Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 10:52 am BST

PDB ID	:	5FFJ
Title	:	Structure of a nuclease-deletion mutant of the Type ISP restriction-modification enzyme LlaGI in complex with a DNA substrate mimic
Authors	:	Saikrishnan, K.; Kulkarni, M.; Nirwan, N.
Deposited on	:	2015-12-18
Resolution	:	2.84 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 following versions of software and data (see references ⓘ) were used in the production of this report:

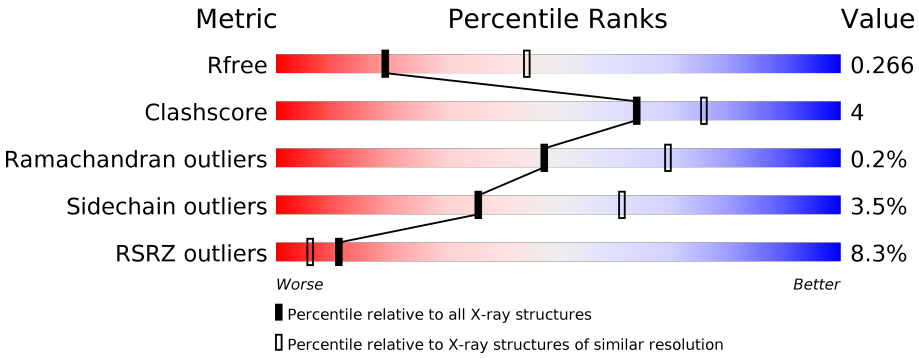
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 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 <=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	1406	7% 64% 10% 26%
1	B	1406	7% 78% 9% 12%
2	D	23	83% 13%
2	E	23	4% 96%
3	C	23	78% 17%
3	F	23	4% 91%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36361 atoms, of which 17133 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 Endonuclease and methylase LlaGI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1044	Total	C	H	N	O	S	0	0	0
			15492	5077	7466	1364	1568	17			
1	B	1232	Total	C	H	N	O	S	0	0	0
			18040	5927	8659	1589	1845	20			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	165	MET	-	expression tag	UNP Q93R01
B	165	MET	-	expression tag	UNP Q93R01

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	22	Total	C	H	N	O	P	0	0	0
			688	212	251	70	134	21			
2	E	23	Total	C	H	N	O	P	0	0	0
			721	222	263	75	139	22			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	22	Total	C	H	N	O	P	0	0	0
			709	218	248	91	130	22			
3	F	22	Total	C	H	N	O	P	0	0	0
			703	218	246	91	127	21			

- Molecule 4 is water.

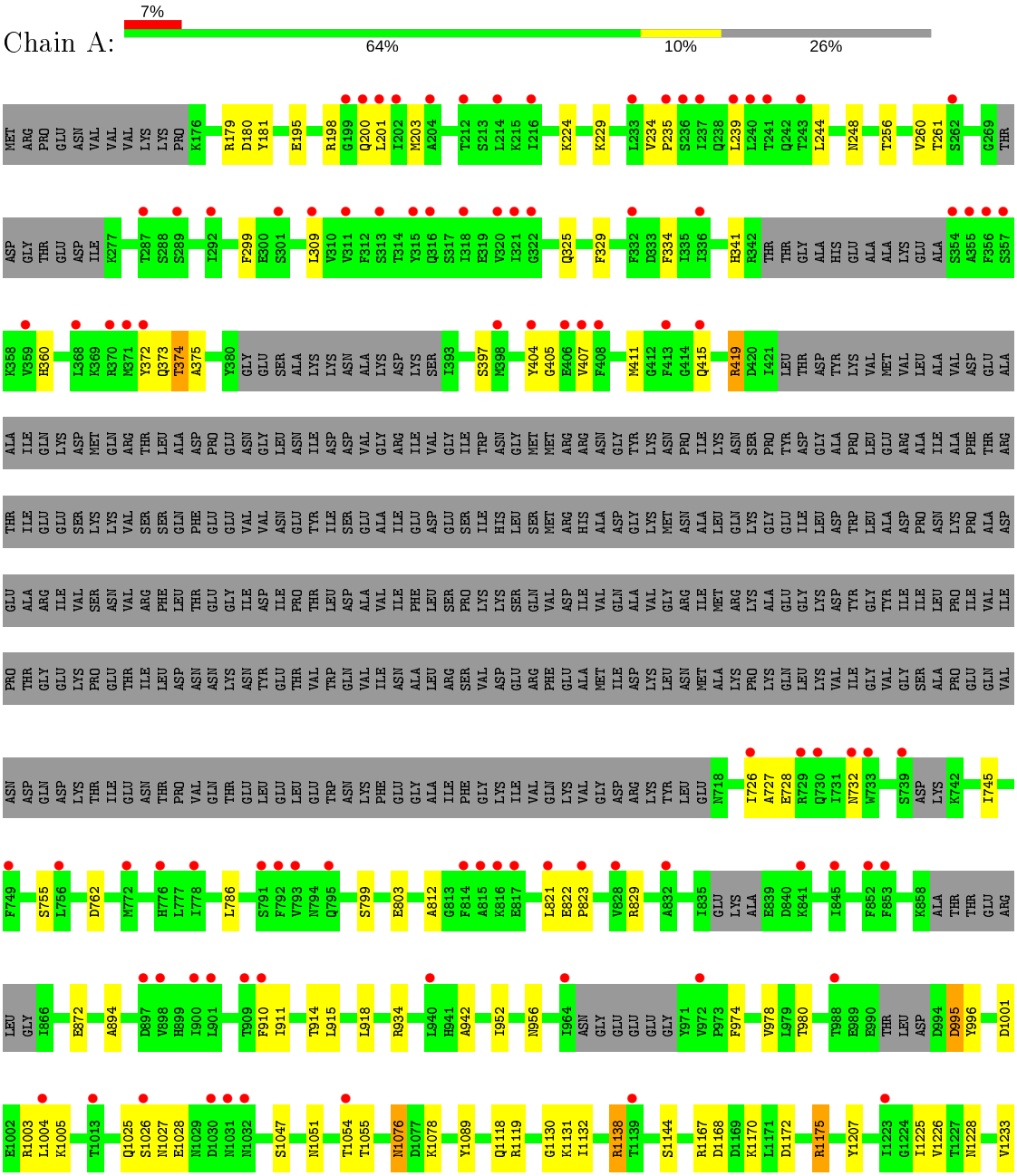
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	1	Total O 1 1	0	0

