



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:33 AM UTC

PDB ID : 8Y0C / pdb_00008y0c
Title : Crystal structure of FnCas12a in complex with pre-crRNA and 18nt target DNA
Authors : Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 3.45 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

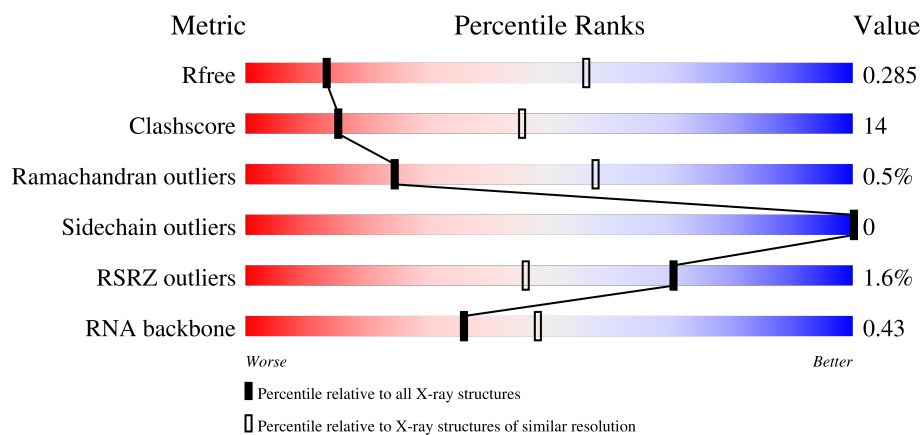
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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 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	B	58	
2	C	27	
3	D	11	
4	A	1300	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12057 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 RNA chain called RNA (42-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	42	Total	C	N	O	P	0	0	0
			890	400	155	294	41			

- Molecule 2 is a DNA chain called DNA (27-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	27	Total	C	N	O	P	0	0	0
			550	265	95	163	27			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	11	Total	C	N	O	P	0	0	0
			221	107	34	69	11			

- Molecule 4 is a protein called CRISPR-associated endonuclease Cas12a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1260	Total	C	N	O	S	0	0	0
			10392	6681	1711	1978	22			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	ALA	GLU	conflict	UNP A0Q7Q2

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		

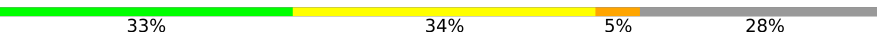
- Molecule 6 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

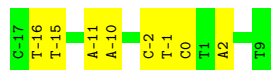
- Molecule 1: RNA (42-MER)

Chain B: 



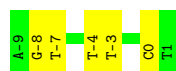
- Molecule 2: DNA (27-MER)

Chain C: 



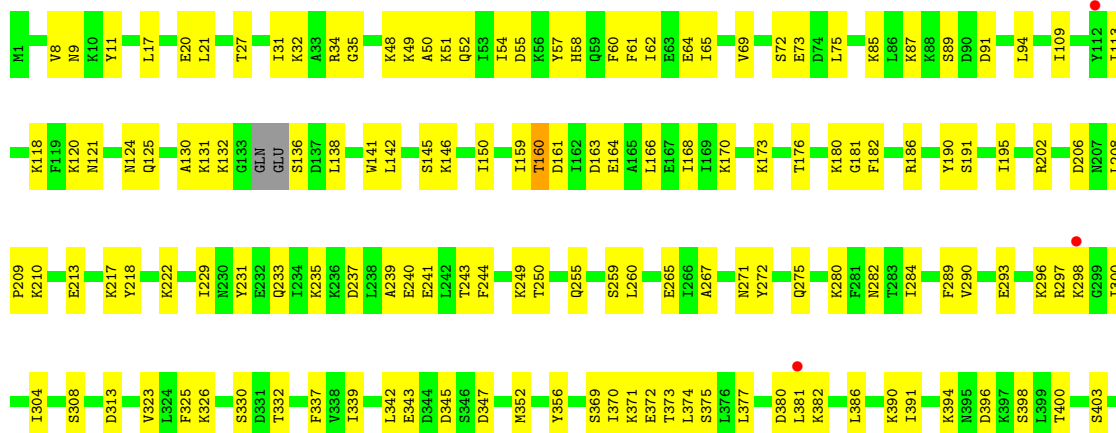
- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*TP*AP*CP*T)-3')

Chain D: 



- Molecule 4: CRISPR-associated endonuclease Cas12a

Chain A: 



