:B:1081:ARG:HD3	1:B:1097:ILE:CG2	2.47	0.44
1:A:610:GLU:HG3	1:A:613:ARG:HH21	1.83	0.44
1:B:1108:GLN:O	1:B:1109:LEU:HD12	2.18	0.44
1:B:273:TYR:CE2	1:B:277:LEU:HD11	2.53	0.44
1:B:283:LEU:HD23	1:B:286:LYS:HD2	2.00	0.44
1:B:65:PRO:CB	1:B:202:ILE:HD12	2.48	0.44
1:B:692:SER:OG	1:B:695:ARG:HB3	2.18	0.44
1:A:1079:LEU:HD23	1:A:1194:LEU:HD21	2.01	0.43
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	2.00	0.43
1:A:150:ALA:O	1:A:154:GLN:HG2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:GLN:O	1:A:330:VAL:HG22	2.18	0.43
1:A:692:SER:OG	1:A:695:ARG:HB3	2.18	0.43
1:A:125:ALA:O	1:A:129:VAL:HG12	2.18	0.43
1:A:808:GLY:HA2	1:A:811:THR:HG22	1.99	0.43
1:B:113:TYR:O	1:B:117:ILE:HG13	2.18	0.43
1:B:1124:ALA:HB2	1:B:1161:TYR:HB2	2.00	0.43
1:B:1040:TYR:HA	1:B:1041:PRO:HD3	1.90	0.43
1:A:925:ARG:HG3	1:B:514:HIS:CD2	2.53	0.43
1:B:957:ALA:O	1:B:961:THR:HG23	2.18	0.43
1:B:975:SER:O	1:B:979:PHE:HB2	2.18	0.43
1:A:289:ILE:O	1:A:293:ILE:HG12	2.18	0.43
1:B:1197:GLU:HB3	1:B:1200:SER:HB3	2.00	0.43
1:A:1036:VAL:N	1:A:1088:GLY:HA3	2.31	0.43
1:A:215:LEU:O	1:A:219:PRO:HD3	2.18	0.43
1:A:726:VAL:O	1:A:730:LYS:HG2	2.18	0.43
1:B:488:ARG:CZ	1:B:491:VAL:HG12	2.49	0.43
1:B:293:ILE:HD12	1:B:767:PHE:HD1	1.83	0.43
1:A:210:LEU:HD21	1:A:327:VAL:HG13	2.01	0.43
1:A:491:VAL:HG11	1:A:542:VAL:CG1	2.48	0.43
1:B:488:ARG:HB3	1:B:491:VAL:HG13	2.00	0.43
1:A:1002:SER:HA	1:A:1005:ILE:HG12	2.01	0.43
1:A:122:LEU:HD12	1:A:123:ILE:N	2.34	0.43
1:A:277:LEU:HA	1:A:277:LEU:HD23	1.86	0.43
1:A:277:LEU:C	1:A:279:GLU:H	2.22	0.43
1:B:1062:LEU:HD11	1:B:1240:VAL:HG23	2.01	0.43
1:B:422:VAL:HG22	1:B:423:GLY:H	1.83	0.43
1:A:488:ARG:NH2	1:A:491:VAL:HG12	2.34	0.43
1:B:156:ILE:HD11	1:B:439:LEU:O	2.17	0.43
1:B:281:LYS:HG3	1:B:782:LYS:HB2	2.01	0.43
1:B:707:PHE:O	1:B:711:ILE:HG13	2.19	0.43
1:B:896:ALA:HB2	1:B:912:PHE:CD2	2.54	0.43
1:B:1022:LEU:O	1:B:1024:PRO:HD3	2.19	0.43
1:B:1061:THR:HG22	1:B:1223:CYS:HB3	2.00	0.43
1:A:1118:LEU:HD12	1:A:1165:VAL:HG11	2.01	0.43
1:A:211:THR:HG22	1:A:334:VAL:HG21	2.00	0.43
1:A:727:ILE:HB	1:A:755:PHE:HE1	1.84	0.43
1:B:691:ALA:HB1	1:B:692:SER:HA	2.01	0.43
1:A:86:LYS:NZ	1:A:739:GLY:HA2	2.33	0.42
1:A:784:LEU:CD2	1:A:821:VAL:HG11	2.48	0.42
1:B:1033:PHE:CE2	1:B:1075:VAL:HG13	2.54	0.42
1:B:1081:ARG:HD3	1:B:1097:ILE:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:488:ARG:NH2	1:B:491:VAL:HG12	2.34	0.42
1:A:54:THR:CG2	1:A:132:TRP:HZ2	2.32	0.42
1:B:828:ARG:HA	1:B:831:VAL:HG22	1.99	0.42
1:A:848:ILE:HG13	1:A:849:TYR:CD1	2.53	0.42
1:B:1064:LEU:HB2	1:B:1226:ILE:HG13	2.01	0.42
1:B:730:LYS:HB3	1:B:751:PHE:CE2	2.54	0.42
1:B:792:MET:CE	1:B:810:LEU:HB3	2.49	0.42
1:A:1070:CYS:HA	1:A:1071:GLY:HA2	1.56	0.42
1:A:303:TYR:HE1	1:A:758:LEU:HD23	1.84	0.42
1:A:980:GLY:O	1:A:984:VAL:HG13	2.19	0.42
1:B:169:THR:O	1:B:173:ASP:HB2	2.19	0.42
1:B:603:VAL:HG13	1:B:604:GLU:H	1.84	0.42
1:A:132:TRP:CZ3	1:A:186:ILE:HD11	2.55	0.42
1:A:372:ASP:HA	1:A:373:SER:HB3	2.01	0.42
1:A:424:ASN:H	1:A:429:LYS:NZ	2.17	0.42
1:A:436:MET:HB3	1:A:549:LEU:HD21	2.02	0.42
1:B:123:ILE:O	1:B:127:ILE:HG12	2.19	0.42
1:B:221:LEU:HD12	1:B:222:GLY:N	2.35	0.42
1:A:1064:LEU:HD22	1:A:1242:ILE:HD11	2.00	0.42
1:A:604:GLU:OE1	1:A:617:ILE:N	2.52	0.42
