



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 07:57 PM EDT

PDB ID : 5FFJ / pdb_00005ffj
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 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:

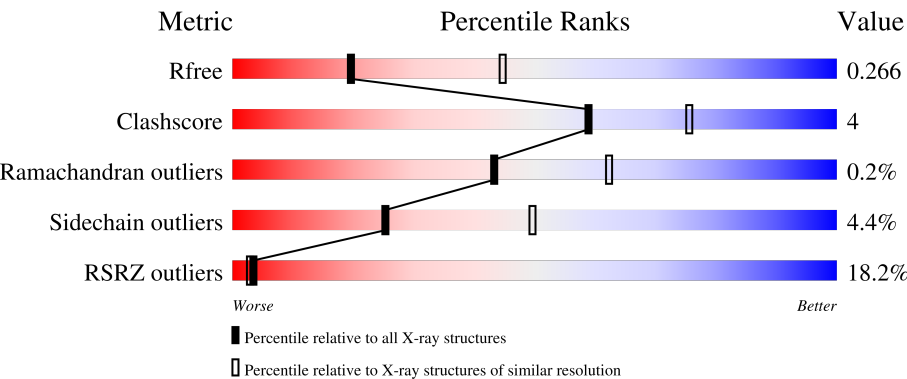
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance 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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (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 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	A	1406	13% 63% 11% • 26%
1	B	1406	17% 77% 10% • 12%
2	D	23	83% 13% •
2	E	23	4% 91% 9%
3	C	23	78% 17% •

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Mol	Chain	Length	Quality of chain
3	F	23	4% 91%

2 Entry composition [i](#)

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			

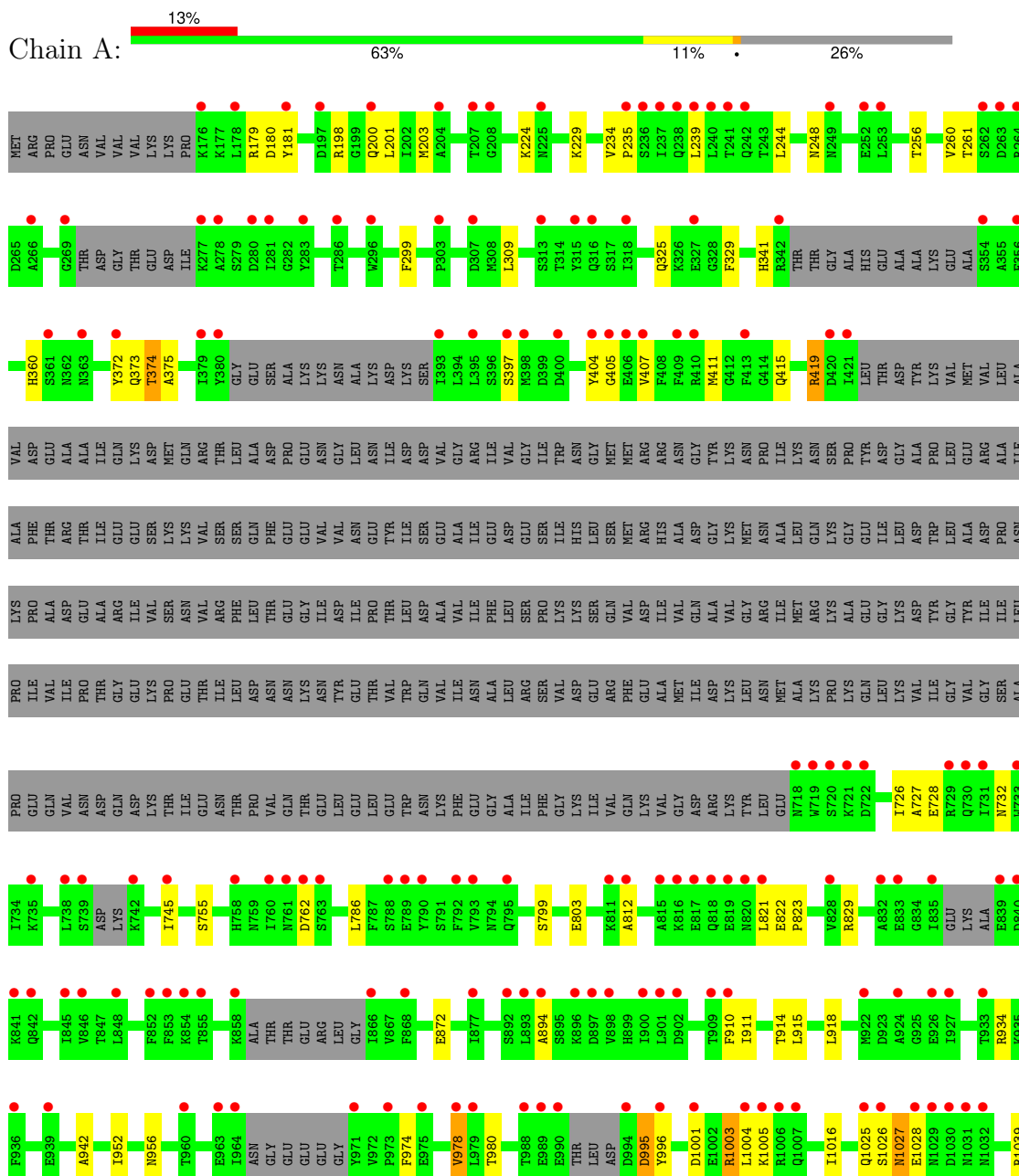
- Molecule 4 is water.

