Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 06:04 PM EDT

PDB ID	:	4OO8
Title	:	Crystal structure of Streptococcus pyogenes Cas9 in complex with guide RNA and target DNA
Authors	:	Nishimasu, H.; Ishitani, R.; Nureki, O.
Deposited on	:	2014-01-31
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

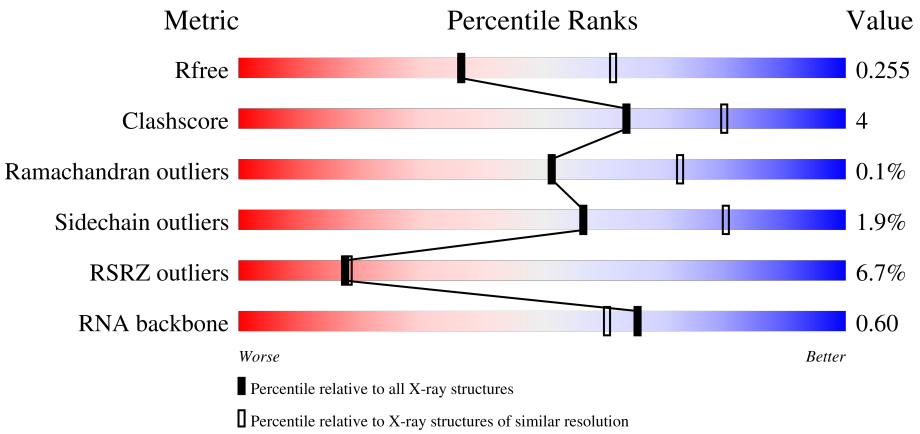
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

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 <=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	1372	8% 81% 13% • 5%
1	D	1372	5% 76% 8% 15%
2	B	98	2% 72% 24% • •
2	E	98	3% 66% 30% • •

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Mol	Chain	Length	Quality of chain
3	C	23	4% 57% 35% 9%
3	F	23	4% 65% 35%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 24153 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1301	9999	6388	1708	1883	20	0	0	0
1	D	1163	8998	5754	1529	1698	17	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	expression tag	UNP Q99ZW2
A	-2	SER	-	expression tag	UNP Q99ZW2
A	-1	GLY	-	expression tag	UNP Q99ZW2
A	0	HIS	-	expression tag	UNP Q99ZW2
A	10	ALA	ASP	engineered mutation	UNP Q99ZW2
A	80	LEU	CYS	engineered mutation	UNP Q99ZW2
A	574	GLU	CYS	engineered mutation	UNP Q99ZW2
A	840	ALA	HIS	engineered mutation	UNP Q99ZW2
D	-3	GLY	-	expression tag	UNP Q99ZW2
D	-2	SER	-	expression tag	UNP Q99ZW2
D	-1	GLY	-	expression tag	UNP Q99ZW2
D	0	HIS	-	expression tag	UNP Q99ZW2
D	10	ALA	ASP	engineered mutation	UNP Q99ZW2
D	80	LEU	CYS	engineered mutation	UNP Q99ZW2
D	574	GLU	CYS	engineered mutation	UNP Q99ZW2
D	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 2 is a RNA chain called RNA (97-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	97	2082	930	380	675	97	0	0	0
2	E	97	2082	930	380	675	97	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	21	404	192	72	120	20	0	0	1
3	F	23	444	211	80	131	22	0	0	1

- Molecule 4 is water.

