



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:24 AM UTC

PDB ID : 8Y0B / pdb_00008y0b
Title : Crystal structure of FnCas12a in complex with pre-crRNA and 12nt target DNA
Authors : Lin, X.; Chen, J.; Liu, L.
Deposited on : 2024-01-22
Resolution : 2.30 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

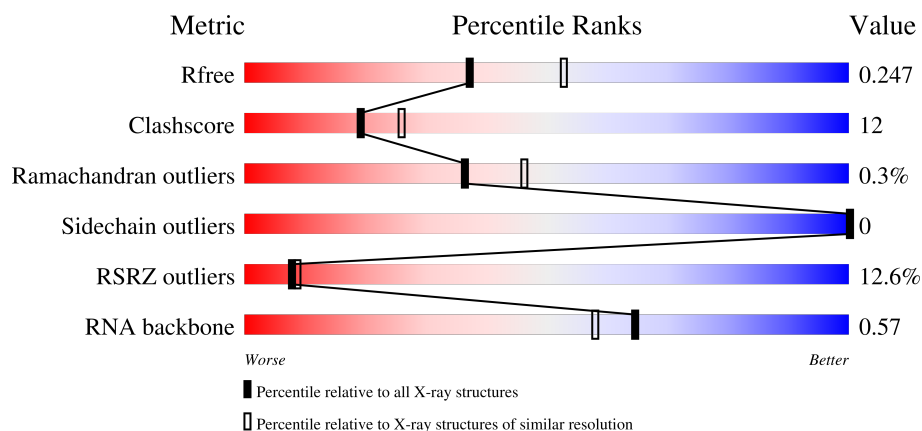
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)
RNA backbone	3983	1090 (2.60-2.00)

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	9% 62% 22% 7% 9%
2	C	21	67% 33%
3	D	18	6% 33% 39% 28%
4	A	1300	13% 79% 18% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12785 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 (53-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	53	Total	C	N	O	P	0	0	0
			1120	504	194	370	52			

- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*AP*AP*TP*GP*AP*CP*TP*TP*CP*TP*CP*TP*AP*AP*AP*GP*GP*AP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	21	Total	C	N	O	P	0	0	0
			430	206	79	124	21			

- Molecule 3 is a DNA chain called DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*TP*AP*GP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	13	Total	C	N	O	P	0	0	0
			266	128	46	79	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1264	Total	C	N	O	S	0	0	0
			10399	6679	1714	1984	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	1	Total 1	Mg 1	0	0
5	A	1	Total 1	Mg 1	0	0

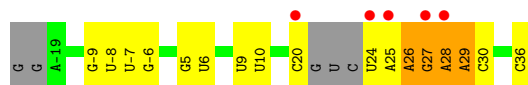
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	91	Total 91	O 91	0	0
6	C	44	Total 44	O 44	0	0
6	D	16	Total 16	O 16	0	0
6	A	417	Total 417	O 417	0	0

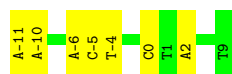
3 Residue-property plots [i](#)

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.

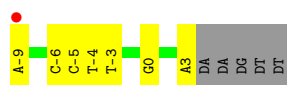
- Molecule 1: RNA (53-MER)



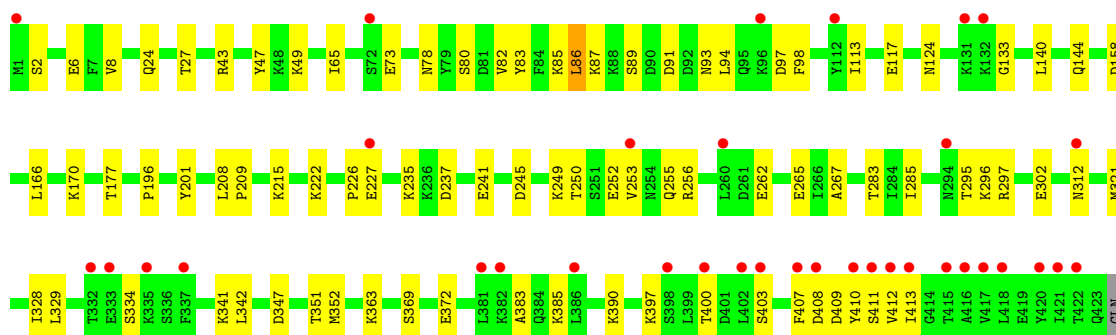
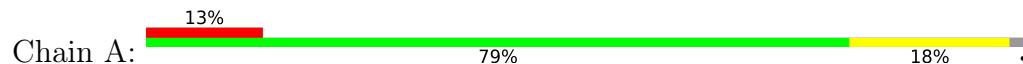
- Molecule 2: DNA (5'-D(P*AP*AP*AP*TP*GP*AP*CP*TP*TP*CP*TP*CP*TP*AP*AP*A P*GP*GP*AP*CP*T)-3')