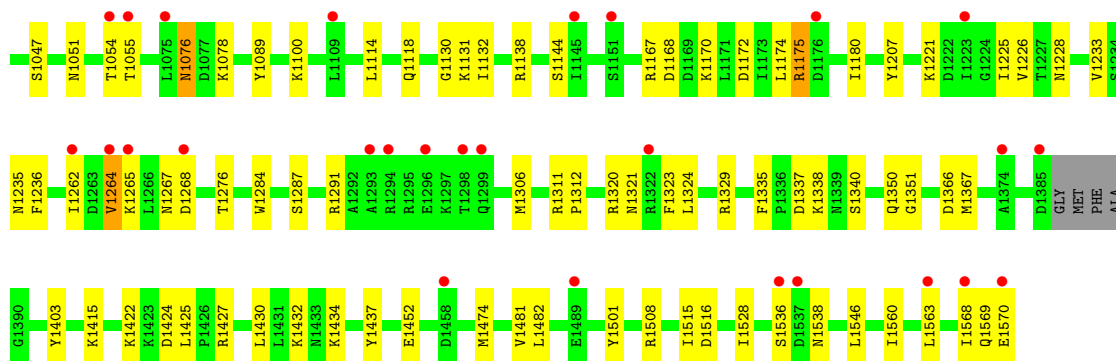
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	7	Total 7	O 7	0	0
4	B	1	Total 1	O 1	0	0

3 Residue-property plots

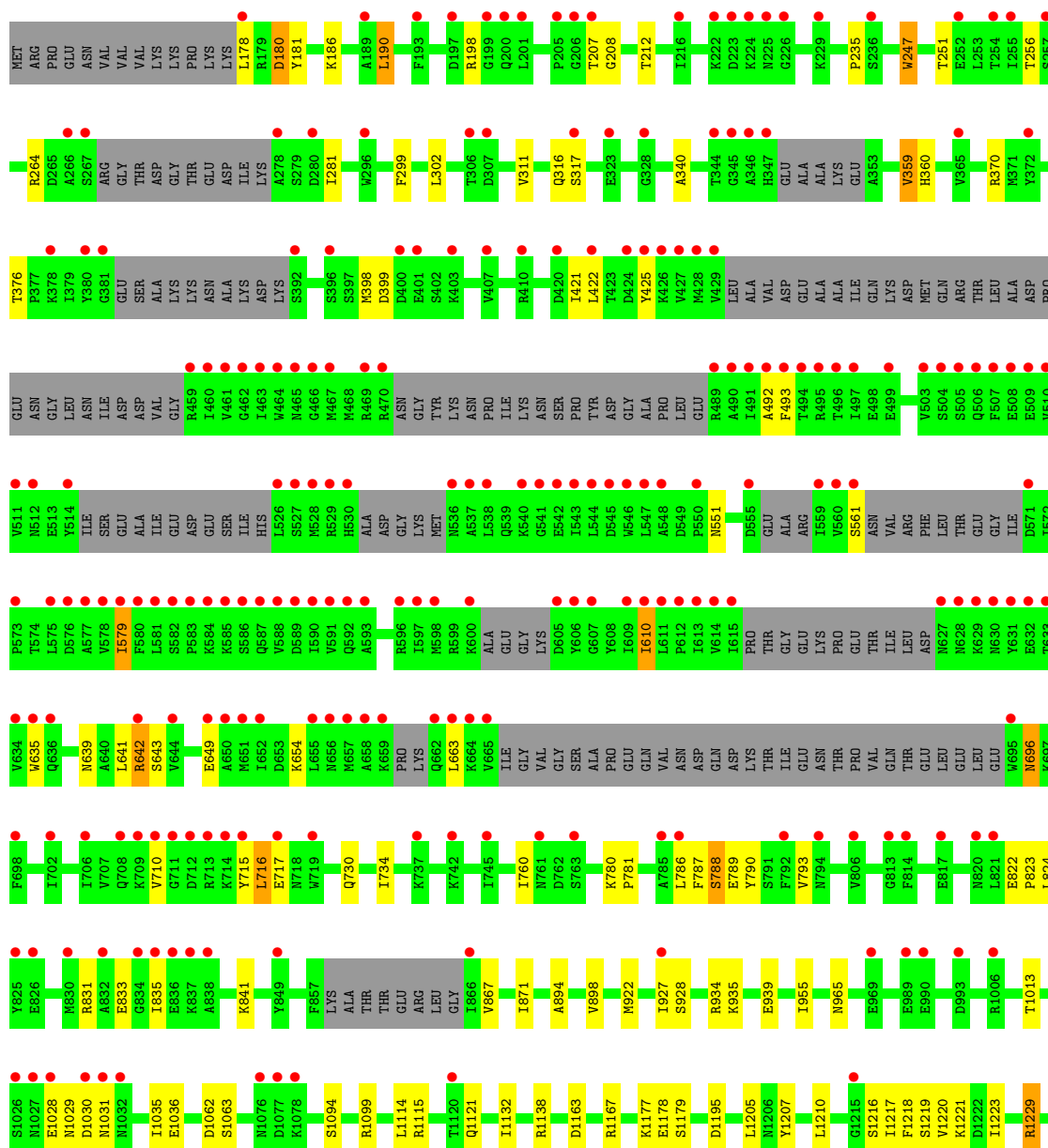
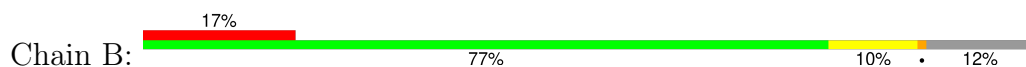
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