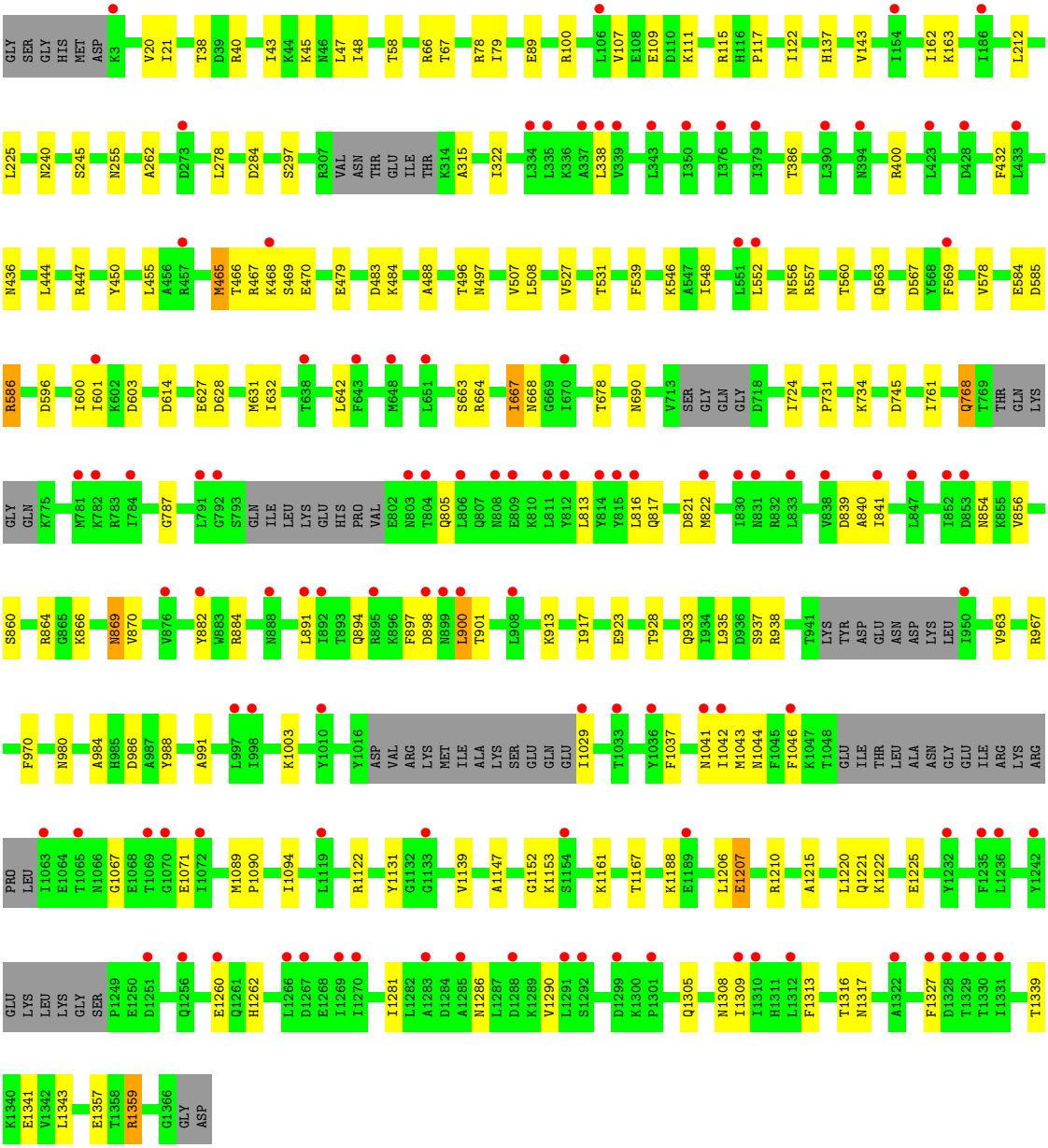
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	32	32	32	0	0
4	B	28	28	28	0	0
4	C	2	2	2	0	0
4	D	49	49	49	0	0
4	E	32	32	32	0	0
4	F	1	1	1	0	0

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.