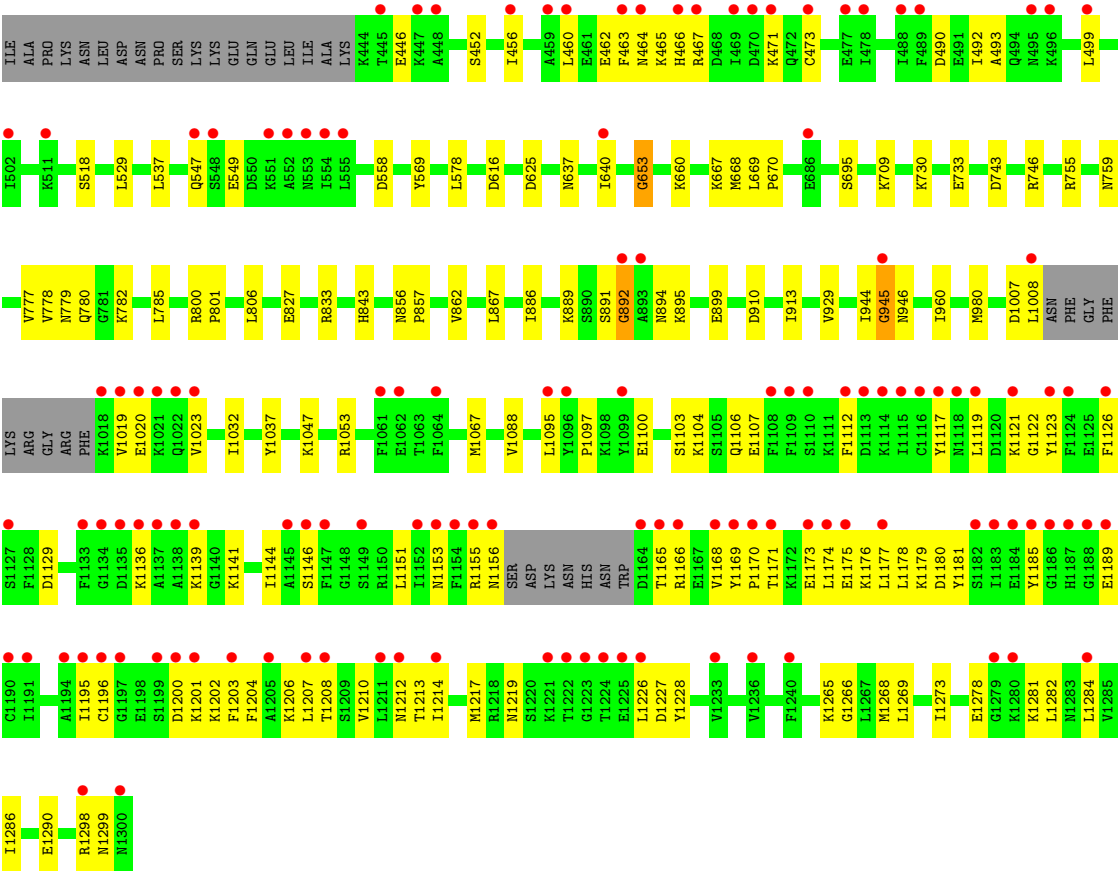


- Molecule 3: DNA (5'-D(P*AP*GP*TP*CP*CP*TP*TP*TP*AP*GP*AP*TP*A)-3')



- Molecule 4: CRISPR-associated endonuclease Cas12a





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	124.73Å 124.73Å 267.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.30 49.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (49.21-2.30) 97.1 (49.21-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.203 , 0.247 0.204 , 0.247	Depositor DCC
R_{free} test set	4589 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	39.9	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12785	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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

5.1 Standard geometry

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	0.40	0/1251	0.64	0/1943
2	C	0.43	0/482	0.65	0/741
3	D	0.54	0/297	0.70	0/456
4	A	0.39	0/10604	0.60	3/14242 (0.0%)
All	All	0.40	0/12634	0.61	3/17382 (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	3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
4	A	945	GLY	CA-C-N	7.10	134.47	121.70
4	A	945	GLY	C-N-CA	7.10	134.47	121.70
4	A	653	GLY	N-CA-C	5.26	125.65	113.18

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	549	GLU	Peptide
4	A	86	LEU	Peptide
4	A	944	ILE	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	1120	0	567	22	0
2	C	430	0	238	6	0
3	D	266	0	149	16	0
4	A	10399	0	10328	245	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	A	417	0	0	79	0
6	B	91	0	0	1	0
6	C	44	0	0	1	0
6	D	16	0	0	8	0
All	All	12785	0	11282	272	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 12.