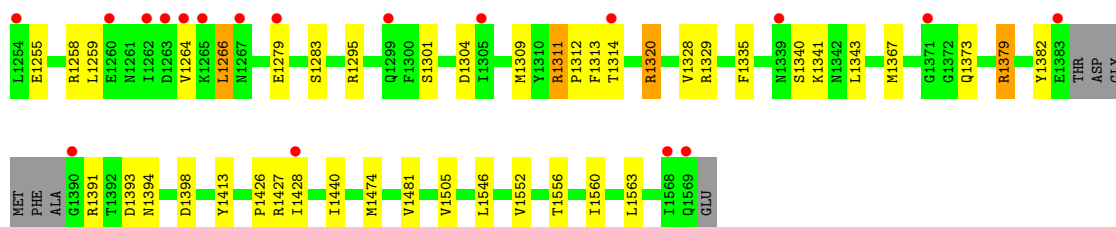
• Molecule 1: Endonuclease and methylase LlaGI





• Molecule 1: Endonuclease and methylase LlaGI





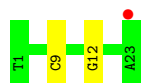
- Molecule 2: DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP*AP*GP*TP*CP*TP*A P*TP*TP*AP*GP*CP*T)-3')

Chain D: 83% 13% .



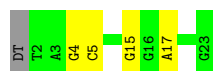
- Molecule 2: DNA (5'-D(P*TP*CP*CP*TP*CP*CP*AP*TP*CP*CP*AP*GP*TP*CP*TP*A P*TP*TP*AP*GP*CP*T)-3')

Chain E: 4% 91% 9%



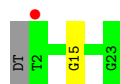
- Molecule 3: DNA (5'-D(P*TP*AP*GP*CP*TP*AP*AP*TP*AP*GP*AP*CP*TP*GP*GP*A P*TP*GP*GP*AP*GP*G)-3')

Chain C: 78% 17% .



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

Chain F: 4% 91% . .



4 Data and refinement statistics

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 50.00 – 2.84	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.84) 99.9 (50.00-2.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.229 , 0.262 0.237 , 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)	0.36 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	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.*

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](#)

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	0.32	0/8178	0.72	2/11106 (0.0%)
1	B	0.31	0/9548	0.69	3/12967 (0.0%)
2	D	0.28	0/486	0.50	0/746
2	E	0.28	0/510	0.49	0/783
3	C	0.25	0/519	0.48	0/801
3	F	0.26	0/515	0.47	0/796
All	All	0.31	0/19756	0.68	5/27199 (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
1	A	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1276	THR	N-CA-C	6.21	118.13	111.36
1	B	1311	ARG	CA-C-N	-5.85	113.91	119.76
1	B	1311	ARG	C-N-CA	-5.85	113.91	119.76
1	A	1027	ASN	N-CA-C	5.76	117.56	111.28
1	B	579	ILE	N-CA-C	5.56	116.31	108.36