D409	K496	I774	T985	Q987	C1086	L1178	D1255
Y410	D497	D775	I886	Y988	P1087	I1183	A1256
L418	K498	S776	N887	D1007	V1088	E1184	M1257
Q423	L499	V777	F888	L1008	T1089	Y1185	G1258
GLN	K505	Q780	K895	ASN	Y1099	E1189	A1259
ILE	Y506	G781	D898	PHE	E1100	I1190	H1261
ALA	G510	K782	L902	GLY	S1101	I1191	K1265
PRO	K511	L783	L902	K1013	S1102	I1191	G1266
LYS	K512	Y784	L902	K1014	S1103	I1195	L1267
ASN	D513	L785	K905	GLY	K1104	I1195	M1268
LEU	S518	L657	E906	ARG	S1105	E1198	L1269
ASP	A519	K667	K907	PHE	Q1106	S1199	L1270
ASN	E520	M668	V911	K1018	E1107	D1200	G1271
PRO	L529	L669	V911	V1019	F1108	F1203	R1272
SER	L529	P670	S915	E1020	F1109	F1204	M1276
LYS	L529	S675	I916	Y1024	S1110	A1205	N1276
GLU	T533	L679	D917	L1027	K1111	L1206	I1286
GLN	L536	P684	R918	L1032	D1113	L1207	Y1291
LEU	F543	L689	H922	I1033	K1114	V1210	F1292
ILE	D550	R690	Y925	E1034	I1115	T1213	E1293
ALA	K551	L691	Y926	L1035	C1116	L1214	F1294
LYS	T445	R692	V929	L1038	K1121	L1215	V1295
K449	A552	K623	I935	L1039	G1122	Q1216	Q1296
Y450	K557	G826	D939	F1040	F1126	M1217	R1298
K457	D568	E827	N942	K1041	S1127	R1218	N1299
L460	E569	A828	I943	D1042	F1128	N1219	M1300
E461	E573	E829	G945	N1043	F1129	S1220	
F462	N574	E832	N946	E1044	Y1130	K1221	
F463	I575	I837	M949	D1046	A1137	THR	
H464	Y585	K840	K956	K1047	A1138	GLY	
K465	K597	A848	I960	T1048	K1141	GLU	
H466	L598	S861	R964	G1049	W1142	D1227	
R467	N602	V862	R968	L1052	T1143	Y1228	
D468	S603	I868	K972	R1053	I1144	L1229	
Y469	T604	K869	K973	A1054	L1151	I1230	
D470	W609	D870	I974	Y1055	F1154	S1231	
K471	N612	K871	N975	P1060	R1155	F1232	
Q472	D616	R872	N976	F1061	N1156	V1233	
F475	T618	D876	K977	E1062	ASP	A1234	
A483	I623	K877	I977	T1063	LYS	G1238	
H486	D626	F878	K978	F1064	ASN	F1241	
F489	M633	F879	E979	K1065	HIS	D1242	
I492		P880	L985	M1067	ASN	S1243	
N495		I884	S986	T1071	TRP	K1247	
				G1072	D1164	P1248	
				I1073	T1165	N1249	
				I1074	R1166	D1253	
				G1080	L1174	A1254	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.28Å 124.28Å 268.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 3.45 47.22 – 3.45	Depositor EDS
% Data completeness (in resolution range)	88.9 (47.22-3.45) 88.8 (47.22-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.216 , 0.285 0.217 , 0.285	Depositor DCC
R_{free} test set	1234 reflections (4.34%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	12057	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	B	0.48	0/995	0.77	2/1548 (0.1%)
2	C	0.55	0/615	0.69	0/946
3	D	0.54	0/245	0.72	0/375
4	A	0.51	0/10595	0.74	2/14220 (0.0%)
All	All	0.51	0/12450	0.74	4/17089 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	A	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	617	ASN	CA-C-N	-7.34	109.08	122.38
4	A	617	ASN	C-N-CA	-7.34	109.08	122.38
1	B	-10	U	P-O3'-C3'	5.63	128.64	120.20
1	B	-10	U	C2'-C3'-O3'	5.26	117.39	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	789	TYR	Peptide