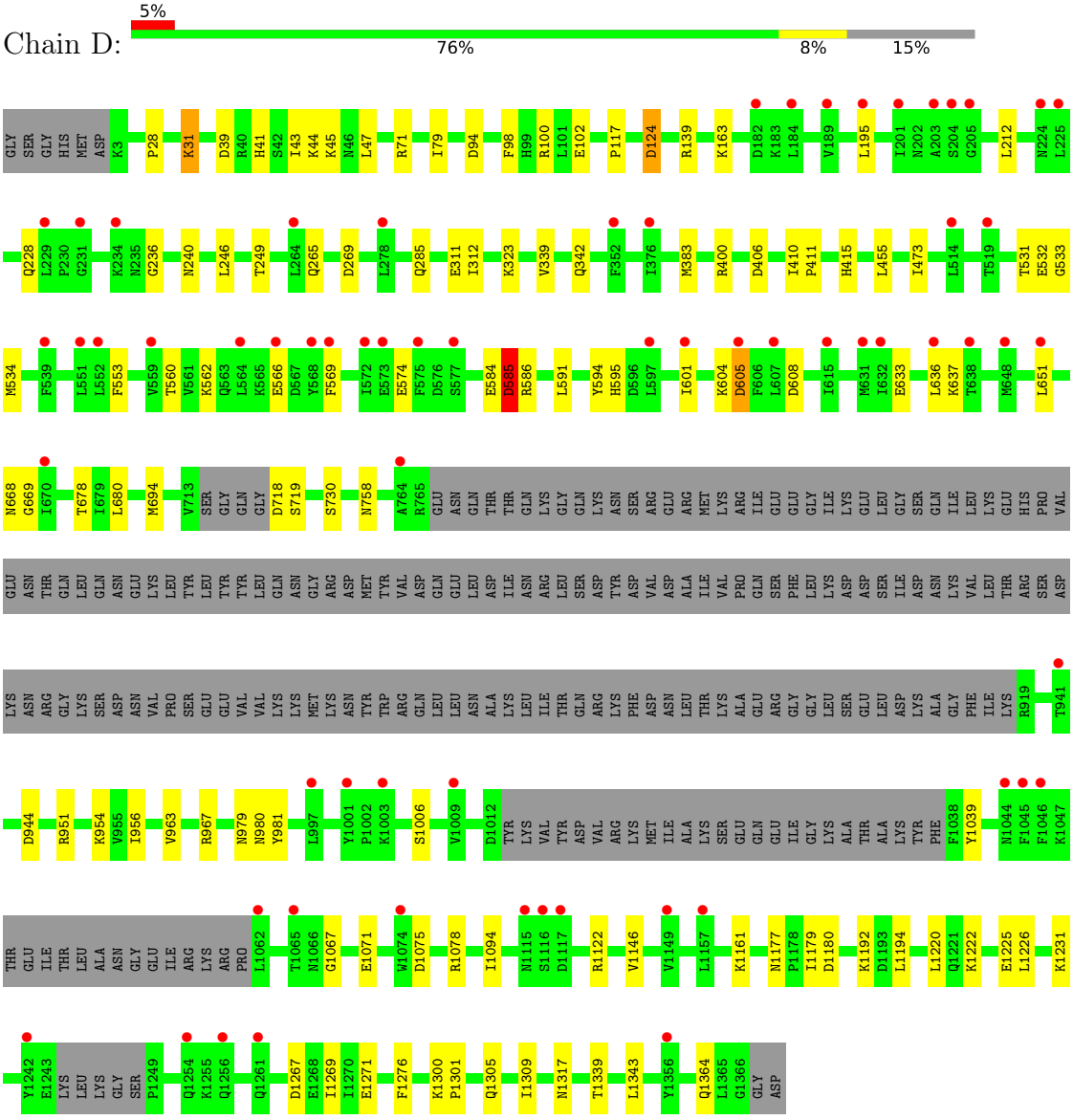
- Molecule 1: CRISPR-associated endonuclease Cas9/Csn1

Chain A:



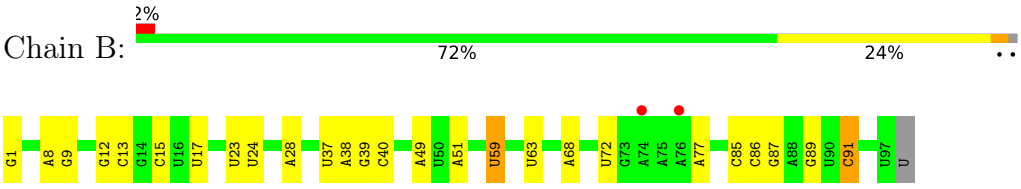
- Molecule 1: CRISPR-associated endonuclease Cas9/Csn1

Chain D:



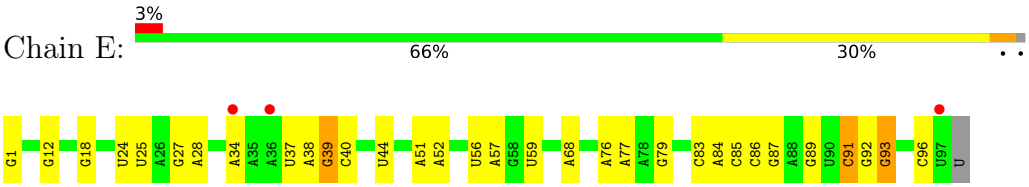
- Molecule 2: RNA (97-MER)

Chain B:



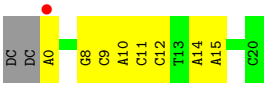
- Molecule 2: RNA (97-MER)