All (272) 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:1117:TYR:OH	4:A:1119:LEU:HD13	1.34	1.22
4:A:1282:LEU:CA	6:A:1502:HOH:O	1.83	1.21
4:A:1281:LYS:HA	6:A:1520:HOH:O	1.39	1.17
3:D:-5:DC:C5'	6:D:101:HOH:O	1.93	1.15
4:A:1282:LEU:HA	6:A:1502:HOH:O	1.40	1.12
4:A:1282:LEU:N	6:A:1502:HOH:O	1.81	1.10
4:A:1170:PRO:HA	6:A:1524:HOH:O	1.61	1.00
4:A:341:LYS:NZ	6:A:1510:HOH:O	1.93	1.00
4:A:1219:ASN:O	6:A:1501:HOH:O	1.81	0.98
4:A:1281:LYS:C	6:A:1502:HOH:O	2.04	0.97
4:A:1196:CYS:C	6:A:1508:HOH:O	2.08	0.97
4:A:1117:TYR:OH	4:A:1119:LEU:CD1	2.13	0.97
4:A:80:SER:OG	6:A:1503:HOH:O	1.82	0.96
4:A:65:ILE:HG21	4:A:113:ILE:HG22	1.46	0.96
4:A:1175:GLU:HB3	6:A:1506:HOH:O	1.66	0.94
4:A:1173:GLU:HB2	6:A:1524:HOH:O	1.68	0.94
4:A:227:GLU:N	6:A:1509:HOH:O	1.92	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1117:TYR:CZ	4:A:1119:LEU:HD13	2.06	0.90
4:A:227:GLU:HB3	6:A:1509:HOH:O	1.71	0.90
4:A:408:ASP:O	6:A:1504:HOH:O	1.88	0.90
4:A:1176:LYS:HA	4:A:1179:LYS:HG2	1.54	0.89
4:A:1228:TYR:N	6:A:1501:HOH:O	2.03	0.89
4:A:1153:ASN:HB3	4:A:1165:THR:HG22	1.55	0.88
3:D:-5:DC:OP1	6:D:101:HOH:O	1.92	0.88
4:A:226:PRO:HD2	6:A:1531:HOH:O	1.75	0.87
3:D:-5:DC:H5'	6:D:101:HOH:O	1.63	0.86
3:D:-9:DA:N7	6:D:102:HOH:O	2.08	0.86
4:A:779:ASN:OD1	6:A:1511:HOH:O	1.94	0.86
4:A:1195:ILE:O	6:A:1508:HOH:O	1.92	0.86
4:A:312:ASN:ND2	6:A:1519:HOH:O	2.09	0.85
3:D:-9:DA:N6	6:D:103:HOH:O	2.10	0.85
4:A:252:GLU:OE2	4:A:256:ARG:NH2	2.12	0.83
4:A:625:ASP:OD1	6:A:1512:HOH:O	1.98	0.82
4:A:227:GLU:CA	6:A:1509:HOH:O	2.27	0.82
4:A:1196:CYS:CA	6:A:1508:HOH:O	2.26	0.81
4:A:227:GLU:CB	6:A:1509:HOH:O	2.27	0.81
4:A:2:SER:OG	6:A:1513:HOH:O	1.99	0.80
4:A:746:ARG:NH2	6:A:1523:HOH:O	2.12	0.80
4:A:1195:ILE:CD1	6:A:1529:HOH:O	2.29	0.80
4:A:245:ASP:OD1	4:A:255:GLN:NE2	2.14	0.79
3:D:-5:DC:P	6:D:101:HOH:O	2.40	0.79
4:A:1298:ARG:NH1	6:A:1505:HOH:O	1.89	0.79
4:A:27:THR:HG21	4:A:785:LEU:H	1.48	0.79
4:A:1155:ARG:HD3	4:A:1155:ARG:C	2.07	0.79
4:A:1196:CYS:HA	6:A:1508:HOH:O	1.84	0.77
4:A:408:ASP:C	6:A:1504:HOH:O	2.24	0.77
4:A:226:PRO:CD	6:A:1531:HOH:O	2.30	0.76
4:A:1227:ASP:HB2	6:A:1501:HOH:O	1.86	0.76
4:A:547:GLN:NE2	6:A:1527:HOH:O	2.16	0.75
4:A:780:GLN:OE1	6:A:1515:HOH:O	2.04	0.75
4:A:1226:LEU:O	6:A:1516:HOH:O	2.05	0.74
4:A:226:PRO:N	6:A:1531:HOH:O	2.21	0.73
4:A:464:ASN:ND2	4:A:473:CYS:O	2.21	0.73
4:A:446:GLU:O	6:A:1514:HOH:O	2.07	0.73
4:A:1117:TYR:CE1	4:A:1119:LEU:HD13	2.23	0.72
4:A:1282:LEU:N	6:A:1520:HOH:O	2.11	0.72
4:A:755:ARG:NH1	4:A:891:SER:HB3	2.04	0.72
4:A:1227:ASP:HB3	6:A:1516:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-9:DA:C8	6:D:102:HOH:O	2.43	0.72
1:B:29:A:H2'	1:B:30:C:C6	2.26	0.71
4:A:24:GLN:O	4:A:27:THR:HG23	1.90	0.71
4:A:1195:ILE:HD13	6:A:1529:HOH:O	1.89	0.70
4:A:1088:VAL:O	4:A:1299:ASN:ND2	2.24	0.70
4:A:1227:ASP:OD1	6:A:1518:HOH:O	2.09	0.70
3:D:3:DA:H1'	4:A:894:ASN:HD22	1.57	0.70
4:A:215:LYS:NZ	6:A:1522:HOH:O	2.12	0.69
4:A:1129:ASP:HB2	4:A:1141:LYS:HE3	1.73	0.69
4:A:463:PHE:HA	4:A:466:HIS:CD2	2.28	0.68
4:A:222:LYS:O	4:A:226:PRO:HG3	1.93	0.68
1:B:27:G:H21	4:A:400:THR:CG2	2.06	0.68
4:A:733:GLU:OE2	6:A:1521:HOH:O	2.11	0.68
2:C:-11:DA:H2'	2:C:-10:DA:C8	2.30	0.67