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	B	890	0	449	18	0
2	C	550	0	308	5	0
3	D	221	0	127	7	0
4	A	10392	0	10350	304	1
5	B	2	0	0	0	0
6	A	2	0	0	1	0
All	All	12057	0	11234	316	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (316) 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)
4:A:371:LYS:HE2	4:A:489:PHE:HB3	1.47	0.93
1:B:19:C:N3	1:B:21:G:N2	2.20	0.89
4:A:518:SER:O	6:A:1401:HOH:O	1.95	0.85
4:A:960:ILE:HG22	4:A:977:ILE:HD12	1.63	0.81
2:C:0:DC:H4'	4:A:827:GLU:HG3	1.63	0.81
4:A:1268:MET:HE1	4:A:1291:TYR:HD1	1.45	0.80
4:A:1063:THR:HG22	4:A:1065:LYS:H	1.46	0.79
4:A:1062:GLU:HG2	4:A:1063:THR:H	1.46	0.79
1:B:-15:U:OP1	4:A:833:ARG:NH2	2.16	0.79
4:A:396:ASP:HB3	4:A:398:SER:H	1.47	0.78
4:A:342:LEU:HD22	4:A:347:ASP:HB3	1.64	0.77
4:A:1102:VAL:O	4:A:1106:GLN:HG3	1.85	0.76
4:A:1265:LYS:HA	4:A:1268:MET:HE3	1.68	0.75
4:A:533:THR:CG2	4:A:575:ILE:HD12	2.17	0.75
4:A:895:LYS:HE3	4:A:898:ASP:OD2	1.85	0.75
4:A:1101:SER:HB3	4:A:1104:LYS:HE3	1.67	0.74
4:A:533:THR:HB	4:A:575:ILE:CD1	2.18	0.74
4:A:390:LYS:HB3	4:A:558:ASP:HB2	1.70	0.73
4:A:533:THR:HG22	4:A:575:ILE:HD12	1.69	0.73
4:A:1267:LEU:HD12	4:A:1294:PHE:HZ	1.54	0.73
4:A:944:ILE:HG21	4:A:987:GLN:HG2	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:643:ASP:HA	4:A:646:ILE:HG12	1.71	0.72
4:A:650:LYS:NZ	4:A:767:GLU:OE2	2.23	0.72
4:A:373:THR:O	4:A:377:LEU:HD13	1.91	0.70
4:A:55:ASP:OD1	4:A:186:ARG:NH1	2.25	0.70
4:A:618:THR:HG21	4:A:633:MET:O	1.91	0.69
4:A:670:PRO:HG3	4:A:724:TYR:OH	1.92	0.69
4:A:1099:TYR:HE2	4:A:1204:PHE:HB2	1.57	0.68
3:D:0:DC:C2	4:A:667:LYS:HE2	2.28	0.68
4:A:1048:THR:HA	4:A:1053:ARG:HB3	1.74	0.68
4:A:275:GLN:HG2	4:A:332:THR:OG1	1.93	0.68
4:A:964:ARG:HD2	4:A:977:ILE:HD11	1.75	0.68
4:A:289:PHE:CE1	4:A:296:LYS:HB2	2.27	0.68
4:A:1045:PHE:CE2	4:A:1052:LEU:HD13	2.28	0.68
4:A:905:LYS:NZ	4:A:1276:ASN:O	2.28	0.67
4:A:356:TYR:HB3	4:A:496:LYS:HD2	1.77	0.66
4:A:533:THR:HB	4:A:575:ILE:HD11	1.76	0.66
4:A:1154:PHE:HE1	4:A:1166:ARG:HB3	1.60	0.66
4:A:87:LYS:NZ	4:A:213:GLU:OE2	2.27	0.66
4:A:180:LYS:HG3	4:A:181:GLY:N	2.10	0.66
4:A:821:VAL:HG23	4:A:887:ASN:HA	1.77	0.65
4:A:275:GLN:OE1	4:A:330:SER:OG	2.13	0.65
4:A:400:THR:HG23	4:A:410:TYR:HB2	1.78	0.64
4:A:960:ILE:CG2	4:A:977:ILE:HD12	2.28	0.64
4:A:1089:THR:HG21	4:A:1233:VAL:HG12	1.80	0.64
4:A:51:LYS:HD2	4:A:182:PHE:CD1	2.33	0.64
4:A:1189:GLU:OE2	4:A:1189:GLU:N	2.22	0.63
4:A:1268:MET:HE2	4:A:1294:PHE:HD2	1.63	0.63
4:A:282:ASN:CG	4:A:323:VAL:HG13	2.23	0.62
4:A:218:TYR:O	4:A:222:LYS:HG3	1.99	0.62
4:A:722:ASP:O	4:A:726:GLN:HG3	1.98	0.62
4:A:916:ILE:O	4:A:1024:TYR:OH	2.15	0.62
4:A:460:LEU:HD11	4:A:475:PHE:HB2	1.81	0.62
4:A:1086:CYS:HG	4:A:1231:SER:HG	1.21	0.61
4:A:1099:TYR:HE2	4:A:1204:PHE:CB	2.13	0.61
1:B:16:A:O2'	4:A:298:LYS:NZ	2.33	0.61
4:A:243:THR:HG23	4:A:255:GLN:HG3	1.83	0.61
4:A:57:TYR:HB2	4:A:141:TRP:CE3	2.36	0.60