Chain E:



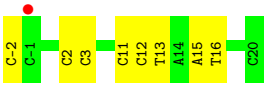
• Molecule 3: DNA (5'-D(*CP*CP*AP*GP*CP*CP*AP*AP*GP*CP*GP*CP*AP*CP*CP*TP*AP*AP*TP*TP*TP*CP*C)-3')

Chain C:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	76.71Å 105.69Å 126.82Å 97.68° 98.43° 100.31°	Depositor
Resolution (Å)	46.70 – 2.50 46.88 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (46.70-2.50) 98.6 (46.88-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.8.3_1479	Depositor
R, R_{free}	0.222 , 0.254 0.226 , 0.255	Depositor DCC
R_{free} test set	6523 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	59.8	Xtriage
Anisotropy	0.201	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 54.8	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	0.94	EDS
Total number of atoms	24153	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.33% 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 (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	0.22	0/10177	0.36	0/13792
1	D	0.22	0/9164	0.37	0/12424
2	B	0.29	1/2332 (0.0%)	0.70	0/3633
2	E	0.30	1/2332 (0.0%)	0.70	0/3633
3	C	0.70	1/451 (0.2%)	0.86	0/693
3	F	0.70	1/496 (0.2%)	0.91	0/762
All	All	0.27	4/24952 (0.0%)	0.48	0/34937

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	G	OP3-P	-10.58	1.48	1.61
3	F	-2	DC	O3'-P	-10.56	1.48	1.61
2	B	1	G	OP3-P	-10.56	1.48	1.61
3	C	0	DA	O3'-P	-10.52	1.48	1.61

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	9999	0	9573	96	1
1	D	8998	0	8657	71	1
2	B	2082	0	1043	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2082	0	1043	13	0
3	C	404	0	225	5	0
3	F	444	0	247	5	0
4	A	32	0	0	2	0
4	B	28	0	0	0	0
4	C	2	0	0	0	0
4	D	49	0	0	0	0
4	E	32	0	0	0	0
4	F	1	0	0	0	0
All	All	24153	0	20788	185	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 4.