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	81	0
1	B	9381	8659	8658	75	0
2	D	437	251	252	4	0
2	E	458	263	263	2	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	158	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 (158) 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:359:VAL:O	1:B:370:ARG:NH1	2.26	0.68
1:B:1132:ILE:O	1:B:1167: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:244:LEU:O	1:A:248:ASN:ND2	2.29	0.66
1:A:1132:ILE:O	1:A:1167:ARG:NH1	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1379:ARG:NH1	1:B:1398:ASP:OD1	2.37	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:180:ASP:OD1	1:A:181:TYR:N	2.38	0.57
1:A:1320:ARG:NH1	1:A:1335:PHE:O	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:A:1367:MET:HE1	2:D:8:DT:O4	2.10	0.52
1:B:894:ALA:CB	1:B:927:ILE:HD11	2.40	0.52
1:B:1264:VAL:O	1:B:1295:ARG:NH2	2.43	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
3:C:4:DG:OP1	1:B:317:SER:OG	2.26	0.51
1:A:1047:SER:O	1:A:1051:ASN:ND2	2.41	0.51
1:B:493:PHE:N	1:B:579:ILE:O	2.42	0.51
1:B:1311:ARG:HB3	1:B:1312:PRO:HD2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:635:TRP:O	1:B:639:ASN:ND2	2.41	0.50
1:A:728:GLU:O	1:A:732:ASN:ND2	2.42	0.50
1:A:1118:GLN:O	1:A:1138:ARG:NH1	2.43	0.50
1:A:201:LEU:HD11	1:A:203:MET:HE2	1.93	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:788:SER:C	1:B:790:TYR:H	2.20	0.49
1:B:399:ASP:OD1	1:B:399:ASP:N	2.44	0.49
1:B:376:THR:O	1:B:376:THR:OG1	2.30	0.49
1:A:1329:ARG:HH21	1:A:1367:MET:HE3	1.78	0.48
1:A:995:ASP:N	1:A:995:ASP:OD1	2.46	0.48
1:A:915:LEU:HD23	1:A:918:LEU:HD12	1.94	0.48
1:A:1311:ARG:HB3	1:A:1312:PRO:HD2	1.96	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:N	1:A:1001:ASP:OD1	2.46	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:B:642:ARG:NH1	1:B:649:GLU:OE2	2.47	0.48
1:B:696:ASN:N	1:B:696:ASN:OD1	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:B:340:ALA:HB3	1:B:398:MET:HE1	1.96	0.46
1:B:1094:SER:OG	2:E:9:DC:OP1	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:726:ILE:CD1	1:A:821:LEU:HD11	2.48	0.43
1:A:1367:MET:HE2	2:D:8:DT:H72	2.00	0.43
1:A:1482:LEU:HB3	1:A:1501:TYR:CE1	2.53	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
1:B:1309:MET:HE1	1:B:1313:PHE:H	1.84	0.43
1:B:1413:TYR:OH	1:B:1427:ARG:O	2.34	0.43
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
1:B:1301:SER:OG	1:B:1304:ASP:OD2	2.37	0.43
1:A:200:GLN:HB2	1:A:407:VAL:HG12	2.01	0.43
1:A:360:HIS:CE1	1:A:404:TYR:HE1	2.37	0.43
1:B:208:GLY:O	1:B:212:THR:HG23	2.18	0.43
1:B:1035:ILE:HG22	1:B:1036:GLU:H	1.84	0.43
1:B:1474:MET:HE3	1:B:1546:LEU:HD22	1.99	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:715:TYR:CE1	1:B:716:LEU:HD13	2.55	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: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:726:ILE:HG13	1:A:727:ALA:N	2.35	0.42
1:A:1168:ASP:OD1	1:A:1168:ASP:N	2.53	0.42
1:A:1560:ILE:O	1:A:1563:LEU:HD23	2.20	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:1001:ASP:O	1:A:1005:LYS:N	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:ARG:NH1	1:B:1283:SER:O	2.53	0.41
1:B:492:ALA:HA	1:B:579:ILE:CB	2.50	0.41
1:B:1219:SER:OG	1:B:1394:ASN:OD1	2.35	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:A:1474:MET:HE2	1:A:1515:ILE:HG12	2.03	0.41
1:B:822:GLU:N	1:B:823:PRO:CD	2.83	0.41
1:B:1216:SER:OG	1:B:1218:PHE:O	2.35	0.40
1:B:1367:MET:HG2	1:B:1373:GLN:HA	2.03	0.40
1:A:1051:ASN:OD1	1:A:1100:LYS:NZ	2.45	0.40
1:A:1432:LYS:HA	1:A:1570:GLU:HA	2.03	0.40
1:A:1536:SER:C	1:A:1538:ASN:H	2.29	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
1:A:1337:ASP:OD1	1:A:1340:SER:OG	2.37	0.40
1:B:181:TYR:OH	1:B:207:THR:OG1	2.33	0.40

There are no symmetry-related clashes.