4:A:282:ASN:OD1	4:A:323:VAL:HG13	2.02	0.60
4:A:602:ASN:ND2	4:A:616:ASP:O	2.18	0.60
4:A:1195:ILE:HG22	4:A:1203:PHE:CZ	2.37	0.59
4:A:64:GLU:OE2	4:A:118:LYS:HD2	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1067:MET:HG3	4:A:1071:THR:HG22	1.84	0.59
4:A:1267:LEU:HD12	4:A:1294:PHE:CZ	2.36	0.59
4:A:467:ARG:HH11	4:A:472:GLN:HA	1.67	0.59
4:A:145:SER:HB3	4:A:150:ILE:HG22	1.84	0.59
4:A:837:ILE:HD11	4:A:870:ASP:HB2	1.85	0.59
4:A:1292:PHE:O	4:A:1296:GLN:HB2	2.03	0.59
4:A:693:ASN:HA	4:A:704:GLN:HB2	1.85	0.58
4:A:1130:TYR:HB3	4:A:1138:ALA:HB1	1.84	0.58
1:B:-2:A:OP2	4:A:1041:LYS:HE3	2.03	0.58
4:A:121:ASN:HA	4:A:124:ASN:HD21	1.68	0.58
4:A:27:THR:HG21	4:A:785:LEU:H	1.68	0.58
4:A:640:ILE:HD11	4:A:782:LYS:HB3	1.86	0.58
1:B:-17:U:H2'	4:A:872:ARG:HD3	1.86	0.57
4:A:520:GLU:HG3	4:A:972:LYS:HG2	1.86	0.57
4:A:125:GLN:HA	4:A:176:THR:HG21	1.86	0.57
4:A:1247:PRO:HB2	4:A:1249:ASN:OD1	2.05	0.57
4:A:380:ASP:HB3	4:A:386:LEU:CD2	2.35	0.57
4:A:381:LEU:HD23	4:A:386:LEU:HB2	1.87	0.57
4:A:623:ILE:HG13	4:A:657:ILE:HD11	1.87	0.57
4:A:717:CYS:O	4:A:721:ILE:HG13	2.05	0.57
4:A:722:ASP:OD2	4:A:744:THR:HG21	2.05	0.57
4:A:371:LYS:HE2	4:A:489:PHE:CB	2.30	0.56
4:A:774:ILE:O	4:A:777:VAL:HG12	2.05	0.56
4:A:352:MET:CE	4:A:499:LEU:HD21	2.35	0.56
4:A:612:ASN:ND2	4:A:733:GLU:OE1	2.33	0.56
4:A:945:GLY:CA	4:A:946:ASN:HB2	2.34	0.56
4:A:1210:VAL:HA	4:A:1213:THR:HG22	1.87	0.56
4:A:690:ARG:NH2	4:A:716:ASP:OD1	2.36	0.56
4:A:1144:ILE:HD12	4:A:1215:LEU:HD21	1.87	0.56
4:A:20:GLU:OE2	4:A:877:LYS:HD3	2.06	0.55
4:A:776:SER:O	4:A:780:GLN:HG3	2.06	0.55
4:A:61:PHE:CE1	4:A:65:ILE:HD13	2.42	0.55
4:A:235:LYS:CE	4:A:259:SER:HA	2.37	0.55
4:A:657:ILE:HG13	4:A:766:PHE:CE1	2.41	0.55
4:A:1045:PHE:CZ	4:A:1052:LEU:HD13	2.42	0.54
4:A:925:TYR:CZ	4:A:1256:ALA:HB2	2.43	0.54
4:A:113:ILE:CD1	4:A:190:TYR:HB3	2.38	0.54
4:A:160:THR:OG1	4:A:161:ASP:N	2.37	0.54
4:A:240:GLU:HB3	4:A:241:GLU:OE2	2.08	0.54
4:A:1130:TYR:CD1	4:A:1138:ALA:HB1	2.43	0.54
4:A:121:ASN:HA	4:A:124:ASN:ND2	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:604:THR:O	4:A:617:ASN:HA	2.08	0.54
4:A:1067:MET:SD	4:A:1071:THR:HG21	2.48	0.54
4:A:356:TYR:CZ	4:A:529:LEU:HD22	2.43	0.54
2:C:-11:DA:H2'	2:C:-10:DA:C8	2.43	0.54
4:A:877:LYS:HB2	4:A:879:PHE:CE2	2.42	0.54
4:A:457:LYS:O	4:A:461:GLU:HB2	2.08	0.53
4:A:1229:LEU:HB2	4:A:1254:ALA:HB2	1.91	0.53
4:A:170:LYS:O	4:A:173:LYS:HG3	2.09	0.53
4:A:922:HIS:HA	4:A:942:ASN:HD21	1.73	0.53
4:A:343:GLU:O	4:A:512:LYS:HD2	2.09	0.53
4:A:1086:CYS:SG	4:A:1231:SER:OG	2.49	0.53
4:A:926:TYR:CE2	4:A:939:ASP:HB3	2.43	0.53
4:A:1269:LEU:CD1	4:A:1286:ILE:HD11	2.39	0.53
4:A:906:GLU:HG3	4:A:907:LYS:HD3	1.90	0.53
4:A:1228:TYR:HB2	4:A:1243:SER:OG	2.09	0.52
4:A:275:GLN:OE1	4:A:326:LYS:HB2	2.08	0.52
4:A:91:ASP:O	4:A:94:LEU:HB2	2.10	0.52
4:A:915:SER:OG	4:A:1259:ALA:O	2.24	0.52
3:D:-4:DT:OP1	4:A:176:THR:OG1	2.26	0.52