4:A:47:TYR:OH	6:A:1517:HOH:O	2.08	0.67
4:A:1155:ARG:HD3	4:A:1156:ASN:N	2.09	0.67
4:A:833:ARG:NH1	6:A:1532:HOH:O	2.22	0.67
4:A:1189:GLU:OE1	4:A:1189:GLU:N	2.22	0.66
4:A:743:ASP:HB3	6:A:1689:HOH:O	1.95	0.66
4:A:518:SER:N	6:A:1507:HOH:O	1.92	0.66
1:B:27:G:H21	4:A:400:THR:HG23	1.61	0.66
4:A:446:GLU:N	6:A:1514:HOH:O	2.00	0.66
4:A:1210:VAL:O	4:A:1213:THR:HG22	1.95	0.65
4:A:733:GLU:OE1	6:A:1525:HOH:O	2.14	0.65
4:A:1169:TYR:O	6:A:1524:HOH:O	2.13	0.65
4:A:65:ILE:CG2	4:A:113:ILE:HG22	2.25	0.64
4:A:892:GLY:N	6:A:1539:HOH:O	2.31	0.64
4:A:889:LYS:NZ	6:A:1538:HOH:O	2.30	0.64
4:A:616:ASP:OD2	6:A:1526:HOH:O	2.14	0.64
3:D:3:DA:H1'	4:A:894:ASN:ND2	2.12	0.64
4:A:86:LEU:HD11	4:A:98:PHE:HB2	1.78	0.64
4:A:1281:LYS:CA	6:A:1520:HOH:O	2.14	0.64
4:A:1273:ILE:HG12	4:A:1282:LEU:HD21	1.80	0.63
4:A:1119:LEU:HD12	4:A:1122:GLY:HA2	1.81	0.63
4:A:1281:LYS:O	6:A:1502:HOH:O	2.11	0.62
4:A:1151:LEU:H	4:A:1219:ASN:HD22	1.47	0.62
4:A:1178:LEU:HD12	4:A:1185:TYR:CD2	2.35	0.62
4:A:1195:ILE:H	4:A:1195:ILE:HD12	1.64	0.62
1:B:29:A:H2'	1:B:30:C:H6	1.65	0.61
4:A:1299:ASN:ND2	6:A:1533:HOH:O	2.33	0.61
4:A:460:LEU:HA	4:A:463:PHE:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:-4:DT:H2'	4:A:177:THR:HG22	1.82	0.61
4:A:1151:LEU:HD12	4:A:1219:ASN:HB3	1.83	0.60
4:A:1146:SER:HB2	4:A:1171:THR:HB	1.83	0.59
4:A:462:GLU:CD	4:A:465:LYS:HZ2	2.10	0.59
4:A:256:ARG:NH1	4:A:262:GLU:OE2	2.35	0.59
4:A:1171:THR:HG22	6:A:1544:HOH:O	2.03	0.59
1:B:27:G:H2'	4:A:410:TYR:HD2	1.67	0.59
4:A:1195:ILE:HG21	4:A:1207:LEU:CD2	2.33	0.58
4:A:1177:LEU:C	4:A:1178:LEU:HD23	2.29	0.58
4:A:886:ILE:HG21	4:A:1037:TYR:CZ	2.38	0.58
3:D:-4:DT:OP2	4:A:177:THR:HG23	2.04	0.57
4:A:1169:TYR:C	6:A:1544:HOH:O	2.46	0.57
4:A:1129:ASP:HB2	4:A:1141:LYS:HG2	1.86	0.56
1:B:-8:U:H5	4:A:862:VAL:O	1.86	0.56
4:A:241:GLU:HG2	4:A:283:THR:HB	1.87	0.56
4:A:295:THR:O	6:A:1528:HOH:O	2.16	0.56
1:B:20:C:N4	1:B:26:A:H2'	2.19	0.56
4:A:403:SER:HB3	4:A:413:ILE:HD12	1.87	0.56
4:A:1171:THR:N	6:A:1544:HOH:O	2.38	0.56
4:A:410:TYR:O	4:A:412:VAL:N	2.39	0.55
4:A:1153:ASN:CB	4:A:1165:THR:HG22	2.33	0.55
4:A:1151:LEU:CD1	4:A:1219:ASN:HB3	2.35	0.55
4:A:467:ARG:NH1	4:A:471:LYS:O	2.39	0.55
4:A:777:VAL:HG22	4:A:782:LYS:HB2	1.88	0.55
4:A:1169:TYR:HB3	6:A:1544:HOH:O	2.06	0.55
4:A:27:THR:HG22	4:A:778:VAL:HG13	1.88	0.55
4:A:1103:SER:O	4:A:1107:GLU:N	2.36	0.55
4:A:1282:LEU:HG	4:A:1284:LEU:HD21	1.88	0.55
1:B:36:C:H2'	2:C:-11:DA:C8	2.42	0.55
4:A:1097:PRO:HG2	4:A:1212:ASN:HB3	1.89	0.54
4:A:801:PRO:HG2	4:A:806:LEU:HD21	1.89	0.54
4:A:49:LYS:HE2	4:A:158:ASP:HB3	1.89	0.54
4:A:73:GLU:OE2	4:A:267:ALA:HB2	2.07	0.53
4:A:256:ARG:HH11	4:A:262:GLU:CD	2.15	0.53
1:B:27:G:H5'	1:B:27:G:H8	1.72	0.53
4:A:1227:ASP:CA	6:A:1516:HOH:O	2.56	0.53
4:A:397:LYS:HA	4:A:400:THR:HB	1.90	0.53
4:A:249:LYS:HD3	4:A:265:GLU:OE1	2.09	0.53
4:A:1179:LYS:HG3	4:A:1180:ASP:N	2.23	0.53
4:A:1195:ILE:N	6:A:1529:HOH:O	2.16	0.53
4:A:352:MET:HE1	4:A:499:LEU:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1177:LEU:HD22	4:A:1206:LYS:HB3	1.91	0.53
4:A:467:ARG:HD3	4:A:471:LYS:O	2.07	0.53
1:B:27:G:O4'	1:B:29:A:H1'	2.10	0.52
4:A:1032:ILE:HD13	4:A:1067:MET:HE1	1.91	0.52
