



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:44 PM GMT

PDB ID : 4YZM
Title : Humanized Roco4 bound to LRRK2-In1
Authors : Gilsbach, B.K.; Messias, A.C.; Ito, G.; Sattler, M.; Alessi, D.R.; Wittinghofer, A.; Kortholt, A.
Deposited on : 2015-03-25
Resolution : 3.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

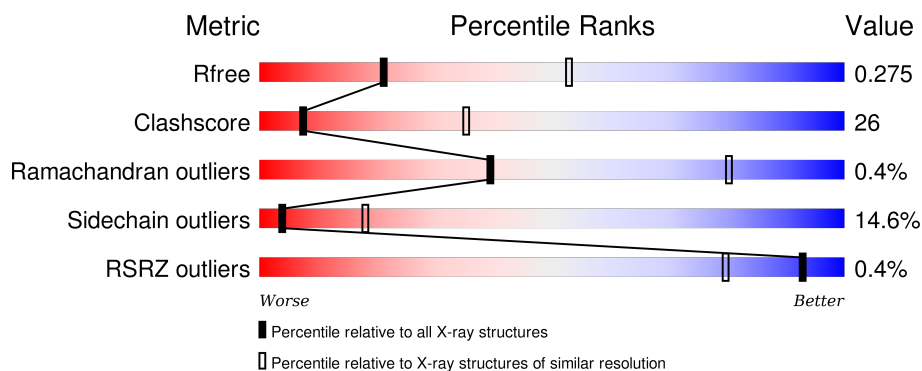
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	287	 49% 32% 9% • 9%
1	B	287	 48% 36% 7% • 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4330 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 Probable serine/threonine-protein kinase roco4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2098	1352	355	377	14			
1	B	262	Total	C	N	O	S	0	1	0
			2110	1359	356	381	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	GLY	-	expression tag	UNP Q6XHB2
A	1007	ALA	-	expression tag	UNP Q6XHB2
A	1008	MET	-	expression tag	UNP Q6XHB2
A	1009	GLY	-	expression tag	UNP Q6XHB2
A	1010	GLY	-	expression tag	UNP Q6XHB2
A	1011	SER	-	expression tag	UNP Q6XHB2
A	1012	GLU	-	expression tag	UNP Q6XHB2
A	1013	PHE	-	expression tag	UNP Q6XHB2
A	1014	PRO	-	expression tag	UNP Q6XHB2
A	1015	LYS	-	expression tag	UNP Q6XHB2
A	1016	SER	-	expression tag	UNP Q6XHB2
A	1017	ARG	-	expression tag	UNP Q6XHB2
A	1018	LEU	-	expression tag	UNP Q6XHB2
A	1107	LEU	PHE	engineered mutation	UNP Q6XHB2
A	1161	LEU	PHE	engineered mutation	UNP Q6XHB2
B	1006	GLY	-	expression tag	UNP Q6XHB2
B	1007	ALA	-	expression tag	UNP Q6XHB2
B	1008	MET	-	expression tag	UNP Q6XHB2
B	1009	GLY	-	expression tag	UNP Q6XHB2
B	1010	GLY	-	expression tag	UNP Q6XHB2
B	1011	SER	-	expression tag	UNP Q6XHB2
B	1012	GLU	-	expression tag	UNP Q6XHB2
B	1013	PHE	-	expression tag	UNP Q6XHB2
B	1014	PRO	-	expression tag	UNP Q6XHB2
B	1015	LYS	-	expression tag	UNP Q6XHB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1016	SER	-	expression tag	UNP Q6XHB2
B	1017	ARG	-	expression tag	UNP Q6XHB2
B	1018	LEU	-	expression tag	UNP Q6XHB2
B	1107	LEU	PHE	engineered mutation	UNP Q6XHB2
B	1161	LEU	PHE	engineered mutation	UNP Q6XHB2

- [illegible]