1:A:482:GLU:HA	1:A:485:ARG:HG2	2.01	0.42
1:B:1181:ALA:O	1:B:1184:ARG:HB3	2.20	0.42
1:B:286:LYS:O	1:B:290:THR:HG23	2.20	0.42
1:B:610:GLU:OE1	1:B:610:GLU:N	2.52	0.42
1:A:1040:TYR:HA	1:A:1041:PRO:HD3	1.73	0.42
1:B:1160:LYS:HB3	1:B:1161:TYR:H	1.65	0.42
1:B:257:ILE:HG13	1:B:261:ILE:HG13	2.02	0.42
1:A:922:ILE:HB	1:A:923:PRO:HD3	2.01	0.42
1:B:703:GLU:HB3	1:B:706:TYR:HD2	1.84	0.42
1:A:282:ARG:N	1:A:282:ARG:HE	2.17	0.41
1:A:484:ILE:HG21	1:A:496:ILE:HG23	2.01	0.41
1:B:508:PHE:O	1:B:512:LEU:HG	2.20	0.41
1:A:335:LEU:HA	1:A:335:LEU:HD12	1.87	0.41
1:A:156:ILE:HD11	1:A:439:LEU:O	2.19	0.41
1:A:200:PHE:CE2	1:A:215:LEU:HD12	2.54	0.41
1:A:390:PHE:O	1:A:410:ASN:HA	2.19	0.41
1:B:289:ILE:HD13	1:B:771:PHE:CE1	2.54	0.41
1:B:46:ASP:OD1	1:B:138:ARG:NH1	2.54	0.41
1:A:484:ILE:HG23	1:A:542:VAL:HG21	2.03	0.41
1:A:54:THR:HG23	1:A:132:TRP:HZ2	1.85	0.41
1:A:136:ALA:HB2	1:A:183:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:ALA:O	1:A:294:SER:OG	2.27	0.41
1:B:1100:LEU:HD13	1:B:1105:LEU:HD13	2.02	0.41
1:B:404:GLN:HB3	1:B:407:LYS:HZ3	1.86	0.41
1:A:1049:LEU:HD21	1:A:1071:GLY:HA3	2.02	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HB3	2.02	0.41
1:A:1157:LEU:HD12	1:A:1158:PRO:HD2	2.03	0.41
1:A:54:THR:O	1:A:58:ILE:HG12	2.21	0.41
1:A:594:ILE:HB	1:A:611:LEU:HD22	2.02	0.41
1:A:719:GLY:C	1:A:722:PRO:HD2	2.40	0.41
1:B:322:TYR:O	1:B:326:GLN:HB3	2.21	0.41
1:A:113:TYR:O	1:A:117:ILE:HG13	2.21	0.41
1:B:1023:LYS:HA	1:B:1024:PRO:HD3	1.82	0.41
1:B:1089:SER:HB3	1:B:1096:GLU:HG2	2.03	0.41
1:B:1217:ALA:O	1:B:1221:ARG:HD2	2.20	0.41
1:B:150:ALA:O	1:B:154:GLN:HG2	2.20	0.41
1:A:550:LEU:HD23	1:A:569:LEU:HD13	2.02	0.41
1:A:64:LEU:HB3	1:A:65:PRO:HD3	2.02	0.41
1:A:67:MET:HE3	1:A:946:TYR:CD2	2.56	0.41
1:B:257:ILE:HG21	1:B:800:PHE:CD2	2.55	0.41
1:B:388:LEU:HB2	1:B:413:VAL:HB	2.02	0.41
1:A:1004:ILE:O	1:A:1008:ILE:HG13	2.20	0.41
1:A:203:GLY:C	1:A:211:THR:HG21	2.41	0.41
1:A:955:PHE:O	1:A:959:LEU:HG	2.20	0.41
1:B:825:THR:OG1	1:B:826:GLY:N	2.53	0.41
1:B:833:PHE:HD1	1:B:836:ILE:HD11	1.86	0.41
1:A:39:PHE:CD1	1:A:50:MET:HE1	2.56	0.41
1:A:828:ARG:HD2	1:A:828:ARG:HA	1.88	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	2.02	0.41
1:A:519:LEU:HD22	1:A:519:LEU:H	1.85	0.41
1:B:156:ILE:H	1:B:156:ILE:HG13	1.59	0.41
1:B:314:THR:HA	1:B:317:VAL:HG12	2.02	0.41
1:B:956:GLY:O	1:B:960:VAL:HG23	2.21	0.41
1:A:1243:GLN:OE1	1:A:1248:LYS:HD2	2.20	0.40
1:B:983:ALA:O	1:B:987:VAL:HG23	2.22	0.40
1:A:140:ILE:HD13	1:A:140:ILE:HA	1.85	0.40
1:A:156:ILE:HG12	1:A:439:LEU:HB3	2.03	0.40
1:A:310:PHE:HD2	1:A:755:PHE:HE2	1.63	0.40
1:A:828:ARG:HG2	1:A:994:TYR:CE2	2.55	0.40
1:A:845:ILE:HG22	1:A:972:LEU:HD21	2.03	0.40
1:B:147:PHE:O	1:B:151:ILE:HG13	2.21	0.40
1:A:1175:GLY:O	1:A:1179:ARG:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:791:SER:O	1:A:795:GLN:HG2	2.20	0.40
1:A:729:SER:OG	1:A:972:LEU:HD12	2.21	0.40
1:B:1096:GLU:OE1	1:B:1097:ILE:N	2.54	0.40
1:B:1090:VAL:O	1:B:1097:ILE:HG13	2.20	0.40
1:A:107:MET:SD	1:A:110:TYR:HD2	2.44	0.40
1:A:139:GLN:O	1:A:143:ILE:HG13	2.22	0.40
1:B:1189:GLN:OE1	1:B:1221:ARG:NH2	2.55	0.40
1:B:829:LEU:O	1:B:832:ILE:HG22	2.21	0.40
1:B:728:PHE:HE2	1:B:971:LEU:HD21	1.87	0.40