3:D:0:DC:O2	4:A:667:LYS:HE2	2.09	0.52
4:A:533:THR:HB	4:A:575:ILE:HD12	1.92	0.52
4:A:976:ASN:C	4:A:977:ILE:HD13	2.35	0.52
1:B:-8:U:O4	4:A:861:SER:HB3	2.10	0.52
4:A:512:LYS:HA	4:A:585:TYR:OH	2.09	0.52
4:A:1183:ILE:HD11	4:A:1198:GLU:OE2	2.09	0.52
4:A:1121:LYS:HB3	4:A:1123:TYR:CE1	2.46	0.51
4:A:146:LYS:HE2	4:A:163:ASP:OD1	2.11	0.51
4:A:381:LEU:HD11	4:A:391:ILE:HD13	1.92	0.51
4:A:916:ILE:HA	4:A:925:TYR:O	2.10	0.51
4:A:964:ARG:HD2	4:A:977:ILE:CD1	2.39	0.51
4:A:229:ILE:HG13	4:A:231:TYR:CE1	2.46	0.51
4:A:533:THR:CB	4:A:575:ILE:HD12	2.41	0.51
4:A:11:TYR:CE1	4:A:1060:PRO:HG3	2.46	0.50
4:A:911:VAL:CG2	4:A:1270:LEU:HD11	2.41	0.50
4:A:166:LEU:O	4:A:170:LYS:HD3	2.11	0.50
4:A:27:THR:HG21	4:A:785:LEU:N	2.26	0.50
4:A:1112:PHE:CE1	4:A:1126:PHE:HB3	2.46	0.50
4:A:1269:LEU:HD13	4:A:1286:ILE:HD11	1.94	0.50
4:A:675:SER:O	4:A:679:ILE:N	2.43	0.50
4:A:876:ASP:OD1	4:A:876:ASP:N	2.43	0.49
1:B:-1:U:O4	4:A:802:ASN:HB3	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:840:LYS:O	4:A:868:ILE:HG23	2.12	0.49
4:A:1234:ALA:HB1	4:A:1238:GLY:HA2	1.94	0.49
4:A:380:ASP:HB3	4:A:386:LEU:HD23	1.94	0.49
4:A:684:PRO:HB2	4:A:689:LEU:HD22	1.94	0.49
4:A:1195:ILE:HG22	4:A:1203:PHE:HZ	1.77	0.49
4:A:21:LEU:HD21	4:A:880:PHE:HB2	1.95	0.49
4:A:48:LYS:O	4:A:52:GLN:HG3	2.12	0.49
4:A:461:GLU:O	4:A:465:LYS:HG3	2.12	0.49
4:A:945:GLY:HA2	4:A:946:ASN:HB2	1.94	0.49
4:A:1007:ASP:O	4:A:1008:LEU:HG	2.13	0.49
4:A:85:LYS:HE3	4:A:94:LEU:HD21	1.95	0.49
4:A:985:LEU:HD22	4:A:1027:LEU:HB2	1.94	0.49
4:A:1032:ILE:HG12	4:A:1074:ILE:HD12	1.94	0.49
4:A:1043:ASN:HD22	4:A:1049:GLY:HA3	1.77	0.48
4:A:213:GLU:O	4:A:217:LYS:HG3	2.12	0.48
4:A:113:ILE:HD11	4:A:190:TYR:HB3	1.95	0.48
4:A:308:SER:OG	4:A:313:ASP:O	2.24	0.48
4:A:1012:PHE:HB2	4:A:1080:GLY:HA2	1.95	0.48
1:B:-11:C:H5'	4:A:852:LYS:HD2	1.96	0.48
4:A:382:LYS:HE3	4:A:483:ALA:CB	2.42	0.48
4:A:1151:LEU:HB2	4:A:1219:ASN:HB3	1.94	0.48
4:A:34:ARG:HH12	4:A:636:LYS:HE3	1.78	0.48
2:C:2:DA:N3	4:A:668:MET:HE1	2.29	0.48
1:B:21:G:H1'	1:B:22:U:H5''	1.96	0.47
4:A:657:ILE:HG13	4:A:766:PHE:HE1	1.78	0.47
1:B:-11:C:OP1	4:A:949:MET:HE2	2.13	0.47
4:A:293:GLU:OE2	4:A:297:ARG:NH1	2.44	0.47
4:A:345:ASP:HB3	4:A:506:TYR:HB3	1.96	0.47
4:A:394:LYS:HD2	4:A:396:ASP:CG	2.39	0.47
4:A:725:LYS:HE3	4:A:744:THR:HG22	1.96	0.47
4:A:925:TYR:CD2	4:A:926:TYR:N	2.82	0.47
4:A:159:ILE:HA	4:A:164:GLU:OE1	2.15	0.47
4:A:711:GLU:HG2	4:A:712:PHE:H	1.79	0.47
4:A:1088:VAL:HG23	4:A:1089:THR:HG23	1.97	0.47
4:A:1113:ASP:O	4:A:1114:LYS:HG2	2.14	0.47
4:A:275:GLN:HG3	4:A:275:GLN:O	2.14	0.47
4:A:762:TYR:CZ	4:A:823:LYS:HG2	2.50	0.47
4:A:386:LEU:HD13	4:A:386:LEU:HA	1.78	0.47
4:A:403:SER:OG	4:A:409:ASP:O	2.31	0.46
4:A:697:HIS:CD2	4:A:697:HIS:H	2.33	0.46
4:A:1111:LYS:HE3	4:A:1111:LYS:HB2	1.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:138:LEU:HD23	4:A:142:LEU:HD13	1.96	0.46
4:A:390:LYS:CB	4:A:558:ASP:HB2	2.40	0.46