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

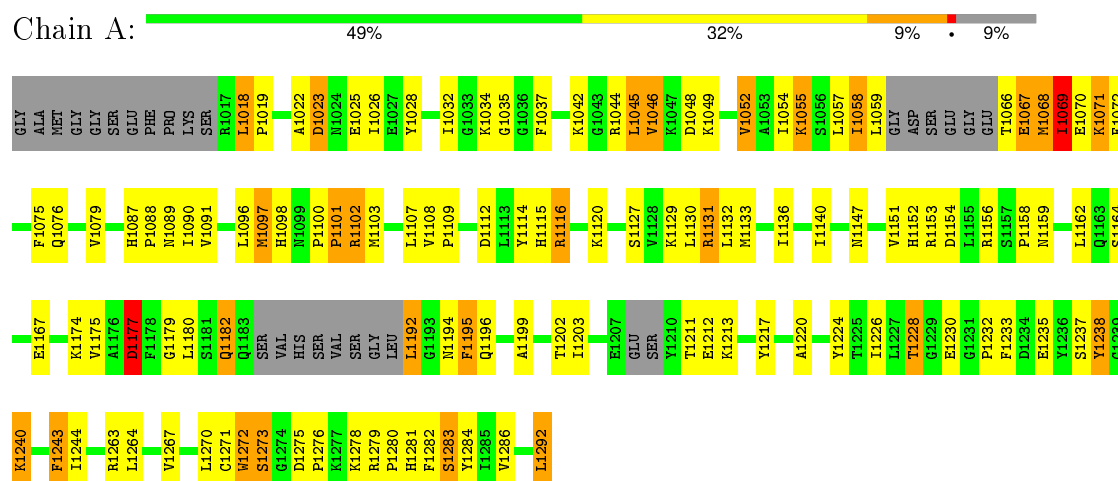
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	23	Total 23	O 23	0	0

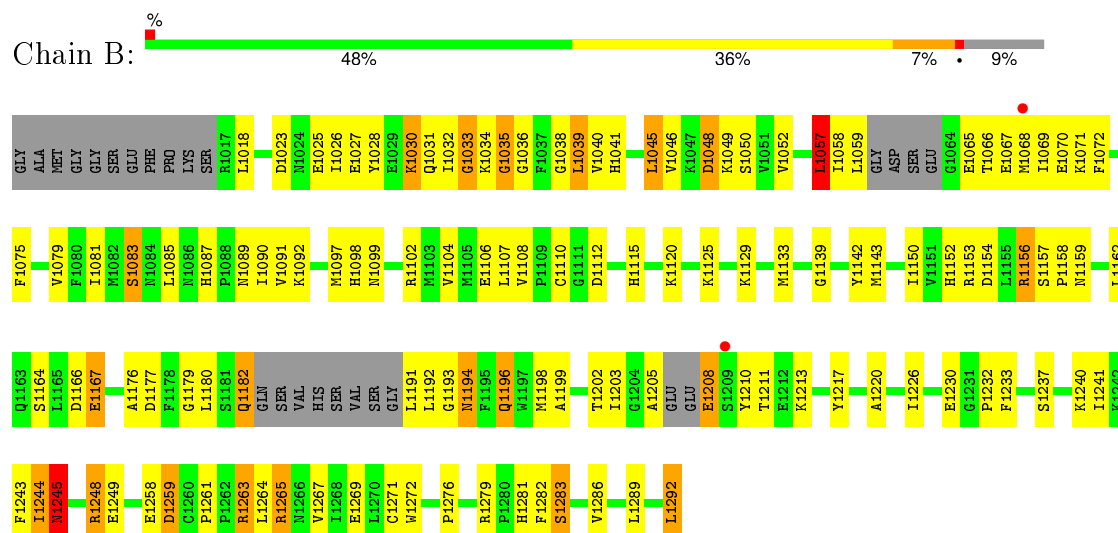
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Probable serine/threonine-protein kinase roco4



- Molecule 1: Probable serine/threonine-protein kinase roco4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.03 Å 89.07 Å 177.71 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 3.00 44.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.43-3.00) 99.9 (44.43-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.282 0.225 , 0.275	Depositor DCC
R_{free} test set	719 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 14409 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4330	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 4K4

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	1.49	3/2145 (0.1%)	1.05	7/2895 (0.2%)
1	B	1.53	3/2160 (0.1%)	1.07	11/2917 (0.4%)
All	All	1.51	6/4305 (0.1%)	1.06	18/5812 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1217	TYR	CE1-CZ	-6.39	1.30	1.38
1	A	1284	TYR	CE1-CZ	-5.88	1.30	1.38
1	B	1035	GLY	N-CA	-5.20	1.38	1.46
1	A	1238	TYR	CE1-CZ	-5.17	1.31	1.38
1	B	1245[A]	ASN	N-CA	5.02	1.56	1.46
1	B	1245[B]	ASN	N-CA	5.02	1.56	1.46