All (185) 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:D:139:ARG:HH22	1:D:415:HIS:HD2	1.29	0.78
1:D:28:PRO:HG2	1:D:47:LEU:HD12	1.73	0.69
1:D:100:ARG:NH1	1:D:117:PRO:O	2.26	0.69
1:A:967:ARG:NH1	1:A:986:ASP:OD1	2.26	0.69
1:A:21:ILE:HD12	1:A:991:ALA:HB3	1.76	0.68
1:D:980:ASN:HB2	1:D:1094:ILE:HD13	1.76	0.67
1:D:1222:LYS:NZ	1:D:1317:ASN:O	2.26	0.66
1:D:31:LYS:HE2	2:E:84:A:H62	1.61	0.66
1:A:1042:ILE:HD12	1:A:1043:MET:HG2	1.79	0.65
1:A:1222:LYS:HD2	1:A:1281:ILE:HD12	1.79	0.63
1:D:1179:ILE:HD11	1:D:1192:LYS:HD2	1.80	0.63
1:D:311:GLU:HG2	1:D:312:ILE:HG23	1.80	0.63
1:A:400:ARG:NH1	4:A:1417:HOH:O	2.32	0.62
1:D:94:ASP:OD2	1:D:100:ARG:NH2	2.33	0.62
1:D:1067:GLY:N	1:D:1071:GLU:O	2.29	0.61
1:A:668:ASN:ND2	1:A:678:THR:OG1	2.33	0.61
1:A:1207:GLU:OE1	1:A:1210:ARG:NH2	2.31	0.60
1:A:745:ASP:OD2	1:A:938:ARG:NH2	2.33	0.60
1:D:553:PHE:HB3	1:D:591:LEU:HD13	1.85	0.59
2:E:38:A:H3'	2:E:39:G:H5"	1.83	0.59
1:A:560:THR:HG23	1:A:563:GLN:H	1.67	0.59
1:A:980:ASN:HB2	1:A:1094:ILE:HD13	1.84	0.57
1:A:66:ARG:NH1	4:A:1405:HOH:O	2.36	0.57
1:A:432:PHE:O	1:A:436:ASN:ND2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:236:GLY:O	1:D:240:ASN:ND2	2.35	0.57
1:D:730:SER:HB3	2:E:12:G:H4'	1.86	0.57
1:D:956:ILE:HG23	1:D:1006:SER:HB3	1.87	0.56
1:A:467:ARG:NH1	2:B:59:U:OP1	2.38	0.56
1:D:758:ASN:HD22	1:D:954:LYS:HB2	1.71	0.56
1:D:531:THR:HG22	1:D:534:MET:HG3	1.88	0.55
1:D:339:VAL:HG22	1:D:383:MET:HE1	1.88	0.55
1:A:584:GLU:O	1:A:586:ARG:N	2.40	0.54
1:D:718:ASP:OD1	1:D:719:SER:N	2.40	0.54
1:A:78:ARG:NH1	1:A:162:ILE:O	2.41	0.54
1:D:1300:LYS:HG3	1:D:1301:PRO:HD2	1.91	0.53
1:A:479:GLU:HG2	1:A:484:LYS:HE3	1.90	0.53
1:A:1122:ARG:NH2	2:B:49:A:N3	2.57	0.53
1:A:894:GLN:NE2	1:A:898:ASP:OD2	2.42	0.52
1:D:1300:LYS:O	1:D:1305:GLN:NE2	2.42	0.52
1:A:614:ASP:OD1	1:A:664:ARG:NH2	2.43	0.52
1:D:43:ILE:HD13	1:D:45:LYS:HE3	1.91	0.52
1:D:531:THR:OG1	1:D:532:GLU:OE1	2.27	0.52
1:D:124:ASP:OD2	1:D:124:ASP:N	2.42	0.51
1:D:71:ARG:NH1	2:E:18:G:N7	2.49	0.51
1:A:869:ASN:HD22	1:A:870:VAL:HG12	1.74	0.51
1:D:604:LYS:NZ	1:D:608:ASP:OD2	2.40	0.51
1:A:1222:LYS:HE2	1:A:1317:ASN:O	2.11	0.51
1:D:633:GLU:O	1:D:637:LYS:NZ	2.44	0.51
1:A:1067:GLY:N	1:A:1071:GLU:O	2.40	0.50
1:A:1041:ASN:HA	1:A:1044:ASN:HB2	1.94	0.50
1:D:249:THR:HG23	1:D:265:GLN:HB2	1.93	0.50
1:A:79:ILE:HD11	1:A:163:LYS:HB2	1.94	0.49
1:D:531:THR:HG23	1:D:533:GLY:H	1.76	0.49
1:D:569:PHE:O	1:D:574:GLU:N	2.44	0.49
3:C:8:DG:H2'	3:C:9:DC:C6	2.47	0.49
1:D:981:TYR:HD1	1:D:1094:ILE:HD11	1.77	0.49
1:A:89:GLU:HG3	1:A:432:PHE:CD1	2.48	0.49
1:D:585:ASP:OD2	1:D:585:ASP:N	2.45	0.49
3:C:9:DC:H2'	3:C:10:DA:C8	2.48	0.49
1:A:923:GLU:HG2	1:A:928:THR:HG21	1.94	0.48
1:A:1220:LEU:HG	1:A:1339:THR:HG22	1.96	0.48
1:A:531:THR:HG22	1:A:578:VAL:HG12	1.95	0.48
1:A:1207:GLU:O	1:A:1210:ARG:HG2	2.14	0.48
1:A:447:ARG:HG3	2:B:17:U:H5'	1.96	0.48
1:D:1146:VAL:HG21	1:D:1194:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD13	1:A:386:THR:HG22	1.96	0.47
1:A:821:ASP:OD1	1:A:822:MET:N	2.47	0.47
1:D:212:LEU:HD22	1:D:246:LEU:HD21	1.96	0.47
1:A:240:ASN:ND2	1:A:255:ASN:OD1	2.46	0.47
1:D:400:ARG:NH2	1:D:406:ASP:OD2	2.47	0.47
2:E:24:U:H2'	2:E:25:U:C6	2.50	0.47
2:E:86:C:H2'	2:E:87:G:O4'	2.15	0.47
1:A:21:ILE:HD11	1:A:988:TYR:CD1	2.50	0.47
2:E:27:G:N2	2:E:44:U:OP2	2.48	0.47
2:E:92:G:O2'	2:E:93:G:H8	1.98	0.47
1:D:44:LYS:HD2	2:E:92:G:N7	2.30	0.46
1:A:497:ASN:HD21	3:C:11:DC:P	2.37	0.46
1:A:1308:ASN:ND2	1:A:1327:PHE:H	2.13	0.46
1:A:560:THR:HA	1:A:586:ARG:HA	1.96	0.46
1:A:897:PHE:O	1:A:901:THR:HG22	2.15	0.46
1:D:694:MET:HA	1:D:694:MET:HE2	1.98	0.46
1:A:839:ASP:OD2	1:A:840:ALA:N	2.48	0.46
1:D:39:ASP:O	1:D:41:HIS:ND1	2.36	0.46
1:A:864:ARG:NH2	1:A:866:LYS:O	2.49	0.46
1:A:933:GLN:NE2	1:A:937:SER:OG	2.48	0.46
2:E:85:C:H2'	2:E:86:C:C6	2.51	0.46
1:A:100:ARG:HB3	1:A:117:PRO:HA	1.97	0.45
1:A:450:TYR:OH	1:A:627:GLU:OE2	2.26	0.45
1:A:468:LYS:HG3	1:A:483:ASP:HB2	1.98	0.45
1:D:560:THR:HG22	1:D:562:LYS:H	1.80	0.45
1:A:245:SER:HA	1:A:297:SER:HB3	1.98	0.45
1:A:854:ASN:O	1:A:854:ASN:ND2	2.48	0.45
1:D:269:ASP:OD1	1:D:269:ASP:N	2.49	0.45