4:A:412:VAL:HG21	4:A:473:CYS:SG	2.50	0.52
4:A:1201:LYS:HE2	4:A:1202:LYS:HG3	1.91	0.52
2:C:0:DC:H4'	4:A:827:GLU:HG3	1.91	0.52
4:A:390:LYS:HB3	4:A:558:ASP:N	2.24	0.52
4:A:1195:ILE:HG23	4:A:1203:PHE:CE2	2.45	0.51
2:C:-5:DC:H2'	2:C:-4:DT:H71	1.92	0.51
4:A:407:PHE:HD2	4:A:412:VAL:HG11	1.74	0.51
4:A:1195:ILE:HD12	6:A:1529:HOH:O	2.02	0.51
4:A:1200:ASP:OD1	4:A:1203:PHE:N	2.42	0.51
4:A:383:ALA:HB3	4:A:385:LYS:HG2	1.93	0.51
4:A:1151:LEU:H	4:A:1219:ASN:ND2	2.08	0.51
4:A:407:PHE:CD2	4:A:412:VAL:HG11	2.45	0.50
4:A:490:ASP:HA	4:A:493:ALA:HB3	1.93	0.50
4:A:1195:ILE:HD12	4:A:1195:ILE:N	2.26	0.50
4:A:1117:TYR:HE1	4:A:1119:LEU:HB2	1.76	0.50
4:A:895:LYS:O	4:A:899:GLU:HG3	2.12	0.50
4:A:166:LEU:O	4:A:170:LYS:HG3	2.12	0.49
4:A:407:PHE:HD2	4:A:412:VAL:CG1	2.25	0.49
4:A:65:ILE:HD12	4:A:113:ILE:HA	1.92	0.49
1:B:6:U:O4	6:B:201:HOH:O	2.19	0.49
4:A:1227:ASP:CB	6:A:1516:HOH:O	2.55	0.49
1:B:20:C:N4	1:B:27:G:C8	2.79	0.49
4:A:913:ILE:HB	4:A:929:VAL:HG22	1.94	0.49
4:A:537:LEU:HD22	4:A:569:TYR:CE1	2.48	0.49
4:A:1181:TYR:CZ	4:A:1203:PHE:HB2	2.48	0.49
4:A:91:ASP:OD2	4:A:93:ASN:HB3	2.13	0.49
4:A:945:GLY:HA3	4:A:946:ASN:HB2	1.95	0.48
4:A:1117:TYR:HE1	4:A:1119:LEU:CB	2.26	0.48
4:A:1136:LYS:O	4:A:1139:LYS:NZ	2.42	0.48
4:A:250:THR:OG1	4:A:252:GLU:HG2	2.14	0.48
4:A:1007:ASP:O	4:A:1008:LEU:HG	2.13	0.48
4:A:43:ARG:NH1	6:A:1560:HOH:O	2.46	0.48
4:A:1106:GLN:HG3	4:A:1204:PHE:CZ	2.49	0.48
4:A:1266:GLY:HA2	4:A:1269:LEU:HD12	1.94	0.48
4:A:1195:ILE:HG23	4:A:1203:PHE:HE2	1.78	0.48
4:A:1278:GLU:H	4:A:1278:GLU:CD	2.21	0.47
1:B:27:G:H4'	1:B:28:A:O5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1020:GLU:O	4:A:1023:VAL:N	2.44	0.47
3:D:-5:DC:H5''	6:D:101:HOH:O	1.79	0.47
4:A:1227:ASP:HA	6:A:1516:HOH:O	2.15	0.47
4:A:253:VAL:HG12	4:A:253:VAL:O	2.15	0.47
4:A:492:ILE:HG23	4:A:529:LEU:HD11	1.96	0.47
4:A:1204:PHE:O	4:A:1208:THR:HG23	2.15	0.47
4:A:285:ILE:HD13	4:A:321:MET:HB2	1.97	0.46
4:A:196:PRO:HA	4:A:201:TYR:CD2	2.50	0.46
4:A:1281:LYS:HG3	6:A:1520:HOH:O	2.14	0.46
4:A:328:ILE:HG22	4:A:329:LEU:HD13	1.97	0.46
4:A:660:LYS:HE2	4:A:660:LYS:HA	1.97	0.46
4:A:730:LYS:HB3	4:A:730:LYS:HE3	1.69	0.46
4:A:1112:PHE:HE1	4:A:1126:PHE:HB3	1.80	0.46
4:A:1146:SER:HA	4:A:1214:ILE:CD1	2.44	0.46
4:A:1178:LEU:HD23	4:A:1178:LEU:N	2.30	0.46
1:B:36:C:OP1	4:A:334:SER:HB2	2.15	0.46
4:A:328:ILE:O	4:A:329:LEU:HB2	2.15	0.46
4:A:1206:LYS:O	4:A:1210:VAL:HG13	2.15	0.46
1:B:27:G:C4	4:A:410:TYR:CG	3.04	0.46
4:A:910:ASP:OD1	6:A:1530:HOH:O	2.21	0.46
4:A:1106:GLN:HG2	6:A:1508:HOH:O	2.16	0.46
4:A:1155:ARG:C	4:A:1155:ARG:CD	2.84	0.46
4:A:537:LEU:CD2	4:A:569:TYR:CE1	2.99	0.45
4:A:1126:PHE:HB2	4:A:1144:ILE:HG12	1.96	0.45
2:C:-6:DA:OP2	6:C:101:HOH:O	2.20	0.45
4:A:755:ARG:NH2	4:A:889:LYS:O	2.49	0.45
4:A:237:ASP:O	4:A:297:ARG:NH1	2.43	0.45
4:A:755:ARG:HE	4:A:759:ASN:HD21	1.63	0.45
4:A:363:LYS:HE3	6:A:1614:HOH:O	2.16	0.45
1:B:24:U:H6	1:B:24:U:H5'	1.80	0.45
4:A:637:ASN:O	4:A:640:ILE:HG12	2.16	0.45
4:A:133:GLY:N	6:A:1548:HOH:O	2.41	0.45
4:A:800:ARG:HH11	4:A:800:ARG:HG3	1.82	0.45
1:B:9:U:H2'	1:B:10:U:C6	2.52	0.45
4:A:1227:ASP:C	6:A:1501:HOH:O	2.49	0.45
4:A:800:ARG:HG3	4:A:800:ARG:NH1	2.32	0.44