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1195	PHE	N-CA-CB	-14.93	83.72	110.60
1	B	1035	GLY	N-CA-C	-12.96	80.69	113.10
1	A	1195	PHE	N-CA-C	11.57	142.24	111.00
1	A	1179	GLY	N-CA-C	-8.63	91.53	113.10
1	B	1176	ALA	N-CA-C	8.49	133.93	111.00
1	B	1179	GLY	N-CA-C	-8.11	92.84	113.10
1	B	1244	ILE	C-N-CA	7.45	140.33	121.70
1	B	1065	GLU	N-CA-C	7.27	130.63	111.00
1	A	1177	ASP	N-CA-C	7.10	130.16	111.00
1	A	1098	HIS	N-CA-C	6.76	129.24	111.00
1	B	1048	ASP	N-CA-C	-5.95	94.94	111.00
1	B	1065	GLU	CB-CA-C	-5.61	99.17	110.40
1	A	1048	ASP	N-CA-C	-5.38	96.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1033	GLY	N-CA-C	5.38	126.56	113.10
1	B	1066	THR	N-CA-C	-5.37	96.52	111.00
1	B	1057	LEU	CA-CB-CG	5.35	127.60	115.30
1	A	1045	LEU	CB-CG-CD2	-5.26	102.06	111.00
1	B	1036	GLY	N-CA-C	-5.12	100.29	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2098	0	2119	112	0
1	B	2110	0	2130	105	0
2	A	42	0	38	4	0
2	B	42	0	38	2	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	13	0	0	0	0
4	B	23	0	0	7	0
All	All	4330	0	4325	221	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 26.