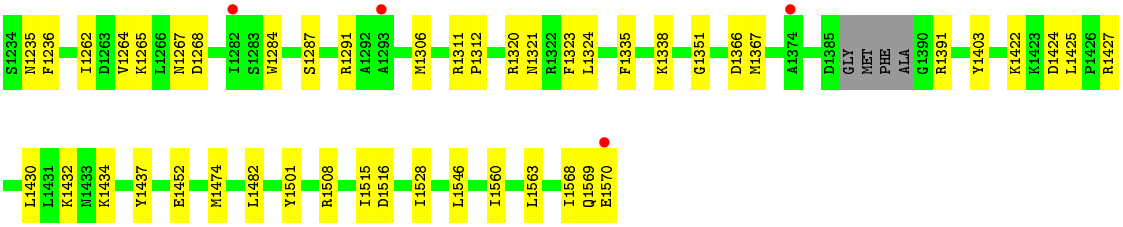
3 Residue-property plots (i)

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.

- Molecule 1: Endonuclease and methylase LlaGI

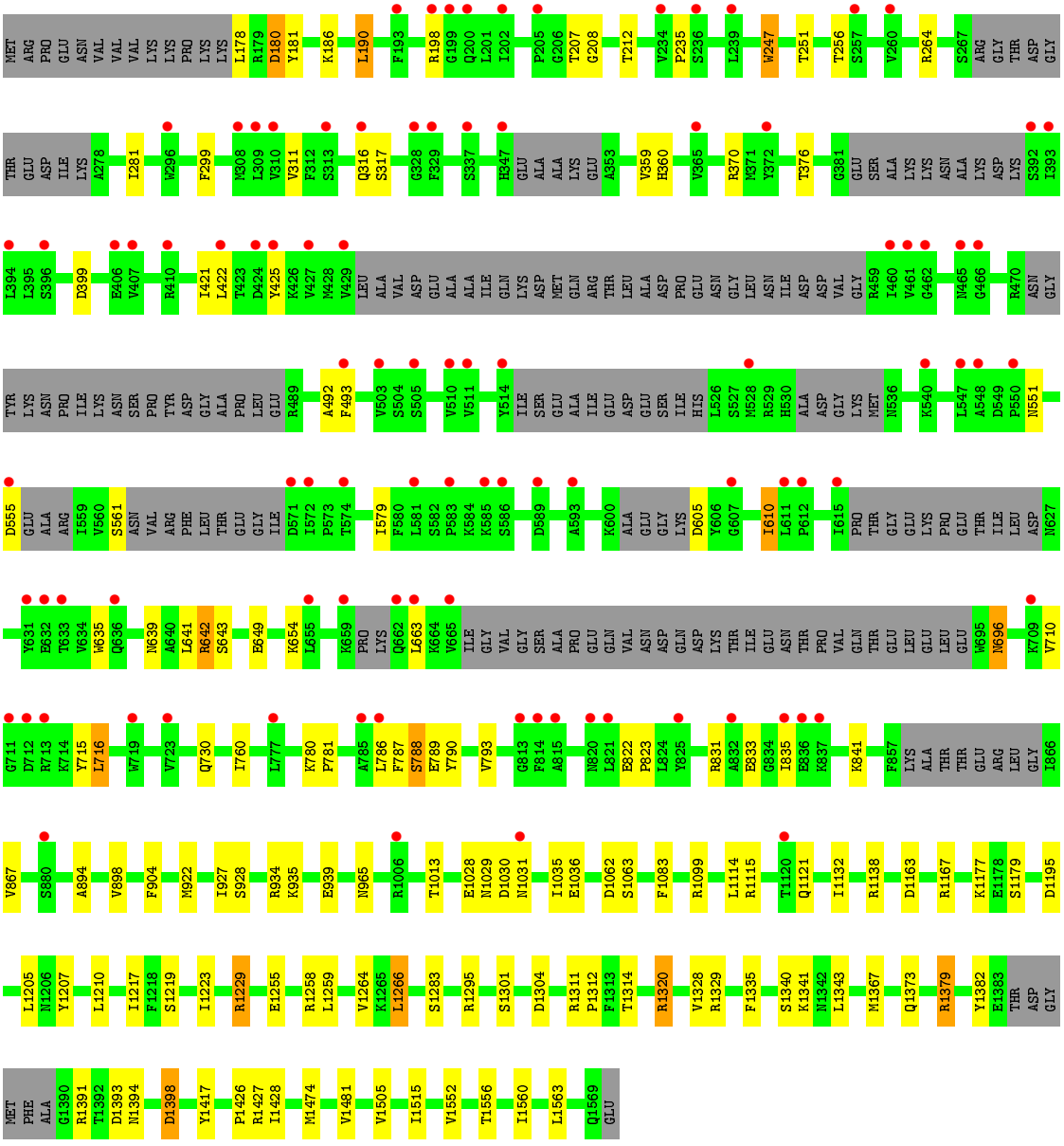
Chain A:





• Molecule 1: Endonuclease and methylase LlaGI

Chain B:

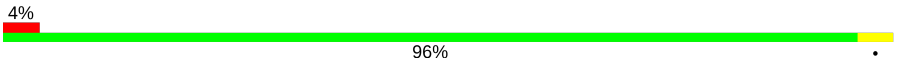


• Molecule 2: DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP*AP*GP*TP*CP*TP*AP*TP*TP*AP*GP*CP*T)-3')

Chain D:

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

Chain E:

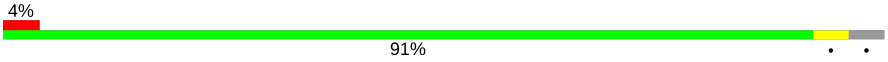


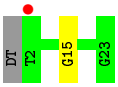
• Molecule 3: DNA (5'-D(P*TP*AP*GP*CP*TP*AP*AP*TP*AP*GP*AP*CP*TP*GP*GP*AP*TP*GP*GP*AP*GP*G)-3')

Chain C:

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

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.40Å 222.29Å 117.41Å 90.00° 105.14° 90.00°	Depositor
Resolution (Å)	50.00 – 2.84 84.37 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.84) 99.9 (84.37-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.229 , 0.262 0.234 , 0.266	Depositor DCC
R_{free} test set	5109 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	66.6	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 60.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	36361	wwPDB-VP
Average B, all atoms (Å^2)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.24	0/8178	0.44	0/11106
1	B	0.24	0/9548	0.43	0/12967
2	D	0.67	0/486	1.05	0/746
2	E	0.66	0/510	1.05	0/783
3	C	0.58	0/519	0.99	0/801
3	F	0.59	0/515	0.98	0/796
All	All	0.30	0/19756	0.54	0/27199

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
1	A	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	GLN	Peptide
1	A	1026	SER	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	A	8026	7466	7460	77	0
1	B	9381	8659	8658	71	0
2	D	437	251	252	3	0
2	E	458	263	263	1	0
3	C	461	248	248	6	0
3	F	457	246	246	1	0
4	A	7	0	0	0	0
4	B	1	0	0	0	0
All	All	19228	17133	17127	150	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 4.