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	
1	A	1022/1406 (73%)	966 (94%)	55 (5%)	1 (0%)	48	69
1	B	1200/1406 (85%)	1152 (96%)	44 (4%)	4 (0%)	36	55
All	All	2222/2812 (79%)	2118 (95%)	99 (4%)	5 (0%)	43	62

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1030	ASP
1	A	235	PRO

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	826/1256 (66%)	796 (96%)	30 (4%)	31	56
1	B	949/1256 (76%)	901 (95%)	48 (5%)	21	44
All	All	1775/2512 (71%)	1697 (96%)	78 (4%)	25	49

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	ARG
1	A	224	LYS
1	A	229	LYS
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	978	VAL
1	A	995	ASP
1	A	1003	ARG
1	A	1016	ILE
1	A	1039	ARG
1	A	1076	ASN
1	A	1114	LEU
1	A	1174	LEU
1	A	1175	ARG
1	A	1180	ILE

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Mol	Chain	Res	Type
1	A	1221	LYS
1	A	1226	VAL
1	A	1233	VAL
1	A	1264	VAL
1	A	1350	GLN
1	A	1415	LYS
1	A	1430	LEU
1	A	1452	GLU
1	A	1481	VAL
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	302	LEU
1	B	311	VAL
1	B	359	VAL
1	B	551	ASN
1	B	561	SER
1	B	610	ILE
1	B	642	ARG
1	B	663	LEU
1	B	696	ASN
1	B	716	LEU
1	B	717	GLU
1	B	730	GLN
1	B	734	ILE
1	B	786	LEU
1	B	788	SER
1	B	789	GLU
1	B	824	LEU
1	B	831	ARG
1	B	867	VAL
1	B	871	ILE
1	B	955	ILE
1	B	965	ASN
1	B	1013	THR
1	B	1028	GLU
1	B	1114	LEU
1	B	1121	GLN

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Mol	Chain	Res	Type
1	B	1178	GLU
1	B	1220	VAL
1	B	1221	LYS
1	B	1223	ILE
1	B	1229	ARG
1	B	1266	LEU
1	B	1279	GLU
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	1440	ILE
1	B	1481	VAL
1	B	1505	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	341	HIS
1	A	362	ASN
1	A	888	HIS
1	A	1157	HIS
1	A	1187	ASN
1	B	238	GLN
1	B	730	GLN
1	B	1093	GLN
1	B	1121	GLN
1	B	1187	ASN
1	B	1206	ASN
1	B	1246	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1044/1406 (74%)	1.06	184 (17%)  	40, 92, 130, 153	0
1	B	1232/1406 (87%)	1.05	245 (19%)  	38, 80, 144, 166	0
2	D	22/23 (95%)	0.24	0  	46, 61, 97, 106	0
2	E	23/23 (100%)	0.15	1 (4%)  	39, 58, 109, 150	0
3	C	22/23 (95%)	0.09	0  	48, 55, 91, 95	0
3	F	22/23 (95%)	0.06	1 (4%)  	40, 59, 95, 130	0
All	All	2365/2904 (81%)	1.02	431 (18%)  	38, 83, 135, 166	0