1:B:27:G:O4'	1:B:29:A:C1'	2.65	0.44
4:A:91:ASP:CG	4:A:93:ASN:HB3	2.41	0.44
4:A:669:LEU:HB2	4:A:670:PRO:HD3	1.98	0.44
4:A:409:ASP:N	6:A:1504:HOH:O	2.48	0.44
3:D:-3:DT:OP1	4:A:124:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:G:H2'	4:A:410:TYR:CD2	2.52	0.44
4:A:113:ILE:HD13	4:A:113:ILE:HG21	1.74	0.43
4:A:94:LEU:HA	4:A:97:ASP:HB2	2.00	0.43
4:A:945:GLY:CA	4:A:946:ASN:HB2	2.49	0.43
4:A:1112:PHE:CE1	4:A:1126:PHE:HB3	2.53	0.43
4:A:518:SER:CB	6:A:1507:HOH:O	2.66	0.43
4:A:464:ASN:HA	4:A:467:ARG:HB2	2.01	0.43
4:A:464:ASN:HD21	4:A:473:CYS:C	2.20	0.43
4:A:1265:LYS:HA	4:A:1268:MET:HE3	2.01	0.43
4:A:83:TYR:CE2	4:A:87:LYS:HE3	2.54	0.43
4:A:27:THR:CG2	4:A:785:LEU:H	2.26	0.43
4:A:78:ASN:O	4:A:82:VAL:HG12	2.18	0.43
4:A:695:SER:HB3	4:A:709:LYS:HE2	2.00	0.42
4:A:342:LEU:HD22	4:A:347:ASP:HB3	2.01	0.42
4:A:1166:ARG:HE	4:A:1168:VAL:CG2	2.32	0.42
4:A:140:LEU:O	4:A:144:GLN:HG3	2.19	0.42
4:A:1095:LEU:HD23	4:A:1095:LEU:HA	1.88	0.42
4:A:208:LEU:HB3	4:A:209:PRO:HD3	2.01	0.42
4:A:452:SER:O	4:A:456:ILE:HG12	2.20	0.42
4:A:1100:GLU:OE2	4:A:1104:LYS:HD2	2.19	0.42
4:A:296:LYS:NZ	4:A:302:GLU:OE2	2.53	0.42
4:A:1047:LYS:HG3	6:A:1685:HOH:O	2.18	0.42
4:A:1217:MET:N	6:A:1549:HOH:O	2.42	0.42
3:D:-4:DT:H1'	3:D:-3:DT:H5''	2.01	0.42
4:A:8:VAL:HG11	4:A:1053:ARG:HB3	2.01	0.42
1:B:27:G:N3	4:A:410:TYR:HB3	2.35	0.41
4:A:85:LYS:O	4:A:89:SER:HB3	2.20	0.41
4:A:1269:LEU:HG	4:A:1286:ILE:HD11	2.02	0.41
4:A:235:LYS:HE3	4:A:235:LYS:HB3	1.75	0.41
4:A:1174:LEU:HA	4:A:1174:LEU:HD23	1.84	0.41
1:B:5:G:H2'	1:B:6:U:O4'	2.20	0.41
4:A:6:GLU:HB2	6:A:1709:HOH:O	2.20	0.41
4:A:1121:LYS:HB3	4:A:1123:TYR:CE1	2.55	0.41
3:D:0:DG:O4'	4:A:667:LYS:HG2	2.20	0.41
4:A:1175:GLU:CB	6:A:1506:HOH:O	2.44	0.41
4:A:397:LYS:O	4:A:400:THR:HB	2.21	0.41
3:D:-6:DC:H2''	3:D:-5:DC:C5	2.55	0.41
4:A:1195:ILE:CD1	4:A:1195:ILE:H	2.32	0.41
4:A:117:GLU:HA	4:A:117:GLU:OE2	2.20	0.41
4:A:351:THR:HG22	4:A:578:LEU:CD1	2.51	0.41
4:A:1290:GLU:H	4:A:1290:GLU:HG3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:843:HIS:HB2	4:A:867:LEU:HB2	2.02	0.40
4:A:856:ASN:OD1	4:A:857:PRO:HD2	2.21	0.40
4:A:1180:ASP:N	4:A:1180:ASP:OD2	2.54	0.40
4:A:285:ILE:HD13	4:A:321:MET:CB	2.51	0.40
2:C:2:DA:N3	4:A:668:MET:HE1	2.36	0.40
4:A:369:SER:OG	4:A:372:GLU:HG3	2.21	0.40
4:A:960:ILE:HD13	4:A:980:MET:HG3	2.04	0.40
4:A:1020:GLU:O	4:A:1023:VAL:HB	2.21	0.40
1:B:26:A:H1'	1:B:30:C:H1'	2.04	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
4	A	1256/1300 (97%)	1216 (97%)	36 (3%)	4 (0%)	36 46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	411	SER
4	A	653	GLY
4	A	1019	VAL
4	A	892	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	1141/1183 (96%)	1141 (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 (22) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	5	GLN
4	A	9	ASN
4	A	134	GLN
4	A	405	GLN
4	A	495	ASN
4	A	508	ASN
4	A	535	ASN
4	A	666	ASN
4	A	700	ASN
4	A	745	GLN
4	A	759	ASN
4	A	818	GLN
4	A	894	ASN
4	A	990	HIS
4	A	1094	GLN
4	A	1118	ASN
4	A	1153	ASN
4	A	1219	ASN
4	A	1261	HIS
4	A	1283	ASN
4	A	1299	ASN
4	A	1300	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	B	51/58 (87%)	8 (15%)	1 (1%)