4:A:964:ARG:HD2	4:A:977:ILE:CG1	2.45	0.46
4:A:964:ARG:O	4:A:968:ARG:HG3	2.15	0.46
4:A:51:LYS:HB3	4:A:182:PHE:CE1	2.51	0.46
4:A:598:LEU:HD21	4:A:832:TYR:HB2	1.97	0.46
4:A:902:LEU:HD23	4:A:902:LEU:HA	1.60	0.46
4:A:72:SER:O	4:A:75:LEU:HB2	2.16	0.46
4:A:968:ARG:HG2	4:A:974:ILE:HD13	1.98	0.46
4:A:1040:PHE:C	4:A:1042:ASP:H	2.23	0.46
4:A:1052:LEU:HD23	4:A:1053:ARG:HH12	1.81	0.46
4:A:1087:PRO:HG2	4:A:1241:PHE:CE2	2.51	0.46
4:A:235:LYS:HZ2	4:A:260:LEU:H	1.64	0.46
4:A:244:PHE:HB3	4:A:271:ASN:ND2	2.31	0.46
4:A:1268:MET:HE1	4:A:1291:TYR:CD1	2.37	0.45
4:A:210:LYS:HE3	4:A:325:PHE:CE2	2.51	0.45
4:A:618:THR:HG22	4:A:618:THR:O	2.15	0.45
4:A:1062:GLU:HG2	4:A:1063:THR:N	2.24	0.45
3:D:-4:DT:H2''	3:D:-3:DT:H5''	1.98	0.45
4:A:142:LEU:HD23	4:A:166:LEU:HD13	1.97	0.45
1:B:-1:U:OP1	4:A:1034:LYS:HD3	2.16	0.45
4:A:1071:THR:O	4:A:1071:THR:OG1	2.29	0.45
4:A:1174:LEU:HG	4:A:1210:VAL:HG11	1.97	0.45
4:A:191:SER:HB3	4:A:195:ILE:HD11	1.98	0.45
4:A:848:ALA:HA	4:A:862:VAL:HG12	1.98	0.45
4:A:280:LYS:O	4:A:284:ILE:HG13	2.17	0.45
4:A:460:LEU:HA	4:A:463:PHE:HB3	1.99	0.45
4:A:1178:LEU:HD12	4:A:1185:TYR:CD2	2.51	0.45
4:A:337:PHE:HE2	4:A:339:ILE:HD13	1.81	0.44
4:A:1038:LEU:HB3	4:A:1055:TYR:HB2	1.98	0.44
4:A:27:THR:HG22	4:A:784:TYR:HA	1.99	0.44
4:A:85:LYS:O	4:A:89:SER:HB2	2.17	0.44
4:A:488:ILE:HD12	4:A:536:LEU:HD13	1.99	0.44
4:A:725:LYS:CE	4:A:744:THR:HG22	2.47	0.44
4:A:1086:CYS:HB2	4:A:1217:MET:HE1	1.98	0.44
4:A:375:SER:HA	4:A:486:PRO:HG3	1.99	0.44
4:A:956:LYS:O	4:A:960:ILE:HG13	2.17	0.44
4:A:58:HIS:O	4:A:62:ILE:HG13	2.18	0.44
4:A:1113:ASP:C	4:A:1114:LYS:HG2	2.43	0.44
4:A:130:ALA:HB2	4:A:136:SER:HB2	1.99	0.44
4:A:609:TRP:CD1	4:A:826:GLY:HA2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1129:ASP:HB2	4:A:1141:LYS:HG2	1.99	0.44
4:A:1200:ASP:HB3	4:A:1203:PHE:HB3	1.99	0.44
4:A:202:ARG:O	4:A:206:ASP:HB2	2.17	0.44
4:A:27:THR:O	4:A:31:ILE:HG13	2.17	0.43
4:A:49:LYS:HD3	4:A:168:ILE:HD13	2.00	0.43
4:A:369:SER:OG	4:A:372:GLU:HG3	2.19	0.43
1:B:-8:U:H5	4:A:862:VAL:O	2.00	0.43
1:B:-5:U:H6	1:B:-5:U:O5'	2.01	0.43
4:A:50:ALA:O	4:A:54:ILE:HG13	2.19	0.43
4:A:468:ASP:O	4:A:472:GLN:HB3	2.18	0.43
4:A:944:ILE:CD1	4:A:988:VAL:HG12	2.48	0.43
4:A:918:ARG:HH21	4:A:1020:GLU:HB2	1.83	0.43
4:A:1104:LYS:H	4:A:1104:LYS:HG3	1.62	0.43
4:A:65:ILE:O	4:A:69:VAL:HG23	2.18	0.43
4:A:249:LYS:HD3	4:A:250:THR:HG23	2.01	0.43
4:A:763:LYS:HB3	4:A:763:LYS:HE2	1.55	0.43
4:A:1063:THR:HB	4:A:1066:LYS:H	1.83	0.43
1:B:7:C:H2'	1:B:8:A:C8	2.53	0.43
4:A:1183:ILE:HG21	4:A:1191:ILE:HG23	1.99	0.43
4:A:1217:MET:O	4:A:1229:LEU:HA	2.18	0.43
4:A:60:PHE:CD2	4:A:141:TRP:NE1	2.86	0.43
4:A:120:LYS:HG3	4:A:121:ASN:N	2.33	0.43
4:A:300:ILE:O	4:A:304:ILE:HG13	2.19	0.43
4:A:208:LEU:HB3	4:A:209:PRO:HD3	2.01	0.43
4:A:290:VAL:HG21	4:A:297:ARG:NH1	2.34	0.43
4:A:1257:ASN:OD1	4:A:1261:HIS:CE1	2.72	0.43