All (431) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1031	ASN	7.9
1	B	662	GLN	7.3
1	B	465	ASN	7.1
1	B	530	HIS	7.0
1	B	199	GLY	7.0
1	B	665	VAL	7.0
1	B	586	SER	6.7
1	A	1030	ASP	6.6
1	B	540	LYS	6.5
1	A	971	TYR	6.2
1	A	380	TYR	6.2
1	A	1026	SER	6.1
1	B	536	ASN	6.1
1	B	628	ASN	5.9
1	B	589	ASP	5.9
1	B	580	PHE	5.9
1	A	820	ASN	5.8
1	A	817	GLU	5.7
1	B	600	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	470	ARG	5.6
1	B	1264	VAL	5.6
1	A	840	ASP	5.5
1	B	583	PRO	5.3
1	B	547	LEU	5.3
1	B	656	ASN	5.3
1	B	429	VAL	5.3
1	B	655	LEU	5.3
1	B	588	VAL	5.1
1	A	421	ILE	5.1
1	B	632	GLU	5.0
1	B	969	GLU	5.0
1	A	1385	ASP	5.0
1	B	197	ASP	5.0
1	A	816	LYS	5.0
1	B	1265	LYS	4.9
1	B	427	VAL	4.9
1	B	593	ALA	4.8
1	B	631	TYR	4.8
1	B	462	GLY	4.8
1	A	939	GLU	4.7
1	B	493	PHE	4.7
1	B	581	LEU	4.7
1	A	280	ASP	4.6
1	B	1077	ASP	4.6
1	B	469	ARG	4.6
1	A	281	ILE	4.6
1	B	587	GLN	4.6
1	B	461	VAL	4.6
1	A	225	ASN	4.6
1	B	267	SER	4.5
1	A	893	LEU	4.5
1	B	510	VAL	4.5
1	B	651	MET	4.5
1	B	508	GLU	4.4
1	B	630	ASN	4.4
1	B	826	GLU	4.3
1	B	514	TYR	4.2
1	B	255	ILE	4.2
1	A	790	TYR	4.2
1	B	492	ALA	4.1
1	A	792	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	316	GLN	4.1
1	B	511	VAL	4.1
1	A	990	GLU	4.1
1	A	718	ASN	4.1
1	A	866	ILE	4.1
1	B	578	VAL	4.1
1	B	989	GLU	4.0
1	A	342	ARG	4.0
1	B	609	ILE	4.0
1	B	489	ARG	4.0
1	B	585	LYS	4.0
1	A	994	ASP	4.0
1	B	252	GLU	4.0
1	B	425	TYR	4.0
1	B	403	LYS	3.9
1	B	710	VAL	3.9
1	B	307	ASP	3.9
1	B	611	LEU	3.9
1	B	659	LYS	3.9
1	B	1299	GLN	3.9
1	B	990	GLU	3.9
1	B	546	TRP	3.9
1	B	1076	ASN	3.9
1	B	1006	ARG	3.9
1	B	993	ASP	3.8
1	A	975	GLU	3.8
1	B	571	ASP	3.8
1	A	788	SER	3.8
1	A	964	ILE	3.8
1	A	406	GLU	3.7
1	B	629	LYS	3.7
1	B	346	ALA	3.7
1	B	584	LYS	3.7
1	A	845	ILE	3.7
1	B	745	ILE	3.7
1	B	400	ASP	3.7
1	B	459	ARG	3.7
1	A	393	ILE	3.7
1	B	559	ILE	3.7
1	B	506	GLN	3.6
1	B	466	GLY	3.6
1	B	537	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
3	F	2	DT	3.6
1	B	627	ASN	3.6
1	A	815	ALA	3.6
1	B	396	SER	3.6
1	B	835	ILE	3.6
1	B	503	VAL	3.6
1	A	239	LEU	3.6
1	B	836	GLU	3.5
1	B	786	LEU	3.5
1	B	698	PHE	3.5
1	A	242	GLN	3.5
1	A	795	GLN	3.5
1	A	208	GLY	3.5
1	B	560	VAL	3.5
1	B	612	PRO	3.5
1	B	834	GLY	3.5
1	A	327	GLU	3.4
1	B	178	LEU	3.4
1	A	315	TYR	3.4
1	B	1305	ILE	3.4
1	A	839	GLU	3.4
1	A	236	SER	3.4
1	B	236	SER	3.4
1	B	464	TRP	3.4
1	A	237	ILE	3.4
1	A	407	VAL	3.3
1	A	1006	ARG	3.3
1	B	392	SER	3.3
1	B	548	ALA	3.3
1	A	269	GLY	3.3
1	B	576	ASP	3.3
1	B	550	PRO	3.3
1	B	837	LYS	3.3
1	B	561	SER	3.3
1	B	813	GLY	3.3
1	A	896	LYS	3.3
1	B	460	ILE	3.3
1	B	490	ALA	3.3
1	B	381	GLY	3.3
1	B	635	TRP	3.3
1	B	222	LYS	3.2