All (150) 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:B:1320:ARG:NH2	1:B:1335:PHE:O	2.13	0.82
1:B:1255:GLU:OE1	1:B:1258:ARG:NH2	2.17	0.77
1:B:922:MET:HA	1:B:927:ILE:HG22	1.65	0.77
1:A:1089:TYR:OH	1:A:1144:SER:OG	2.06	0.73
1:A:198:ARG:NH1	1:A:360:HIS:O	2.25	0.70
1:A:974:PHE:O	1:A:1003:ARG:NH2	2.25	0.69
1:A:1001:ASP:OD2	1:A:1005:LYS:NZ	2.26	0.69
1:B:1132:ILE:O	1:B:1167:ARG:NH1	2.26	0.68
1:B:359:VAL:O	1:B:370:ARG:NH1	2.26	0.68
1:A:1321:ASN:ND2	1:A:1323:PHE:O	2.27	0.67
1:A:1235:ASN:OD1	1:A:1236:PHE:N	2.28	0.67
1:B:247:TRP:O	1:B:251:THR:OG1	2.12	0.66
1:B:898:VAL:O	1:B:935:LYS:NZ	2.29	0.66
1:A:1132:ILE:O	1:A:1167:ARG:NH1	2.28	0.66
1:A:244:LEU:O	1:A:248:ASN:ND2	2.29	0.66
1:B:922:MET:CA	1:B:927:ILE:HG22	2.26	0.65
1:A:1028:GLU:OE1	1:A:1284:TRP:N	2.28	0.64
1:A:1054:THR:O	1:A:1055:THR:OG1	2.12	0.64
1:B:894:ALA:HB1	1:B:927:ILE:HD11	1.80	0.64
1:A:894:ALA:O	1:A:934:ARG:NH2	2.32	0.63
1:A:1172:ASP:OD1	1:A:1175:ARG:NH1	2.33	0.61
1:A:1424:ASP:OD1	1:A:1425:LEU:N	2.33	0.61
1:A:822:GLU:OE2	1:A:829:ARG:NH1	2.35	0.60
1:A:415:GLN:O	1:A:419:ARG:N	2.34	0.60
1:A:1131:LYS:NZ	2:D:12:DG:O6	2.35	0.59
1:A:910:PHE:O	1:A:914:THR:OG1	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1379:ARG:NH1	1:B:1398:ASP:OD1	2.37	0.58
1:A:201:LEU:HD11	1:A:203:MET:HE2	1.85	0.58
1:B:654:LYS:NZ	1:B:833:GLU:O	2.21	0.57
1:A:1076:ASN:ND2	1:A:1078:LYS:O	2.37	0.57
1:A:1207:TYR:O	1:A:1427:ARG:NH1	2.38	0.57
1:A:1320:ARG:NH1	1:A:1335:PHE:O	2.38	0.57
1:A:180:ASP:OD1	1:A:181:TYR:N	2.38	0.57
1:A:1351:GLY:N	1:A:1422:LYS:O	2.38	0.56
1:B:934:ARG:NH1	1:B:939:GLU:OE2	2.38	0.56
1:B:1207:TYR:O	1:B:1427:ARG:NH1	2.39	0.56
1:B:1311:ARG:NH1	3:F:15:DG:OP2	2.38	0.56
1:A:980:THR:HG21	1:A:1004:LEU:HD13	1.86	0.56
1:B:1115:ARG:NH1	1:B:1163:ASP:OD1	2.38	0.55
1:A:374:THR:OG1	1:A:375:ALA:N	2.39	0.55
1:A:1267:ASN:OD1	1:A:1268:ASP:N	2.41	0.54
1:B:180:ASP:OD1	1:B:180:ASP:N	2.37	0.54
1:A:201:LEU:N	1:A:372:TYR:O	2.40	0.53
1:A:755:SER:CB	1:A:996:TYR:HB2	2.38	0.53
1:B:1205:LEU:O	1:B:1427:ARG:NH1	2.42	0.52
1:B:316:GLN:N	1:B:316:GLN:OE1	2.39	0.52
1:B:780:LYS:CE	1:B:793:VAL:HG11	2.39	0.52
1:B:1138:ARG:HD2	2:E:12:DG:C4	2.45	0.52
1:B:1264:VAL:O	1:B:1295:ARG:NH2	2.43	0.52
1:B:894:ALA:CB	1:B:927:ILE:HD11	2.40	0.52
1:A:1264:VAL:HG12	1:A:1265:LYS:H	1.74	0.52