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	1184/1282 (92%)	1124 (95%)	54 (5%)	6 (0%)	29	66
1	B	1176/1282 (92%)	1111 (94%)	57 (5%)	8 (1%)	22	60
All	All	2360/2564 (92%)	2235 (95%)	111 (5%)	14 (1%)	25	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1036	VAL
1	B	32	ALA
1	B	1136	VAL
1	A	1070	CYS
1	A	1120	ASP
1	B	393	ILE
1	A	278	GLU
1	A	838	ASN
1	B	278	GLU

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Mol	Chain	Res	Type
1	B	383	ASN
1	B	1172	LEU
1	B	128	GLN
1	B	33	VAL
1	A	1046	ILE

### 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	978/1062 (92%)	953 (97%)	25 (3%)	46	69
1	B	972/1062 (92%)	953 (98%)	19 (2%)	55	75
All	All	1950/2124 (92%)	1906 (98%)	44 (2%)	50	72

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	206	ARG
1	A	258	ARG
1	A	283	LEU
1	A	310	PHE
1	A	374	PHE
1	A	383	ASN
1	A	396	SER
1	A	435	LEU
1	A	478	THR
1	A	520	VAL
1	A	681	LYS
1	A	688	VAL
1	A	695	ARG
1	A	700	ASN
1	A	817	ASP
1	A	852	GLN
1	A	942	GLN
1	A	965	MET