1	B	428	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	379	ILE	3.2
1	A	745	ILE	3.2
1	A	996	TYR	3.2
1	B	1383	GLU	3.2
1	A	761	ASN	3.2
1	B	543	ILE	3.2
1	A	742	LYS	3.2
1	B	345	GLY	3.2
1	A	739	SER	3.2
1	A	1536	SER	3.2
1	A	197	ASP	3.2
1	B	663	LEU	3.2
1	B	614	VAL	3.2
1	A	841	LYS	3.2
1	A	858	LYS	3.2
1	A	989	GLU	3.2
1	A	404	TYR	3.2
1	A	240	LEU	3.2
1	B	1028	GLU	3.2
1	A	722	ASP	3.1
1	B	280	ASP	3.1
1	A	363	ASN	3.1
1	A	398	MET	3.1
1	A	318	ILE	3.1
1	A	733	TRP	3.1
1	B	410	ARG	3.1
1	B	708	GLN	3.1
1	B	226	GLY	3.1
1	A	264	ARG	3.1
1	B	223	ASP	3.1
1	B	504	SER	3.1
1	B	1030	ASP	3.1
1	B	206	GLY	3.1
1	A	793	VAL	3.1
1	B	592	GLN	3.1
1	A	1570	GLU	3.1
1	B	714	LYS	3.1
1	B	507	PHE	3.0
1	B	495	ARG	3.0
1	B	529	ARG	3.0
1	A	249	ASN	3.0
1	A	842	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	819	GLU	3.0
1	B	785	ALA	3.0
1	B	615	ILE	3.0
1	B	597	ILE	3.0
1	B	526	LEU	3.0
1	A	307	ASP	3.0
1	A	763	SER	3.0
1	A	253	LEU	2.9
1	B	278	ALA	2.9
1	A	1563	LEU	2.9
1	B	607	GLY	2.9
1	B	512	ASN	2.9
1	B	542	GLU	2.9
1	A	1458	ASP	2.9
1	A	898	VAL	2.9
1	A	833	GLU	2.9
2	E	23	DA	2.9
1	A	1031	ASN	2.9
1	B	1027	ASN	2.9
1	B	596	ARG	2.9
1	A	241	THR	2.9
1	B	1428	ILE	2.9
1	B	719	TRP	2.8
1	A	252	GLU	2.8
1	B	737	LYS	2.8
1	B	825	TYR	2.8
1	B	407	VAL	2.8
1	B	193	PHE	2.8
1	A	892	SER	2.8
1	A	738	LEU	2.8
1	B	575	LEU	2.8
1	B	636	GLN	2.8
1	B	1078	LYS	2.8
1	A	1176	ASP	2.8
1	B	201	LEU	2.8
1	A	354	SER	2.8
1	B	1026	SER	2.8
1	B	380	TYR	2.8
1	A	413	PHE	2.8
1	A	868	PHE	2.8
1	B	266	ALA	2.8
1	B	1390	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	205	PRO	2.8
1	A	852	PHE	2.8
1	A	1025	GLN	2.7
1	A	729	ARG	2.7
1	A	926	GLU	2.7
1	B	817	GLU	2.7
1	B	499	GLU	2.7
1	A	901	LEU	2.7
1	A	1568	ILE	2.7
1	B	224	LYS	2.7
1	A	405	GLY	2.7
1	A	410	ARG	2.7
1	A	238	GLN	2.7
1	A	818	GLN	2.7
1	B	544	LEU	2.7
1	B	658	ALA	2.7
1	A	176	LYS	2.7
1	B	494	THR	2.7
1	A	902	ASP	2.7
1	A	1264	VAL	2.7
1	B	229	LYS	2.7
1	B	695	TRP	2.7
1	B	633	THR	2.7
1	B	1339	ASN	2.7
1	B	426	LYS	2.6
1	B	866	ILE	2.6
1	A	894	ALA	2.6
1	A	758	HIS	2.6
1	A	1054	THR	2.6
1	B	1032	ASN	2.6
1	A	835	ILE	2.6
1	A	1145	ILE	2.6
1	A	812	ALA	2.6
1	B	577	ALA	2.6
1	A	719	TRP	2.6
1	B	509	GLU	2.6
1	B	605	ASP	2.6
1	B	792	PHE	2.6
1	A	848	LEU	2.6
1	A	1489	GLU	2.6
1	A	420	ASP	2.6
1	A	361	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	634	VAL	2.6
1	B	1267	ASN	2.6
1	B	541	GLY	2.5
1	B	613	ILE	2.5
1	B	207	THR	2.5
1	B	832	ALA	2.5
1	B	820	ASN	2.5
1	A	897	ASP	2.5
1	A	735	LYS	2.5
1	B	505	SER	2.5
1	A	235	PRO	2.5
1	B	579	ILE	2.5
1	B	200	GLN	2.5
1	B	712	ASP	2.5
1	A	922	MET	2.5
1	B	652	ILE	2.5
1	B	323	GLU	2.5
1	A	1075	LEU	2.5
1	A	303	PRO	2.5