1:A:768:GLN:H	1:A:768:GLN:HG3	1.56	0.45
1:D:1146:VAL:HG22	1:D:1161:LYS:HG3	1.99	0.45
1:D:1161:LYS:HE3	1:D:1343:LEU:HB3	1.99	0.45
1:A:488:ALA:HB3	1:A:631:MET:HE1	1.99	0.45
3:C:11:DC:H2'	3:C:12:DC:C6	2.52	0.45
1:D:668:ASN:ND2	1:D:678:THR:OG1	2.50	0.45
1:A:817:GLN:O	1:A:882:TYR:OH	2.34	0.45
1:A:45:LYS:NZ	1:A:1357:GLU:OE2	2.48	0.44
1:A:663:SER:O	1:A:667:ILE:HG22	2.17	0.44
1:A:1139:VAL:HA	1:A:1167:THR:HA	1.99	0.44
1:D:1220:LEU:HG	1:D:1339:THR:HG22	1.99	0.44
1:D:1305:GLN:O	1:D:1309:ILE:HG12	2.17	0.44
1:A:841:ILE:HD11	1:A:856:VAL:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:12:DC:H2'	3:F:13:DT:C6	2.53	0.44
1:D:139:ARG:HH22	1:D:415:HIS:CD2	2.20	0.44
1:D:951:ARG:HD3	1:D:951:ARG:HA	1.84	0.44
1:D:1177:ASN:HB3	1:D:1180:ASP:HB3	2.00	0.44
1:A:628:ASP:O	1:A:632:ILE:HG12	2.17	0.44
1:D:605:ASP:N	1:D:605:ASP:OD1	2.50	0.44
1:A:38:THR:HG23	1:A:40:ARG:H	1.83	0.44
1:A:107:VAL:HG23	1:A:1131:TYR:CZ	2.52	0.44
1:A:1161:LYS:HD2	1:A:1343:LEU:HB3	1.99	0.44
1:A:465:MET:HG2	1:A:466:THR:N	2.33	0.44
3:C:14:DA:H2"	3:C:15:DA:C8	2.53	0.44
1:D:1269:ILE:HD12	1:D:1309:ILE:HG21	2.00	0.43
1:D:584:GLU:O	1:D:586:ARG:N	2.51	0.43
1:D:1075:ASP:OD1	1:D:1078:ARG:N	2.52	0.43
1:A:970:PHE:HZ	1:A:1046:PHE:HB3	1.83	0.43
1:D:591:LEU:HB3	1:D:594:TYR:HB3	2.00	0.43
1:D:979:ASN:HB2	1:D:1225:GLU:HG3	2.00	0.43
1:A:48:ILE:HG12	1:A:984:ALA:HB1	2.01	0.43
1:A:508:LEU:HD21	1:A:664:ARG:HB2	2.00	0.43
1:A:539:PHE:HB3	1:A:690:ASN:ND2	2.33	0.43
1:A:557:ARG:NH2	1:A:596:ASP:OD1	2.28	0.43
1:A:601:ILE:HG13	1:A:603:ASP:H	1.84	0.43
1:A:43:ILE:HD11	2:B:91:C:H5'	2.01	0.43
1:A:813:LEU:HD23	1:A:816:LEU:HD12	2.00	0.43
1:D:981:TYR:CD1	1:D:1094:ILE:HD11	2.54	0.43
1:A:724:ILE:O	1:A:734:LYS:HE3	2.19	0.43
1:A:841:ILE:HG12	1:A:900:LEU:HD22	2.01	0.43
1:A:913:LYS:O	1:A:917:ILE:HG12	2.19	0.43
1:A:787:GLY:HA3	1:A:891:LEU:HD21	2.00	0.42
1:D:963:VAL:O	1:D:967:ARG:HG3	2.19	0.42
1:A:761:ILE:HD11	1:A:935:LEU:HD12	2.00	0.42
1:D:43:ILE:HD11	2:E:91:C:H5'	2.00	0.42
3:F:2:DC:H2'	3:F:3:DC:C6	2.54	0.42
1:A:66:ARG:NH2	2:B:15:C:OP2	2.52	0.42
1:D:98:PHE:O	1:D:102:GLU:HG2	2.20	0.42
1:A:1357:GLU:OE1	1:A:1359:ARG:NH1	2.46	0.42
1:D:31:LYS:HD3	2:E:83:C:N4	2.34	0.42
1:A:137:HIS:HA	1:A:322:ILE:HD11	2.01	0.42
1:A:143:VAL:HG11	1:A:315:ALA:HB2	2.01	0.42
1:D:455:LEU:HB3	1:D:473:ILE:HD12	2.01	0.42
1:A:58:THR:HA	1:A:731:PRO:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD21	1:A:225:LEU:HD13	2.01	0.42
1:A:469:SER:OG	1:A:470:GLU:N	2.53	0.42
1:A:596:ASP:O	1:A:600:ILE:HG12	2.19	0.42
1:D:79:ILE:HD11	1:D:163:LYS:HB2	2.01	0.42
1:D:1226:LEU:HD13	1:D:1276:PHE:CG	2.55	0.42
1:A:548:ILE:HG23	1:A:552:LEU:HD12	2.02	0.42
3:F:2:DC:H2'	3:F:3:DC:H6	1.84	0.42
1:A:1089:MET:HA	1:A:1090:PRO:HD3	1.94	0.42
1:A:1152:GLY:HA2	1:A:1153:LYS:HA	1.81	0.41
1:A:262:ALA:HB1	1:A:278:LEU:HD13	2.01	0.41
2:B:12:G:H2'	2:B:13:C:C6	2.55	0.41
1:D:668:ASN:HA	1:D:669:GLY:HA3	1.87	0.41
1:D:1122:ARG:O	2:E:52:A:H5"	2.20	0.41
1:A:162:ILE:HD13	1:A:444:LEU:HD12	2.02	0.41
1:A:1147:ALA:HB1	1:A:1188:LYS:O	2.21	0.41
1:A:1206:LEU:HD21	1:A:1341:GLU:HB3	2.01	0.41
1:D:342:GLN:HE22	1:D:383:MET:HA	1.85	0.41
3:F:15:DA:H2'	3:F:16:DT:C6	2.54	0.41
1:A:1215:ALA:HB2	1:A:1221:GLN:HG3	2.03	0.41
1:D:410:ILE:HA	1:D:411:PRO:HD3	1.87	0.41
1:A:111:LYS:HD2	1:A:115:ARG:HA	2.03	0.41
1:D:195:LEU:HD21	1:D:285:GLN:O	2.20	0.41
3:F:11:DC:H2'	3:F:12:DC:H6	1.85	0.41
1:A:963:VAL:O	1:A:967:ARG:HG3	2.21	0.41
1:A:1286:ASN:O	1:A:1290:VAL:HG23	2.21	0.41
1:D:636:LEU:HD21	1:D:651:LEU:HD23	2.03	0.41
1:D:1231:LYS:H	1:D:1231:LYS:HG3	1.66	0.41
1:A:20:VAL:HB	1:A:47:LEU:HB3	2.03	0.41
1:A:1094:ILE:HD12	1:A:1225:GLU:HG3	2.03	0.41
1:A:1305:GLN:O	1:A:1309:ILE:HG12	2.21	0.41
1:D:668:ASN:HD22	1:D:680:LEU:HB3	1.86	0.41
1:A:805:GLN:HE21	1:A:805:GLN:HB2	1.71	0.40
1:D:1267:ASP:O	1:D:1271:GLU:HG2	2.21	0.40
1:A:109:GLU:OE2	1:A:109:GLU:N	2.52	0.40
1:A:1313:PHE:HA	1:A:1316:THR:HG22	2.03	0.40
2:B:23:U:H2'	2:B:24:U:C6	2.56	0.40
2:B:85:C:H2'	2:B:86:C:C6	2.57	0.40
1:D:1364:GLN:N	1:D:1364:GLN:OE1	2.54	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)
1:A:860:SER:OG	1:D:944:ASP:O[1_454]	2.16	0.04