All (221) 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:1192:LEU:CD2	1:A:1196:GLN:HE21	1.50	1.24
1:B:1035:GLY:HA3	1:B:1038:GLY:O	1.36	1.20
1:A:1058:ILE:O	1:A:1071:LYS:NZ	1.78	1.16
1:A:1199:ALA:O	1:A:1202:THR:OG1	1.67	1.12
1:B:1075:PHE:O	1:B:1079:VAL:HG23	1.47	1.10
1:A:1192:LEU:CD2	1:A:1196:GLN:NE2	2.17	1.07
1:B:1248:ARG:HH11	1:B:1248:ARG:HB2	1.18	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1192:LEU:HD22	1:A:1196:GLN:HE21	1.15	1.05
1:B:1112:ASP:OD2	1:B:1115:HIS:HD2	1.43	1.02
1:A:1154:ASP:O	1:A:1159:ASN:ND2	1.93	1.01
1:A:1087:HIS:HD2	1:A:1089:ASN:H	1.09	0.93
1:B:1048:ASP:OD1	1:B:1050:SER:OG	1.86	0.93
1:B:1129:LYS:HE2	1:B:1226:ILE:O	1.70	0.92
1:A:1025:GLU:O	1:A:1046:VAL:HG22	1.69	0.92
1:A:1192:LEU:HD23	1:A:1196:GLN:NE2	1.82	0.91
1:B:1156:ARG:HB2	1:B:1158:PRO:HD2	1.51	0.91
1:A:1067:GLU:O	1:A:1070:GLU:HG2	1.69	0.91
1:B:1092:LYS:N	1:B:1106:GLU:OE2	2.06	0.88
1:A:1087:HIS:CD2	1:A:1089:ASN:H	1.90	0.88
1:A:1075:PHE:O	1:A:1079:VAL:HG23	1.76	0.86
1:A:1068:MET:O	1:A:1070:GLU:N	2.08	0.86
1:A:1025:GLU:O	1:A:1046:VAL:CG2	2.23	0.86
1:A:1224:TYR:O	1:A:1228:THR:OG1	1.93	0.86
1:B:1248:ARG:CB	1:B:1248:ARG:HH11	1.88	0.85
1:B:1033:GLY:HA3	1:B:1040:VAL:H	1.40	0.85
1:B:1035:GLY:CA	1:B:1038:GLY:O	2.23	0.84
1:A:1232:PRO:O	1:A:1233:PHE:HB2	1.77	0.84
1:A:1068:MET:C	1:A:1070:GLU:H	1.83	0.82
1:A:1112:ASP:OD1	1:A:1115:HIS:HD2	1.62	0.82
1:B:1112:ASP:OD2	1:B:1115:HIS:CD2	2.32	0.81
1:A:1032:ILE:HD13	1:A:1042:LYS:HB2	1.62	0.81
1:A:1100:PRO:HG2	1:A:1102:ARG:HD3	1.61	0.81
1:A:1273:SER:O	1:A:1279:ARG:NH2	2.13	0.81
1:A:1132:LEU:O	1:A:1136:ILE:HG13	1.79	0.81
1:B:1232:PRO:O	1:B:1233:PHE:HB2	1.80	0.80
1:B:1030:LYS:HG2	1:B:1031:GLN:N	1.94	0.79
1:A:1282:PHE:O	1:A:1286:VAL:HG23	1.82	0.79
1:B:1167:GLU:CG	4:B:1408:HOH:O	2.31	0.79
1:B:1167:GLU:HG2	4:B:1408:HOH:O	1.84	0.78
1:A:1152:HIS:O	1:A:1153:ARG:HB2	1.84	0.77
1:A:1045:LEU:N	1:A:1045:LEU:HD22	2.00	0.76
1:A:1058:ILE:HG23	1:A:1071:LYS:NZ	2.01	0.76
1:A:1129:LYS:O	1:A:1133:MET:HG3	1.85	0.76
1:A:1087:HIS:HB3	1:A:1090:ILE:HG12	1.69	0.74
1:B:1208:GLU:O	1:B:1208:GLU:HG3	1.86	0.74
1:B:1182:GLN:NE2	1:B:1192:LEU:O	2.21	0.74
1:B:1120:LYS:NZ	1:B:1230:GLU:OE2	2.20	0.74
1:A:1153:ARG:O	1:A:1182:GLN:HG2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1159:ASN:OD1	1:A:1177:ASP:OD2	2.08	0.72
1:B:1194:ASN:HB3	1:B:1196:GLN:OE1	1.90	0.72
1:B:1282:PHE:O	1:B:1286:VAL:HG23	1.90	0.71
1:A:1032:ILE:CD1	1:A:1042:LYS:HB2	2.21	0.71
1:A:1087:HIS:HD2	1:A:1089:ASN:N	1.87	0.70
1:A:1151:VAL:O	1:A:1180:LEU:HD22	1.92	0.70
1:B:1265:ARG:O	1:B:1269:GLU:HG3	1.92	0.69
1:A:1035:GLY:O	1:A:1055:LYS:HE2	1.92	0.69
1:A:1034:LYS:HG3	1:A:1034:LYS:O	1.93	0.68
1:B:1067:GLU:HA	1:B:1070:GLU:HG3	1.76	0.68
1:B:1240:LYS:O	1:B:1244:ILE:HG13	1.94	0.67
1:A:1270:LEU:O	1:A:1273:SER:OG	2.12	0.67
1:A:1045:LEU:HD21	1:A:1052:VAL:CG2	2.25	0.67
1:A:1070:GLU:OE1	1:A:1070:GLU:HA	1.94	0.67
1:B:1248:ARG:HB2	1:B:1248:ARG:NH1	2.03	0.67
1:A:1044:ARG:NH1	1:A:1049:LYS:O	2.27	0.67
1:B:1057:LEU:HD21	1:B:1072:PHE:HD1	1.59	0.67
1:B:1281:HIS:ND1	1:B:1283:SER:OG	2.27	0.66
1:B:1129:LYS:O	1:B:1133:MET:HG3	1.96	0.65
1:A:1159:ASN:CG	1:A:1177:ASP:OD2	2.36	0.64
1:A:1112:ASP:OD1	1:A:1115:HIS:CD2	2.50	0.64
1:B:1079:VAL:O	1:B:1083:SER:OG	2.14	0.64
1:A:1114:TYR:HB2	1:A:1158:PRO:HD3	1.80	0.64
1:A:1025:GLU:C	1:A:1046:VAL:HG22	2.17	0.64
1:A:1087:HIS:HB3	1:A:1090:ILE:CG1	2.28	0.63
1:A:1025:GLU:C	1:A:1046:VAL:CG2	2.66	0.63