1	A	1223	ILE	2.5
1	B	590	ILE	2.5
1	B	702	ILE	2.5
1	A	283	TYR	2.5
1	A	356	PHE	2.5
1	A	988	THR	2.5
1	B	664	LYS	2.5
1	A	1268	ASP	2.4
1	A	927	ILE	2.4
1	A	1151	SER	2.4
1	A	1004	LEU	2.4
1	A	262	SER	2.4
1	A	1055	THR	2.4
1	B	657	MET	2.4
1	B	794	ASN	2.4
1	A	978	VAL	2.4
1	B	401	GLU	2.4
1	A	204	ALA	2.4
1	A	1293	ALA	2.4
1	B	528	MET	2.4
1	B	422	LEU	2.4
1	B	538	LEU	2.4
1	A	1294	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	555	ASP	2.4
1	B	642	ARG	2.4
1	B	317	SER	2.4
1	B	1569	GLN	2.4
1	B	254	THR	2.4
1	B	216	ILE	2.4
1	B	706	ILE	2.4
1	B	1262	ILE	2.4
1	B	365	VAL	2.3
1	B	838	ALA	2.3
1	A	909	THR	2.3
1	B	821	LEU	2.3
1	A	877	ILE	2.3
1	B	927	ILE	2.3
1	B	1215	GLY	2.3
1	A	1109	LEU	2.3
1	B	527	SER	2.3
1	B	582	SER	2.3
1	B	328	GLY	2.3
1	A	1029	ASN	2.3
1	B	761	ASN	2.3
1	B	378	LYS	2.3
1	B	763	SER	2.3
1	B	1568	ILE	2.3
1	A	286	THR	2.3
1	A	910	PHE	2.3
1	A	266	ALA	2.3
1	B	1260	GLU	2.3
1	A	760	ILE	2.3
1	A	296	TRP	2.3
1	A	181	TYR	2.3
1	B	372	TYR	2.3
1	B	606	TYR	2.3
1	B	715	TYR	2.3
1	B	467	MET	2.2
1	B	598	MET	2.2
1	A	1028	GLU	2.2
1	B	649	GLU	2.2
1	A	277	LYS	2.2
1	B	424	ASP	2.2
1	B	463	ILE	2.2
1	B	610	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	933	THR	2.2
1	A	397	SER	2.2
1	A	973	PRO	2.2
1	B	849	TYR	2.2
1	B	814	PHE	2.2
1	A	721	LYS	2.2
1	A	1032	ASN	2.2
1	A	1322	ARG	2.2
1	B	644	VAL	2.2
1	A	720	SER	2.2
1	B	711	GLY	2.2
1	A	178	LEU	2.2
1	A	789	GLU	2.2
1	A	924	ALA	2.2
1	A	979	LEU	2.2
1	B	225	ASN	2.2
1	A	1007	GLN	2.2
1	B	420	ASP	2.2
1	A	828	VAL	2.2
1	B	573	PRO	2.2
1	B	1120	THR	2.2
1	A	313	SER	2.2
1	A	409	PHE	2.2
1	A	821	LEU	2.2
1	A	1374	ALA	2.2
1	A	1001	ASP	2.2
1	B	806	VAL	2.2
1	B	830	MET	2.2
1	A	1265	LYS	2.2
1	B	650	ALA	2.2
1	A	731	ILE	2.1
1	A	730	GLN	2.1
1	A	1537	ASP	2.1
1	B	1263	ASP	2.1
1	B	306	THR	2.1
1	B	1371	GLY	2.1
1	A	853	PHE	2.1
1	B	296	TRP	2.1
1	A	372	TYR	2.1
1	A	1262	ILE	2.1
1	B	709	LYS	2.1
1	A	400	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	207	THR	2.1
1	B	1254	LEU	2.1
1	B	713	ARG	2.1
1	A	963	GLU	2.1
1	A	1296	GLU	2.1
1	B	257	SER	2.1
1	B	497	ILE	2.1
1	A	1299	GLN	2.1
1	A	854	LYS	2.1
1	A	263	ASP	2.1
1	A	395	LEU	2.1
1	A	855	THR	2.1
1	A	278	ALA	2.1
1	A	832	ALA	2.1
1	A	900	ILE	2.1
1	B	347	HIS	2.1
1	A	936	PHE	2.1
1	A	960	THR	2.1
1	B	496	THR	2.1
1	B	491	ILE	2.1
1	B	344	THR	2.0
1	B	1314	THR	2.0
1	A	811	LYS	2.0
1	B	742	LYS	2.0
1	A	200	GLN	2.0
1	A	846	VAL	2.0
1	B	591	VAL	2.0
1	A	1298	THR	2.0
1	B	189	ALA	2.0
1	A	762	ASP	2.0
1	B	545	ASP	2.0
1	A	1005	LYS	2.0
1	B	717	GLU	2.0
1	B	1279	GLU	2.0

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

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.