All (8) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	B	-9	G

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Mol	Chain	Res	Type
1	B	-7	U
1	B	-6	G
1	B	25	A
1	B	26	A
1	B	27	G
1	B	28	A
1	B	29	A

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	B	27	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 [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	B	53/58 (91%)	-0.33	5 (9%) 14 15	26, 35, 109, 138	0
2	C	21/21 (100%)	-0.47	0 100 100	28, 36, 65, 85	0
3	D	13/18 (72%)	-0.08	1 (7%) 19 21	37, 40, 78, 94	0
4	A	1264/1300 (97%)	0.63	164 (12%) 7 8	25, 49, 104, 124	0
All	All	1351/1397 (96%)	0.56	170 (12%) 8 9	25, 48, 104, 138	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	A	499	LEU	5.5
4	A	469	ILE	5.4
4	A	552	ALA	5.4
4	A	1154	PHE	5.1
4	A	554	ILE	4.8
4	A	1019	VAL	4.6
4	A	1099	TYR	4.5
4	A	1137	ALA	4.3
4	A	1169	TYR	4.3
4	A	1096	TYR	4.1
4	A	421	ILE	4.1
4	A	1124	PHE	4.0
4	A	1156	ASN	4.0
4	A	1119	LEU	4.0
4	A	1207	LEU	4.0
4	A	410	TYR	4.0
4	A	447	LYS	3.9
4	A	418	LEU	3.9
4	A	460	LEU	3.9
4	A	1134	GLY	3.9
1	B	27	G	3.9