1:B:1081:ILE:O	1:B:1085:LEU:HG	1.98	0.63
1:A:1058:ILE:HD12	1:A:1059:LEU:N	2.13	0.63
1:A:1058:ILE:HG23	1:A:1071:LYS:HZ1	1.64	0.62
1:B:1248:ARG:HH11	1:B:1248:ARG:CG	2.12	0.62
1:A:1088:PRO:O	1:A:1174:LYS:HE3	1.97	0.62
1:A:1240:LYS:O	1:A:1244:ILE:HG12	1.98	0.62
1:B:1110:CYS:HB2	1:B:1162:LEU:O	1.99	0.62
1:B:1263:ARG:O	1:B:1267:VAL:HG23	1.99	0.62
1:B:1157:SER:OG	1:B:1158:PRO:HD3	2.00	0.62
1:A:1097:MET:HB2	1:A:1102:ARG:HB2	1.82	0.61
1:A:1068:MET:C	1:A:1070:GLU:N	2.48	0.61
1:B:1033:GLY:N	1:B:1040:VAL:O	2.34	0.61
1:A:1018:LEU:HD22	1:A:1019:PRO:HD2	1.83	0.60
1:A:1023:ASP:N	1:A:1023:ASP:OD1	2.32	0.60
1:B:1068:MET:CB	4:B:1421:HOH:O	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1177:ASP:OD2	3:B:1302:MG:MG	1.44	0.60
1:A:1213:LYS:HD2	1:A:1276:PRO:O	2.02	0.59
1:A:1264:LEU:HB2	1:A:1292:LEU:HD21	1.85	0.59
1:A:1057:LEU:HD21	1:A:1075:PHE:CD2	2.38	0.59
1:B:1153:ARG:NH1	1:B:1180:LEU:O	2.36	0.59
1:A:1263:ARG:HB3	1:A:1292:LEU:HD11	1.84	0.59
1:B:1152:HIS:O	1:B:1153:ARG:HB2	2.03	0.59
1:B:1030:LYS:HG2	1:B:1031:GLN:H	1.68	0.59
1:A:1045:LEU:HD21	1:A:1052:VAL:HG21	1.84	0.59
1:B:1199:ALA:O	1:B:1202:THR:OG1	2.21	0.59
1:A:1263:ARG:O	1:A:1267:VAL:HG23	2.03	0.58
1:A:1037:PHE:HZ	1:A:1103:MET:CE	2.16	0.58
1:B:1069:ILE:HG13	1:B:1070:GLU:N	2.17	0.58
1:B:1143:MET:HB3	1:B:1150:ILE:HB	1.85	0.58
1:A:1042:LYS:HG3	1:A:1107:LEU:HD22	1.86	0.57
1:A:1058:ILE:C	1:A:1058:ILE:HD12	2.24	0.57
1:B:1034:LYS:HD3	1:B:1035:GLY:O	2.05	0.57
1:A:1058:ILE:HG23	1:A:1071:LYS:HZ3	1.70	0.57
1:B:1068:MET:HB3	4:B:1421:HOH:O	2.05	0.57
1:B:1081:ILE:HG22	1:B:1085:LEU:HD11	1.87	0.56
1:B:1039:LEU:HD23	1:B:1041:HIS:CE1	2.41	0.55
1:A:1045:LEU:H	1:A:1045:LEU:HD22	1.71	0.54
1:A:1087:HIS:CD2	1:A:1089:ASN:HB2	2.42	0.54
1:B:1213:LYS:HD2	1:B:1276:PRO:O	2.07	0.54
1:A:1263:ARG:HB3	1:A:1292:LEU:CD1	2.38	0.54
1:A:1018:LEU:HD22	1:A:1019:PRO:CD	2.37	0.54
1:B:1081:ILE:HG22	1:B:1085:LEU:CD1	2.38	0.54
1:B:1087:HIS:CD2	1:B:1089:ASN:H	2.26	0.54
1:B:1091:VAL:HG13	1:B:1106:GLU:HG2	1.90	0.53
1:A:1025:GLU:O	1:A:1046:VAL:HG23	2.06	0.53
1:A:1281:HIS:ND1	1:A:1283:SER:OG	2.38	0.53
1:A:1108:VAL:HG13	1:A:1109:PRO:HD2	1.90	0.53
1:B:1097:MET:HE2	1:B:1104:VAL:HG22	1.91	0.53
1:A:1116:ARG:O	1:A:1116:ARG:HD2	2.09	0.53
1:A:1022:ALA:N	1:A:1025:GLU:OE1	2.37	0.52
1:B:1230:GLU:HB3	4:B:1403:HOH:O	2.08	0.52
1:B:1108:VAL:O	2:B:1301:4K4:H27	2.10	0.52
1:B:1033:GLY:HA3	1:B:1040:VAL:N	2.19	0.52
1:B:1033:GLY:HA2	1:B:1040:VAL:HB	1.91	0.52
1:B:1248:ARG:NH1	1:B:1248:ARG:CG	2.71	0.52
1:B:1027:GLU:HG3	1:B:1046:VAL:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1205:ALA:C	1:B:1208:GLU:HA	2.30	0.52
1:B:1153:ARG:HG2	1:B:1210:TYR:CD2	2.44	0.52
1:B:1045:LEU:O	1:B:1049:LYS:HA	2.11	0.51
1:B:1153:ARG:HG2	1:B:1210:TYR:CE2	2.45	0.51
1:B:1259:ASP:OD1	1:B:1259:ASP:N	2.44	0.51
1:B:1045:LEU:O	1:B:1048:ASP:O	2.29	0.51
1:A:1045:LEU:CD2	1:A:1045:LEU:N	2.73	0.50
1:A:1037:PHE:CD1	1:A:1037:PHE:C	2.86	0.50
1:B:1081:ILE:CG2	1:B:1085:LEU:HD11	2.42	0.49
1:B:1075:PHE:O	1:B:1079:VAL:CG2	2.40	0.49
1:A:1177:ASP:OD1	1:A:1177:ASP:O	2.29	0.49
1:B:1026:ILE:HD11	1:B:1028:TYR:CE1	2.47	0.49
1:A:1018:LEU:HD12	1:A:1096:LEU:HG	1.95	0.49
1:B:1058:ILE:O	1:B:1071:LYS:NZ	2.35	0.49
1:B:1035:GLY:HA3	1:B:1038:GLY:C	2.22	0.49
1:A:1072:PHE:O	1:A:1075:PHE:HB3	2.12	0.49
1:B:1057:LEU:HD21	1:B:1072:PHE:CD1	2.45	0.48
1:A:1203:ILE:HG21	1:A:1244:ILE:HD12	1.95	0.48
1:A:1018:LEU:CD1	1:A:1096:LEU:HG	2.43	0.48