1:A:872:GLU:OE2	1:A:1175:ARG:NH2	2.43	0.51
1:A:1047:SER:O	1:A:1051:ASN:ND2	2.41	0.51
1:B:1311:ARG:HB3	1:B:1312:PRO:HD2	1.92	0.51
1:B:493:PHE:N	1:B:579:ILE:O	2.42	0.51
1:B:1341:LYS:O	1:B:1382:TYR:OH	2.25	0.51
1:A:1323:PHE:O	1:A:1324:LEU:HB2	2.11	0.51
1:B:1029:ASN:O	1:B:1031:ASN:N	2.44	0.51
1:B:198:ARG:NH2	1:B:360:HIS:O	2.43	0.50
1:B:635:TRP:O	1:B:639:ASN:ND2	2.41	0.50
1:A:1118:GLN:O	1:A:1138:ARG:NH1	2.43	0.50
1:A:728:GLU:O	1:A:732:ASN:ND2	2.42	0.50
1:A:260:VAL:O	1:A:261:THR:OG1	2.24	0.49
1:A:1228:ASN:ND2	3:C:17:DA:OP2	2.42	0.49
1:B:399:ASP:OD1	1:B:399:ASP:N	2.44	0.49
1:B:376:THR:OG1	1:B:376:THR:O	2.30	0.49
1:A:995:ASP:OD1	1:A:995:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:ARG:HB3	1:A:1312:PRO:HD2	1.96	0.48
1:A:915:LEU:HD23	1:A:918:LEU:HD12	1.94	0.48
1:A:1437:TYR:CE1	1:A:1563:LEU:HD12	2.49	0.48
1:B:186:LYS:O	1:B:190:LEU:HD12	2.13	0.48
1:A:1001:ASP:OD1	1:A:1001:ASP:N	2.46	0.48
1:A:1226:VAL:HG21	1:A:1367:MET:HE3	1.96	0.48
1:B:787:PHE:HB3	1:B:790:TYR:HB2	1.96	0.48
1:B:1552:VAL:O	1:B:1556:THR:OG1	2.16	0.48
1:A:1367:MET:HE1	2:D:8:DT:O4	2.14	0.48
1:B:642:ARG:NH1	1:B:649:GLU:OE2	2.47	0.48
1:B:696:ASN:OD1	1:B:696:ASN:N	2.47	0.48
1:A:200:GLN:NE2	1:A:405:GLY:O	2.47	0.47
1:A:203:MET:HA	1:A:411:MET:HB3	1.96	0.47
1:A:952:ILE:O	1:A:956:ASN:ND2	2.44	0.47
1:A:978:VAL:HG11	1:A:1004:LEU:HB2	1.97	0.47
1:A:1403:TYR:CE1	1:A:1434:LYS:HG3	2.50	0.46
1:B:421:ILE:HG22	1:B:422:LEU:CD1	2.45	0.46
1:A:1311:ARG:NH1	3:C:15:DG:OP2	2.47	0.46
2:D:20:DG:N2	3:C:5:DC:N3	2.49	0.46
1:B:1343:LEU:O	1:B:1379:ARG:N	2.47	0.46
1:B:579:ILE:HA	1:B:610:ILE:HD12	1.98	0.45
1:B:780:LYS:HE3	1:B:793:VAL:HG11	1.97	0.45
3:C:4:DG:H1'	3:C:5:DC:C6	2.51	0.45
1:B:1210:LEU:HD11	1:B:1426:PRO:HG2	1.97	0.45
1:A:745:ILE:HD11	1:A:812:ALA:HB2	1.99	0.45
1:B:1177:LYS:O	1:B:1179:SER:N	2.43	0.45
1:B:788:SER:C	1:B:790:TYR:H	2.20	0.45
1:A:1287:SER:OG	1:A:1291:ARG:NH2	2.48	0.45
1:B:425:TYR:CE2	1:B:641:LEU:HD22	2.51	0.45
1:A:1568:ILE:HG22	1:A:1569:GLN:N	2.32	0.45
1:A:911:ILE:HD11	1:A:942:ALA:HB2	1.99	0.44
1:A:1027:ASN:N	3:C:17:DA:H5"	2.32	0.44
1:B:256:THR:HG21	1:B:299:PHE:CE1	2.53	0.44
1:A:234:VAL:HG21	1:A:239:LEU:HB3	2.00	0.43
1:A:1054:THR:HG23	1:A:1055:THR:N	2.33	0.43
1:B:835:ILE:HD11	1:B:841:LYS:CE	2.47	0.43
1:A:1482:LEU:HB3	1:A:1501:TYR:CE1	2.53	0.43