4:A:1253:ASP:OD2	4:A:1253:ASP:N	2.52	0.42
3:D:-3:DT:OP1	4:A:124:ASN:HB2	2.19	0.42
4:A:449:LYS:NZ	4:A:550:ASP:HB2	2.34	0.42
4:A:394:LYS:HD2	4:A:396:ASP:OD1	2.19	0.42
4:A:511:LYS:HE2	4:A:513:ASP:OD2	2.19	0.42
1:B:7:C:H6	1:B:7:C:O5'	2.02	0.42
4:A:32:LYS:C	4:A:35:GLY:H	2.26	0.42
4:A:61:PHE:HD1	4:A:118:LYS:HD3	1.84	0.42
4:A:1035:LEU:HD13	4:A:1073:ILE:HD11	2.01	0.42
4:A:233:GLN:O	4:A:237:ASP:N	2.49	0.42
4:A:390:LYS:HA	4:A:390:LYS:HD3	1.89	0.42
4:A:49:LYS:HB3	4:A:159:ILE:HD11	2.02	0.42
4:A:1272:ARG:HH22	4:A:1286:ILE:HA	1.85	0.42
4:A:495:ASN:C	4:A:497:ASP:H	2.27	0.42
4:A:1032:ILE:CG1	4:A:1074:ILE:HD12	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1154:PHE:CE1	4:A:1166:ARG:HB3	2.47	0.42
3:D:-3:DT:OP1	4:A:125:GLN:N	2.30	0.42
4:A:816:ASN:HD22	4:A:817:LEU:CD1	2.33	0.42
1:B:-3:G:OP1	4:A:1041:LYS:HD2	2.20	0.42
4:A:17:LEU:HD13	4:A:808:TRP:HB2	2.02	0.42
4:A:131:LYS:HG3	4:A:132:LYS:HE3	2.02	0.42
4:A:396:ASP:C	4:A:398:SER:N	2.76	0.42
4:A:356:TYR:OH	4:A:529:LEU:HD22	2.20	0.41
4:A:573:ALA:C	4:A:575:ILE:H	2.28	0.41
4:A:691:ILE:HG23	4:A:696:THR:OG1	2.19	0.41
4:A:1108:PHE:HA	4:A:1111:LYS:HE3	2.01	0.41
1:B:5:G:H2'	1:B:6:U:O4'	2.20	0.41
2:C:-16:DT:H2'	2:C:-15:DT:C6	2.55	0.41
4:A:370:ILE:O	4:A:374:LEU:HD12	2.21	0.41
4:A:505:LYS:HE3	4:A:506:TYR:CE2	2.55	0.41
4:A:852:LYS:HB2	4:A:949:MET:HE1	2.01	0.41
4:A:394:LYS:HG2	4:A:450:TYR:CE1	2.56	0.41
4:A:1142:TRP:CH2	4:A:1296:GLN:HG2	2.54	0.41
1:B:10:U:H2'	1:B:11:U:C6	2.56	0.41
3:D:-8:DG:C8	3:D:-7:DT:H72	2.55	0.41
4:A:235:LYS:O	4:A:239:ALA:HB2	2.20	0.41
4:A:249:LYS:CB	4:A:265:GLU:HG2	2.51	0.41
4:A:968:ARG:HG2	4:A:974:ILE:CD1	2.50	0.41
4:A:557:LYS:HE3	4:A:559:GLU:OE2	2.20	0.41
4:A:597:LYS:HD2	4:A:829:GLU:HG2	2.03	0.41
4:A:244:PHE:CZ	4:A:272:TYR:HE1	2.38	0.41
4:A:790:ASN:H	4:A:793:PHE:HD1	1.68	0.41
4:A:978:LYS:HE3	4:A:979:GLU:OE2	2.21	0.41
4:A:8:VAL:O	4:A:9:ASN:C	2.64	0.41
4:A:17:LEU:HD11	4:A:884:ILE:HD13	2.02	0.41
4:A:735:LYS:H	4:A:735:LYS:HG2	1.58	0.41
4:A:925:TYR:HD2	4:A:926:TYR:N	2.19	0.41
4:A:929:VAL:HG12	4:A:935:ILE:HG12	2.03	0.41
4:A:887:ASN:O	4:A:888:PHE:C	2.63	0.40
4:A:27:THR:CG2	4:A:785:LEU:H	2.33	0.40
4:A:249:LYS:HB2	4:A:265:GLU:HG2	2.03	0.40
4:A:391:ILE:HD11	4:A:543:PHE:CE2	2.55	0.40
4:A:884:ILE:HG13	4:A:886:ILE:HD11	2.02	0.40
4:A:1116:CYS:HA	4:A:1190:CYS:HA	2.04	0.40
4:A:94:LEU:HD23	4:A:94:LEU:HA	1.86	0.40
4:A:109:ILE:O	4:A:113:ILE:HG23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:488:ILE:O	4:A:492:ILE:HG13	2.21	0.40
2:C:-2:DC:H2'	2:C:-1:DT:C6	2.57	0.40
4:A:75:LEU:HA	4:A:75:LEU:HD23	1.88	0.40
4:A:471:LYS:HB2	4:A:471:LYS:HE3	1.95	0.40
4:A:762:TYR:CE1	4:A:823:LYS:HG2	2.56	0.40
4:A:1294:PHE:O	4:A:1298:ARG:HG2	2.21	0.40
4:A:54:ILE:HD13	4:A:54:ILE:HG21	1.84	0.40
4:A:73:GLU:OE1	4:A:267:ALA:HB2	2.21	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:72:SER:OG	4:A:1046:ASP:OD1[5_454]	2.11	0.09