1:B:1281:HIS:CE1	1:B:1283:SER:OG	2.67	0.48
1:B:1033:GLY:CA	1:B:1040:VAL:H	2.20	0.48
1:B:1026:ILE:HG22	1:B:1045:LEU:HD12	1.95	0.47
1:B:1241:ILE:O	1:B:1245[A]:ASN:HB2	2.14	0.47
1:A:1108:VAL:CG1	1:A:1109:PRO:HD2	2.45	0.47
1:B:1154:ASP:O	1:B:1159:ASN:ND2	2.48	0.47
1:A:1026:ILE:HD11	1:A:1028:TYR:CE1	2.50	0.47
1:B:1097:MET:CE	1:B:1104:VAL:HG22	2.45	0.46
1:A:1136:ILE:O	1:A:1140:ILE:HG13	2.14	0.46
1:B:1289:LEU:HA	1:B:1292:LEU:HD23	1.97	0.46
1:A:1177:ASP:O	1:A:1177:ASP:CG	2.54	0.46
1:A:1034:LYS:HE3	1:A:1034:LYS:HB2	1.79	0.46
1:A:1066:THR:O	1:A:1067:GLU:HG2	2.16	0.46
1:B:1034:LYS:HB3	1:B:1035:GLY:O	2.15	0.46
1:B:1097:MET:HB2	1:B:1102:ARG:HB2	1.96	0.46
1:B:1157:SER:N	1:B:1158:PRO:CD	2.79	0.46
1:B:1199:ALA:HA	1:B:1217:TYR:CD1	2.50	0.46
1:A:1054:ILE:HA	1:A:1103:MET:O	2.16	0.46
1:B:1087:HIS:HD2	1:B:1089:ASN:H	1.63	0.46
1:A:1130:LEU:HA	1:A:1130:LEU:HD23	1.77	0.46
1:A:1220:ALA:HB2	1:A:1271:CYS:HB2	1.99	0.45
1:B:1196:GLN:H	1:B:1196:GLN:CD	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:ILE:HG23	1:A:1058:ILE:O	2.16	0.45
1:B:1032:ILE:CD1	1:B:1107:LEU:HD11	2.47	0.45
1:B:1264:LEU:HD12	1:B:1264:LEU:O	2.17	0.45
1:A:1192:LEU:HD22	1:A:1196:GLN:NE2	2.00	0.45
2:A:1301:4K4:H19	2:A:1301:4K4:CAI	2.47	0.44
1:A:1129:LYS:HE2	1:A:1226:ILE:O	2.17	0.44
1:A:1059:LEU:O	1:A:1069:ILE:HG23	2.17	0.44
1:B:1194:ASN:O	1:B:1198:MET:HG3	2.18	0.44
1:A:1069:ILE:O	1:A:1070:GLU:OE1	2.36	0.44
1:A:1101:PRO:O	1:A:1102:ARG:HG3	2.18	0.44
1:B:1046:VAL:O	1:B:1046:VAL:HG12	2.18	0.43
1:B:1087:HIS:HB3	1:B:1090:ILE:HG12	2.01	0.43
1:A:1037:PHE:HZ	1:A:1103:MET:HE1	1.84	0.43
1:A:1182:GLN:C	1:A:1182:GLN:NE2	2.72	0.43
1:B:1068:MET:HB2	4:B:1421:HOH:O	2.18	0.43
1:A:1045:LEU:HD21	1:A:1052:VAL:HG23	1.98	0.43
1:A:1087:HIS:CG	1:A:1088:PRO:HD2	2.54	0.42
1:A:1097:MET:HB3	1:A:1102:ARG:NH2	2.33	0.42
2:A:1301:4K4:N3	2:A:1301:4K4:CAJ	2.80	0.42
1:A:1112:ASP:OD2	1:A:1114:TYR:HB3	2.19	0.42
1:A:1279:ARG:HA	1:A:1280:PRO:HD3	1.81	0.42
1:B:1194:ASN:HA	1:B:1194:ASN:HD22	1.63	0.42
1:B:1220:ALA:HB2	1:B:1271:CYS:HB2	2.00	0.42
1:A:1131:ARG:HD2	1:A:1131:ARG:HA	1.58	0.42
1:A:1057:LEU:CD2	1:A:1075:PHE:CD2	3.01	0.42
1:B:1156:ARG:CZ	1:B:1193:GLY:HA2	2.50	0.42
1:B:1166:ASP:OD1	1:B:1167:GLU:N	2.52	0.42
2:B:1301:4K4:H2	2:B:1301:4K4:H17	1.85	0.42
1:B:1028:TYR:OH	1:B:1102:ARG:HD2	2.19	0.42
1:B:1098:HIS:O	1:B:1099:ASN:HB2	2.19	0.42
1:B:1203:ILE:O	1:B:1248:ARG:NH2	2.53	0.42
1:B:1139:GLY:O	1:B:1142:TYR:HB3	2.20	0.42
1:A:1275:ASP:HB3	1:A:1278:LYS:HG3	2.00	0.42
1:A:1108:VAL:HG12	1:A:1162:LEU:O	2.19	0.42
1:A:1177:ASP:HB3	2:A:1301:4K4:H36	2.02	0.41
1:B:1182:GLN:C	1:B:1182:GLN:NE2	2.73	0.41
1:B:1087:HIS:HB3	1:B:1090:ILE:CG1	2.51	0.41
1:A:1292:LEU:HA	1:A:1292:LEU:HD12	1.86	0.41
1:A:1120:LYS:NZ	1:A:1230:GLU:OE2	2.53	0.41
1:A:1238:TYR:HB2	1:A:1243:PHE:CD2	2.56	0.41
1:B:1276:PRO:O	1:B:1279:ARG:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1220:ALA:HB2	1:B:1271:CYS:CB	2.50	0.41
2:A:1301:4K4:CAI	2:A:1301:4K4:CAR	2.99	0.41
1:B:1167:GLU:HG3	4:B:1408:HOH:O	2.07	0.41
1:A:1091:VAL:HG23	1:A:1175:VAL:O	2.21	0.41
1:A:1067:GLU:O	1:A:1070:GLU:CG	2.55	0.41
1:B:1034:LYS:CG	1:B:1035:GLY:O	2.69	0.41
1:A:1272:TRP:O	1:A:1272:TRP:CD1	2.74	0.41
1:B:1035:GLY:HA2	1:B:1040:VAL:HG23	2.02	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	252/287 (88%)	240 (95%)	10 (4%)	2 (1%)	24	66
1	B	255/287 (89%)	252 (99%)	3 (1%)	0	100	100
All	All	507/574 (88%)	492 (97%)	13 (3%)	2 (0%)	39	80