1:A:726:ILE:CD1	1:A:821:LEU:HD11	2.48	0.43
1:B:927:ILE:HG13	1:B:928:SER:H	1.82	0.43
1:B:376:THR:HB	1:B:643:SER:HB3	2.01	0.43
1:A:1306:MET:HB3	1:A:1338:LYS:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:THR:HG21	1:A:299:PHE:CE1	2.53	0.43
1:B:579:ILE:HA	1:B:610:ILE:CD1	2.48	0.43
3:C:4:DG:OP1	1:B:317:SER:OG	2.26	0.43
1:B:1301:SER:OG	1:B:1304:ASP:OD2	2.37	0.43
1:B:1474:MET:HE2	1:B:1515:ILE:HG12	1.99	0.43
1:A:360:HIS:CE1	1:A:404:TYR:HE1	2.37	0.43
1:A:200:GLN:HB2	1:A:407:VAL:HG12	2.01	0.43
1:B:1035:ILE:HG22	1:B:1036:GLU:H	1.84	0.43
1:B:208:GLY:O	1:B:212:THR:HG23	2.18	0.43
1:A:325:GLN:HA	1:A:329:PHE:HB3	2.00	0.42
1:A:822:GLU:N	1:A:823:PRO:HD2	2.34	0.42
1:B:1062:ASP:OD1	1:B:1063:SER:N	2.52	0.42
1:B:1379:ARG:NH2	1:B:1393:ASP:OD1	2.53	0.42
1:B:715:TYR:CE1	1:B:716:LEU:HD13	2.55	0.42
1:A:1508:ARG:NH1	1:A:1516:ASP:OD2	2.51	0.42
1:B:1259:LEU:HD22	1:B:1266:LEU:HD21	2.02	0.42
1:A:256:THR:HG23	1:A:309:LEU:HA	2.01	0.42
1:A:799:SER:O	1:A:803:GLU:N	2.35	0.42
1:B:780:LYS:HB3	1:B:781:PRO:HD3	2.00	0.42
1:B:1311:ARG:HB3	1:B:1312:PRO:CD	2.50	0.42
1:A:1168:ASP:N	1:A:1168:ASP:OD1	2.53	0.42
1:A:1560:ILE:O	1:A:1563:LEU:HD23	2.20	0.42
1:A:726:ILE:HG13	1:A:727:ALA:N	2.35	0.42
1:B:1217:ILE:HD13	1:B:1428:ILE:HD11	2.01	0.42
1:A:1262:ILE:O	1:A:1264:VAL:HG23	2.20	0.42
1:B:1560:ILE:HA	1:B:1563:LEU:HD23	2.01	0.42
1:B:1217:ILE:CD1	1:B:1428:ILE:HD11	2.49	0.41
1:A:1225:ILE:HG22	1:A:1366:ASP:HA	2.02	0.41
1:A:1474:MET:HE2	1:A:1515:ILE:HG12	2.02	0.41
1:A:1001:ASP:O	1:A:1005:LYS:N	2.39	0.41
1:B:1229:ARG:NH1	1:B:1283:SER:O	2.53	0.41
1:B:1219:SER:OG	1:B:1394:ASN:OD1	2.35	0.41
1:B:492:ALA:HA	1:B:579:ILE:CB	2.50	0.41
1:B:1311:ARG:HB2	1:B:1314:THR:CG2	2.50	0.41
1:A:1474:MET:CE	1:A:1546:LEU:HD22	2.51	0.41
1:B:822:GLU:N	1:B:823:PRO:CD	2.83	0.41
1:B:1207:TYR:HH	1:B:1417:TYR:HH	1.69	0.40
1:B:1367:MET:HG2	1:B:1373:GLN:HA	2.03	0.40
1:A:1432:LYS:HA	1:A:1570:GLU:HA	2.03	0.40
1:B:1099:ARG:NH2	1:B:1195:ASP:OD1	2.55	0.40
1:A:1130:GLY:O	1:A:1170:LYS:NZ	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:TYR:OH	1:B:207:THR:OG1	2.33	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	1022/1406 (73%)	966 (94%)	55 (5%)	1 (0%)	51 75
1	B	1200/1406 (85%)	1152 (96%)	44 (4%)	4 (0%)	41 61
All	All	2222/2812 (79%)	2118 (95%)	99 (4%)	5 (0%)	47 69