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	1283/1372 (94%)	1252 (98%)	30 (2%)	1 (0%)	51	73
1	D	1151/1372 (84%)	1108 (96%)	42 (4%)	1 (0%)	51	73
All	All	2434/2744 (89%)	2360 (97%)	72 (3%)	2 (0%)	51	73

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	585	ASP
1	A	585	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1013/1227 (83%)	987 (97%)	26 (3%)	46	72
1	D	921/1227 (75%)	911 (99%)	10 (1%)	73	89
All	All	1934/2454 (79%)	1898 (98%)	36 (2%)	57	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	THR
1	A	122	ILE
1	A	284	ASP
1	A	455	LEU
1	A	465	MET
1	A	496	THR
1	A	507	VAL
1	A	527	VAL
1	A	546	LYS
1	A	556	ASN
1	A	567	ASP
1	A	569	PHE
1	A	586	ARG
1	A	642	LEU
1	A	667	ILE
1	A	768	GLN
1	A	869	ASN
1	A	884	ARG
1	A	900	LEU
1	A	1003	LYS
1	A	1029	ILE
1	A	1037	PHE
1	A	1207	GLU
1	A	1260	GLU
1	A	1262	HIS
1	A	1359	ARG
1	D	31	LYS
1	D	124	ASP
1	D	228	GLN
1	D	323	LYS
1	D	566	GLU
1	D	585	ASP
1	D	595	HIS
1	D	601	ILE
1	D	605	ASP
1	D	1039	TYR