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	ILE
1	A	1195	PHE

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	232/253 (92%)	196 (84%)	36 (16%)	3	16
1	B	234/253 (92%)	201 (86%)	33 (14%)	4	19
All	All	466/506 (92%)	397 (85%)	69 (15%)	4	17

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1018	LEU
1	A	1023	ASP
1	A	1046	VAL
1	A	1052	VAL
1	A	1055	LYS
1	A	1058	ILE
1	A	1067	GLU
1	A	1068	MET
1	A	1069	ILE
1	A	1071	LYS
1	A	1076	GLN
1	A	1097	MET
1	A	1101	PRO
1	A	1102	ARG
1	A	1116	ARG
1	A	1127	SER
1	A	1131	ARG
1	A	1147	ASN
1	A	1156	ARG
1	A	1164	SER
1	A	1167	GLU
1	A	1177	ASP
1	A	1182	GLN
1	A	1192	LEU
1	A	1194	ASN
1	A	1211	THR
1	A	1212	GLU
1	A	1228	THR
1	A	1235	GLU
1	A	1237	SER
1	A	1240	LYS
1	A	1243	PHE
1	A	1272	TRP
1	A	1273	SER

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Mol	Chain	Res	Type
1	A	1283	SER
1	A	1292	LEU
1	B	1018	LEU
1	B	1023	ASP
1	B	1025	GLU
1	B	1030	LYS
1	B	1039	LEU
1	B	1045	LEU
1	B	1052	VAL
1	B	1057	LEU
1	B	1059	LEU
1	B	1083	SER
1	B	1125	LYS
1	B	1156	ARG
1	B	1164	SER
1	B	1167	GLU
1	B	1182	GLN
1	B	1191	LEU
1	B	1194	ASN
1	B	1196	GLN
1	B	1208	GLU
1	B	1211	THR
1	B	1237	SER
1	B	1243	PHE
1	B	1245[A]	ASN
1	B	1245[B]	ASN
1	B	1248	ARG
1	B	1258	GLU
1	B	1259	ASP
1	B	1261	PRO
1	B	1263	ARG
1	B	1265	ARG
1	B	1272	TRP
1	B	1283	SER
1	B	1292	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1041	HIS
1	A	1087	HIS
1	A	1098	HIS