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1030	ASP
1	A	235	PRO
1	B	710	VAL
1	B	235	PRO
1	B	760	ILE

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	826/1256 (66%)	804 (97%)	22 (3%)	44	69
1	B	949/1256 (76%)	908 (96%)	41 (4%)	29	54
All	All	1775/2512 (71%)	1712 (96%)	63 (4%)	36	61

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	195	GLU
1	A	224	LYS
1	A	229	LYS
1	A	334	PHE
1	A	341	HIS
1	A	373	GLN
1	A	374	THR
1	A	397	SER
1	A	419	ARG
1	A	762	ASP
1	A	786	LEU
1	A	995	ASP
1	A	1076	ASN
1	A	1119	ARG
1	A	1138	ARG
1	A	1175	ARG
1	A	1233	VAL
1	A	1391	ARG
1	A	1430	LEU
1	A	1452	GLU
1	A	1528	ILE
1	B	178	LEU
1	B	180	ASP
1	B	190	LEU
1	B	247	TRP
1	B	264	ARG
1	B	281	ILE
1	B	311	VAL
1	B	551	ASN
1	B	555	ASP
1	B	561	SER

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Mol	Chain	Res	Type
1	B	605	ASP
1	B	610	ILE
1	B	642	ARG
1	B	663	LEU
1	B	696	ASN
1	B	716	LEU
1	B	730	GLN
1	B	786	LEU
1	B	788	SER
1	B	789	GLU
1	B	831	ARG
1	B	867	VAL
1	B	904	PHE
1	B	965	ASN
1	B	1013	THR
1	B	1028	GLU
1	B	1083	PHE
1	B	1114	LEU
1	B	1121	GLN
1	B	1223	ILE
1	B	1229	ARG
1	B	1266	LEU
1	B	1320	ARG
1	B	1328	VAL
1	B	1329	ARG
1	B	1340	SER
1	B	1379	ARG
1	B	1391	ARG
1	B	1398	ASP
1	B	1481	VAL
1	B	1505	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS

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

There are no ligands in this entry.