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Mol	Chain	Res	Type	RSRZ
4	A	1018	LYS	3.9
4	A	1185	TYR	3.7
4	A	1147	PHE	3.7
4	A	1191	ILE	3.7
4	A	1211	LEU	3.6
4	A	445	THR	3.6
4	A	1138	ALA	3.6
4	A	1008	LEU	3.5
4	A	495	ASN	3.5
4	A	1226	LEU	3.5
4	A	892	GLY	3.4
4	A	1115	ILE	3.4
4	A	1224	THR	3.4
4	A	420	TYR	3.4
4	A	332	THR	3.3
1	B	28	A	3.3
4	A	1155	ARG	3.2
4	A	1222	THR	3.2
4	A	1022	GLN	3.1
4	A	1205	ALA	3.1
4	A	1021	LYS	3.0
4	A	1196	CYS	3.0
4	A	1194	ALA	3.0
4	A	413	ILE	3.0
4	A	1183	ILE	3.0
4	A	1221	LYS	2.9
4	A	1300	ASN	2.9
4	A	1109	PHE	2.9
4	A	1187	HIS	2.9
4	A	551	LYS	2.9
4	A	470	ASP	2.9
4	A	1190	CYS	2.9
4	A	1135	ASP	2.9
4	A	1188	GLY	2.8
4	A	408	ASP	2.8
4	A	1236	VAL	2.8
4	A	473	CYS	2.8
4	A	1116	CYS	2.8
4	A	1197	GLY	2.8
4	A	1123	TYR	2.8
4	A	1	MET	2.8
4	A	1108	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
4	A	466	HIS	2.8
4	A	1152	ILE	2.8
4	A	463	PHE	2.8
4	A	1153	ASN	2.7
4	A	1139	LYS	2.7
4	A	1061	PHE	2.7
4	A	1168	VAL	2.7
4	A	1223	GLY	2.7
4	A	132	LYS	2.7
4	A	1199	SER	2.7
4	A	553	ASN	2.6
4	A	422	THR	2.6
4	A	1171	THR	2.6
1	B	20	C	2.6
1	B	24	U	2.6
4	A	1203	PHE	2.6
4	A	471	LYS	2.6
4	A	467	ARG	2.6
4	A	459	ALA	2.6
4	A	337	PHE	2.6
4	A	1170	PRO	2.6
4	A	496	LYS	2.6
4	A	1114	LYS	2.6
4	A	477	GLU	2.5
4	A	335	LYS	2.5
4	A	1146	SER	2.5
4	A	1182	SER	2.5
4	A	511	LYS	2.5
4	A	411	SER	2.5
4	A	1127	SER	2.5
4	A	1145	ALA	2.5
4	A	1186	GLY	2.5
4	A	1225	GLU	2.5
4	A	416	ALA	2.5
4	A	400	THR	2.4
4	A	1110	SER	2.4
4	A	1133	PHE	2.4
4	A	893	ALA	2.4
4	A	1165	THR	2.4
4	A	1149	SER	2.4
4	A	1195	ILE	2.4
4	A	1214	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
4	A	1164	ASP	2.4
4	A	1023	VAL	2.4
4	A	1233	VAL	2.4
1	B	25	A	2.4
4	A	1212	ASN	2.4
4	A	478	ILE	2.4
4	A	488	ILE	2.4
4	A	72	SER	2.3
4	A	417	VAL	2.3
4	A	1166	ARG	2.3
4	A	1298	ARG	2.3
4	A	1095	LEU	2.3
4	A	1173	GLU	2.3
4	A	1184	GLU	2.3
4	A	548	SER	2.3
4	A	407	PHE	2.3
4	A	1064	PHE	2.3
4	A	1284	LEU	2.3
4	A	1117	TYR	2.3
4	A	403	SER	2.3
4	A	1062	GLU	2.3
4	A	1240	PHE	2.3
4	A	112	TYR	2.3
4	A	686	GLU	2.3
4	A	456	ILE	2.3
4	A	253	VAL	2.3
4	A	555	LEU	2.2
4	A	382	LYS	2.2
4	A	547	GLN	2.2
3	D	-9	DA	2.2
4	A	381	LEU	2.2
4	A	502	ILE	2.2
4	A	640	ILE	2.2
4	A	294	ASN	2.2
4	A	1113	ASP	2.2
4	A	415	THR	2.2
4	A	448	ALA	2.2
4	A	402	LEU	2.1
4	A	1174	LEU	2.1
4	A	412	VAL	2.1
4	A	489	PHE	2.1
4	A	1112	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	A	1177	LEU	2.1
4	A	464	ASN	2.1
4	A	1175	GLU	2.1
4	A	1189	GLU	2.1
4	A	1126	PHE	2.1
4	A	398	SER	2.1
4	A	1280	LYS	2.1
4	A	260	LEU	2.1
4	A	386	LEU	2.1
4	A	1020	GLU	2.1
4	A	1118	ASN	2.1
4	A	945	GLY	2.1
4	A	1279	GLY	2.1
4	A	1208	THR	2.1
4	A	1136	LYS	2.1
4	A	131	LYS	2.0
4	A	1201	LYS	2.0
4	A	312	ASN	2.0
4	A	227	GLU	2.0
4	A	333	GLU	2.0
4	A	1200	ASP	2.0
4	A	96	LYS	2.0
4	A	1121	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	B	101	1/1	0.77	0.12	32,32,32,32	0
5	MG	A	1401	1/1	0.82	0.10	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.