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Mol	Chain	Res	Type
1	A	1115	HIS
1	A	1182	GLN
1	A	1196	GLN
1	B	1041	HIS
1	B	1087	HIS
1	B	1115	HIS
1	B	1194	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	4K4	A	1301	-	40,47,47	1.83	8 (20%)	49,68,68	2.09	14 (28%)
2	4K4	B	1301	-	40,47,47	1.87	5 (12%)	49,68,68	2.54	13 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means

no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4K4	A	1301	-	-	0/18/38/38	0/5/6/6
2	4K4	B	1301	-	-	0/18/38/38	1/5/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	4K4	CBB-CBA	-5.46	1.41	1.50
2	A	1301	4K4	CBB-CBA	-5.06	1.41	1.50
2	B	1301	4K4	CBG-CBH	-4.33	1.38	1.41
2	A	1301	4K4	CBG-CBH	-3.05	1.39	1.41
2	A	1301	4K4	CBC-NAY	-2.49	1.33	1.39
2	A	1301	4K4	OAZ-CBE	2.23	1.40	1.37
2	A	1301	4K4	CAQ-NBM	2.41	1.51	1.47
2	B	1301	4K4	CAQ-NBM	2.53	1.51	1.47
2	B	1301	4K4	CAR-NBM	2.69	1.51	1.47
2	A	1301	4K4	CAR-NBM	3.20	1.52	1.47
2	A	1301	4K4	CAC-NBO	3.36	1.54	1.47
2	A	1301	4K4	C6-N1	4.70	1.40	1.32
2	B	1301	4K4	C6-N1	6.44	1.43	1.32

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4K4	N1-C2-N3	-6.12	119.85	126.62
2	B	1301	4K4	N1-C2-N3	-4.65	121.47	126.62
2	B	1301	4K4	OAE-CBA-CBB	-3.88	112.83	120.17
2	A	1301	4K4	CBC-NAY-C2	-2.38	122.94	129.22
2	A	1301	4K4	OAE-CBA-CBB	-2.32	115.77	120.17
2	B	1301	4K4	CAQ-NBM-CBA	-2.07	116.33	122.80
2	B	1301	4K4	CAB-NBL-CAS	2.02	113.77	110.63
2	B	1301	4K4	CAB-NBL-CAT	2.06	113.84	110.63
2	A	1301	4K4	CAL-CBH-CBG	2.15	123.01	119.97
2	A	1301	4K4	CAJ-CBC-CBE	2.28	121.71	119.05
2	A	1301	4K4	CAT-CAV-NBN	2.28	116.14	110.79
2	A	1301	4K4	CAR-NBM-CAQ	2.89	117.92	112.56
2	B	1301	4K4	CAP-CAR-NBM	3.12	115.60	111.07
2	A	1301	4K4	CAO-CAQ-NBM	3.14	115.63	111.07
2	A	1301	4K4	C6-N1-C2	3.16	121.83	115.97
2	A	1301	4K4	CAP-CAR-NBM	3.24	115.78	111.07
2	A	1301	4K4	CAU-NBN-CBK	3.36	118.96	112.37
2	A	1301	4K4	CBB-CBA-NBM	3.44	123.35	118.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	4K4	CAS-NBL-CAT	3.50	114.12	109.53
2	B	1301	4K4	CAA-OAZ-CBE	3.62	123.03	117.54
2	B	1301	4K4	CAO-CAQ-NBM	4.09	117.01	111.07
2	B	1301	4K4	CAR-NBM-CAQ	4.31	120.56	112.56
2	A	1301	4K4	C2-N3-C4	4.71	120.77	115.09
2	B	1301	4K4	C2-N3-C4	4.98	121.08	115.09
2	A	1301	4K4	CAU-NBN-CAV	5.30	118.84	109.23
2	B	1301	4K4	CBB-CBA-NBM	5.86	126.58	118.76
2	B	1301	4K4	CAK-CBG-CBH	10.09	122.70	118.06

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1301	4K4	CAS-CAT-CAU-CAV-NBL-NBN

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1301	4K4	4	0
2	B	1301	4K4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	260/287 (90%)	-0.18	0	100 100	21, 32, 69, 93	0
1	B	262/287 (91%)	-0.24	2 (0%)	87 67	17, 33, 62, 94	0
All	All	522/574 (90%)	-0.21	2 (0%)	93 80	17, 33, 64, 94	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1209	SER	2.5
1	B	1068	MET	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	4K4	A	1301	42/42	0.94	0.29	1.07	24,37,98,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	4K4	B	1301	42/42	0.95	0.21	0.35	24,30,71,72	0
3	MG	A	1302	1/1	0.88	0.19	-0.07	26,26,26,26	0
3	MG	B	1302	1/1	0.97	0.19	-0.27	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.