5.7 Other polymers

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, 95^{th} 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	1044/1406 (74%)	0.72	98 (9%) 8 4	38, 84, 121, 139	0
1	B	1232/1406 (87%)	0.72	97 (7%) 12 8	34, 74, 134, 150	0
2	D	22/23 (95%)	0.55	0 100 100	44, 57, 92, 100	0
2	E	23/23 (100%)	0.77	1 (4%) 35 27	37, 54, 102, 144	0
3	C	22/23 (95%)	0.57	0 100 100	46, 53, 86, 91	0
3	F	22/23 (95%)	0.64	1 (4%) 33 25	39, 56, 89, 121	0
All	All	2365/2904 (81%)	0.72	197 (8%) 11 6	34, 76, 126, 150	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	SER	9.5
1	B	547	LEU	8.9
1	B	631	TYR	7.1
1	B	615	ILE	6.6
1	B	427	VAL	6.2
1	B	466	GLY	6.1
1	B	462	GLY	5.8
1	B	465	ASN	5.7
1	A	239	LEU	5.5
1	B	540	LYS	5.3
1	A	1030	ASP	5.2
1	A	236	SER	5.1
1	B	607	GLY	5.1
1	B	511	VAL	5.0
1	A	240	LEU	4.9
1	B	1031	ASN	4.7
1	B	425	TYR	4.6
1	A	318	ILE	4.6
1	A	1031	ASN	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	407	VAL	4.5
1	B	665	VAL	4.5
1	B	585	LYS	4.5
1	B	514	TYR	4.4
1	A	792	PHE	4.4
1	B	589	ASP	4.4
1	A	793	VAL	4.3
1	B	581	LEU	4.2
1	B	837	LYS	4.2
1	A	815	ALA	4.1
1	A	315	TYR	4.1
1	A	852	PHE	4.0
1	B	583	PRO	4.0
1	B	199	GLY	3.9
1	B	611	LEU	3.9
1	A	235	PRO	3.8
1	A	237	ILE	3.8
1	B	593	ALA	3.8
1	A	988	THR	3.8
1	B	655	LEU	3.8
1	B	813	GLY	3.7
1	A	845	ILE	3.7
1	B	236	SER	3.7
1	A	729	ARG	3.7
1	B	407	VAL	3.6
1	B	555	ASP	3.6
1	B	461	VAL	3.6
1	A	733	TRP	3.5
1	B	503	VAL	3.5
1	B	612	PRO	3.5
1	B	820	ASN	3.5
1	B	712	ASP	3.5
1	B	713	ARG	3.5
1	B	347	HIS	3.4
1	A	413	PHE	3.4
1	A	322	GLY	3.4
1	A	817	GLU	3.4
1	A	821	LEU	3.4
1	B	328	GLY	3.4
1	A	832	ALA	3.4
1	B	662	GLN	3.3
1	B	309	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	505	SER	3.3
1	B	571	ASP	3.3
1	B	785	ALA	3.3
1	A	204	ALA	3.3
1	B	711	GLY	3.2
1	B	1006	ARG	3.2
1	B	308	MET	3.2
1	A	1032	ASN	3.2
1	A	233	LEU	3.2
1	B	510	VAL	3.1
1	B	550	PRO	3.1
1	A	408	PHE	3.1
2	E	23	DA	3.1
1	B	200	GLN	3.1
1	B	337	SER	3.1
1	A	201	LEU	3.1
1	B	429	VAL	3.1
1	B	663	LEU	3.0
1	B	825	TYR	3.0
1	A	320	VAL	3.0
1	A	372	TYR	3.0
1	A	816	LYS	3.0
1	A	202	ILE	3.0