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
4	A	1246/1300 (96%)	1185 (95%)	55 (4%)	6 (0%)	24 57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	574	ASN
4	A	160	THR
4	A	626	ASP
4	A	1013	LYS
4	A	1137	ALA
4	A	510	GLY

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	
4	A	1144/1183 (97%)	1144 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	52	GLN
4	A	77	GLN
4	A	183	HIS
4	A	185	ASN
4	A	255	GLN
4	A	305	ASN
4	A	358	GLN
4	A	405	GLN
4	A	516	GLN
4	A	584	ASN
4	A	666	ASN
4	A	693	ASN
4	A	697	HIS
4	A	704	GLN
4	A	713	ASN
4	A	748	ASN
4	A	780	GLN
4	A	804	HIS
4	A	901	ASN
4	A	1043	ASN
4	A	1187	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	41/58 (70%)	6 (14%)	2 (4%)

All (6) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	-9	G
1	B	-7	U
1	B	-6	G
1	B	21	G
1	B	22	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	-10	U
1	B	0	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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 ⓘ

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	B	42/58 (72%)	-0.70	0	100 100	19, 27, 101, 139	0
2	C	27/27 (100%)	-0.38	0	100 100	21, 39, 70, 98	0
3	D	11/11 (100%)	-0.36	0	100 100	33, 38, 78, 95	0
4	A	1260/1300 (96%)	-0.05	22 (1%)	69 44	14, 44, 112, 152	0
All	All	1340/1396 (95%)	-0.08	22 (1%)	70 46	14, 43, 112, 152	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	1207	LEU	5.5
4	A	1203	PHE	3.9
4	A	1213	THR	3.0
4	A	1214	ILE	3.0
4	A	298	LYS	2.9
4	A	1206	LYS	2.8
4	A	1109	PHE	2.7
4	A	1156	ASN	2.6
4	A	1191	ILE	2.6
4	A	112	TYR	2.6
4	A	1127	SER	2.5
4	A	1221	LYS	2.5
4	A	647	LYS	2.4
4	A	552	ALA	2.4
4	A	469	ILE	2.3
4	A	445	THR	2.3
4	A	1012	PHE	2.3
4	A	381	LEU	2.2
4	A	1154	PHE	2.1
4	A	418	LEU	2.1
4	A	1183	ILE	2.1
4	A	1018	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	102	1/1	0.94	0.20	9,9,9,9	0
5	MG	B	101	1/1	0.95	0.28	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.