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Mol	Chain	Res	Type
1	A	966	THR
1	A	1020	GLN
1	A	1037	VAL
1	A	1111	ILE
1	A	1163	THR
1	A	1167	ASP
1	A	1168	LYS
1	B	258	ARG
1	B	310	PHE
1	B	335	LEU
1	B	373	SER
1	B	383	ASN
1	B	435	LEU
1	B	478	THR
1	B	603	VAL
1	B	755	PHE
1	B	817	ASP
1	B	828	ARG
1	B	886	LEU
1	B	908	ARG
1	B	944	MET
1	B	966	THR
1	B	967	PHE
1	B	1022	LEU
1	B	1111	ILE
1	B	1163	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	514	HIS
1	A	515	GLN
1	A	608	HIS
1	A	852	GLN
1	B	347	ASN
1	B	514	HIS
1	B	515	GLN
1	B	838	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](#)

Of 13 ligands modelled in this entry, 13 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

### 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, 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	1188/1282 (92%)	-0.16	29 (2%) 59 50	83, 141, 236, 375	0
1	B	1180/1282 (92%)	-0.02	36 (3%) 49 40	86, 152, 247, 420	0
All	All	2368/2564 (92%)	-0.09	65 (2%) 54 45	83, 146, 241, 420	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	598	ASP	5.2
1	B	423	GLY	4.9
1	B	1114	GLN	4.9
1	A	963	GLN	4.3
1	B	1196	ASP	4.1
1	B	1020	GLN	3.9
1	A	1046	ILE	3.6
1	B	1156	SER	3.6
1	B	1068	SER	3.4
1	A	1123	ILE	3.4
1	B	1159	ASP	3.3
1	B	1229	ARG	3.3
1	B	878	GLN	3.3
1	B	1113	SER	3.2
1	B	1227	ALA	3.2
1	A	1227	ALA	3.1
1	A	36	LEU	3.1
1	A	1045	SER	3.0
1	B	1162	ASN	3.0
1	A	1244	ASN	3.0
1	B	1230	LEU	3.0
1	B	1164	ARG	2.9
1	B	1233	ILE	2.9
1	A	1124	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	965	MET	2.8
1	A	1226	ILE	2.8
1	B	1158	PRO	2.8
1	B	1212	GLU	2.7
1	B	876	SER	2.7
1	B	1021	GLY	2.7
1	A	796	ASP	2.7
1	B	875	LEU	2.6
1	A	443	LEU	2.6
1	B	1169	GLY	2.6
1	B	874	MET	2.5
1	A	383	ASN	2.5
1	A	964	LEU	2.5
1	B	1178	GLN	2.5
1	A	1228	HIS	2.5
1	A	108	THR	2.4
1	B	105	GLU	2.4
1	A	1172	LEU	2.4
1	A	1063	ALA	2.4
1	A	278	GLU	2.4
1	B	108	THR	2.4
1	B	597	PHE	2.3
1	A	279	GLU	2.3
1	A	1241	VAL	2.3
1	B	425	SER	2.3
1	A	1162	ASN	2.2
1	A	1171	GLN	2.2
1	A	359	TYR	2.2
1	A	423	GLY	2.2
1	B	1127	ILE	2.2
1	B	989	SER	2.2
1	B	402	GLU	2.2
1	B	1226	ILE	2.2
1	A	526	GLN	2.1
1	B	97	ARG	2.1
1	B	1172	LEU	2.1
1	A	690	PRO	2.1
1	B	109	THR	2.1
1	B	1199	THR	2.0
1	A	1161	TYR	2.0
1	A	489	GLU	2.0

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B	1302	1/1	0.75	0.23	189,189,189,189	1
2	HG	A	1307	1/1	0.81	0.82	138,138,138,138	1
2	HG	A	1302	1/1	0.85	0.48	71,71,71,71	1
2	HG	B	1306	1/1	0.90	0.27	71,71,71,71	1
2	HG	A	1306	1/1	0.90	0.50	96,96,96,96	1
2	HG	B	1303	1/1	0.93	0.09	198,198,198,198	1
2	HG	A	1304	1/1	0.95	0.33	38,38,38,38	1
2	HG	A	1305	1/1	0.96	0.44	65,65,65,65	1
2	HG	A	1303	1/1	0.96	0.33	102,102,102,102	1
2	HG	A	1301	1/1	0.98	0.13	164,164,164,164	1
2	HG	B	1305	1/1	0.98	0.62	46,46,46,46	1
2	HG	B	1304	1/1	0.98	0.25	107,107,107,107	1
2	HG	B	1301	1/1	0.99	0.18	129,129,129,129	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.