1	B	296	TRP	3.0
1	A	791	SER	3.0
1	A	900	ILE	3.0
1	A	243	THR	2.9
1	A	262	SER	2.9
1	B	424	ASP	2.9
1	A	726	ILE	2.9
1	B	659	LYS	2.9
1	B	814	PHE	2.8
1	A	316	GLN	2.8
1	A	355	ALA	2.8
1	A	1026	SER	2.8
1	A	841	LYS	2.8
1	B	394	LEU	2.8
1	A	823	PRO	2.7
1	B	392	SER	2.7
1	A	1223	ILE	2.7
1	B	460	ILE	2.7
1	A	200	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1293	ALA	2.7
1	A	354	SER	2.7
1	A	356	PHE	2.7
1	A	332	PHE	2.6
1	A	406	GLU	2.6
1	A	756	LEU	2.6
1	B	572	ILE	2.6
1	A	292	ILE	2.6
1	A	357	SER	2.6
1	B	372	TYR	2.6
1	B	786	LEU	2.6
1	A	199	GLY	2.6
1	B	815	ALA	2.6
1	A	897	ASP	2.6
1	A	898	VAL	2.6
1	A	1570	GLU	2.6
1	B	310	VAL	2.6
1	B	316	GLN	2.5
1	B	632	GLU	2.5
1	B	777	LEU	2.5
1	B	234	VAL	2.5
1	B	836	GLU	2.5
1	A	398	MET	2.5
1	A	828	VAL	2.5
1	A	311	VAL	2.5
1	B	723	VAL	2.5
1	B	719	TRP	2.5
1	A	336	ILE	2.4
1	B	260	VAL	2.4
1	A	778	ILE	2.4
1	B	835	ILE	2.4
1	B	202	ILE	2.4
1	B	709	LYS	2.4
1	B	548	ALA	2.4
1	B	528	MET	2.4
1	A	1282	ILE	2.4
1	A	359	VAL	2.4
1	B	313	SER	2.4
1	A	1054	THR	2.4
1	B	193	PHE	2.3
1	B	821	LEU	2.3
1	A	910	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	301	SER	2.3
1	B	396	SER	2.3
1	A	415	GLN	2.3
3	F	2	DT	2.3
1	B	205	PRO	2.3
1	A	371	MET	2.3
1	A	404	TYR	2.3
1	A	1374	ALA	2.3
1	B	257	SER	2.3
1	B	329	PHE	2.3
1	A	772	MET	2.3
1	B	636	GLN	2.3
1	A	368	LEU	2.2
1	A	739	SER	2.2
1	B	832	ALA	2.2
1	B	1120	THR	2.2
1	A	940	LEU	2.2
1	A	370	ARG	2.2
1	A	241	THR	2.2
1	A	853	PHE	2.2
1	A	730	GLN	2.2
1	B	198	ARG	2.2
1	A	313	SER	2.2
1	A	909	THR	2.2
1	B	633	THR	2.2
1	A	214	LEU	2.2
1	A	321	ILE	2.2
1	B	422	LEU	2.2
1	B	493	PHE	2.2
1	A	289	SER	2.2
1	B	880	SER	2.1
1	A	212	THR	2.1
1	A	1139	THR	2.1
1	B	239	LEU	2.1
1	A	776	HIS	2.1
1	A	901	LEU	2.1
1	A	814	PHE	2.1
1	A	972	VAL	2.1
1	B	365	VAL	2.1
1	A	795	GLN	2.1
1	B	410	ARG	2.1
1	A	309	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1004	LEU	2.1
1	A	287	THR	2.0
1	A	732	ASN	2.0
1	A	216	ILE	2.0
1	A	1013	THR	2.0
1	B	574	THR	2.0
1	A	749	PHE	2.0
1	A	964	ILE	2.0
1	B	393	ILE	2.0
1	B	406	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.