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

Mol	Chain	Res	Type
1	A	194	GLN
1	A	281	GLN
1	A	285	GLN

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Mol	Chain	Res	Type
1	A	497	ASN
1	A	556	ASN
1	A	668	ASN
1	A	726	ASN
1	A	758	ASN
1	A	805	GLN
1	A	869	ASN
1	A	899	ASN
1	A	933	GLN
1	A	1234	ASN
1	A	1308	ASN
1	D	354	GLN
1	D	415	HIS
1	D	426	GLN
1	D	668	ASN
1	D	758	ASN
1	D	985	HIS
1	D	1254	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	96/98 (97%)	15 (15%)	1 (1%)
2	E	96/98 (97%)	17 (17%)	0
All	All	192/196 (97%)	32 (16%)	1 (0%)

All (32) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	8	A
2	B	9	G
2	B	28	A
2	B	37	U
2	B	39	G
2	B	40	C
2	B	51	A
2	B	59	U
2	B	63	U
2	B	68	A
2	B	72	U
2	B	77	A

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Mol	Chain	Res	Type
2	B	87	G
2	B	89	G
2	B	91	C
2	E	28	A
2	E	34	A
2	E	37	U
2	E	39	G
2	E	40	C
2	E	51	A
2	E	56	U
2	E	57	A
2	E	59	U
2	E	68	A
2	E	76	A
2	E	77	A
2	E	79	G
2	E	89	G
2	E	91	C
2	E	93	G
2	E	96	C

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	38	A

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1301/1372 (94%)	0.62	110 (8%)	10	10	36, 82, 120, 160	0
1	D	1163/1372 (84%)	0.50	65 (5%)	24	25	40, 75, 117, 166	0
2	B	97/98 (98%)	0.20	2 (2%)	63	66	40, 75, 146, 168	0
2	E	97/98 (98%)	0.15	3 (3%)	49	52	44, 77, 172, 189	0
3	C	21/23 (91%)	0.36	1 (4%)	30	32	49, 65, 102, 108	0
3	F	23/23 (100%)	0.40	1 (4%)	35	38	53, 64, 131, 152	0
All	All	2702/2986 (90%)	0.54	182 (6%)	17	18	36, 78, 121, 189	0

All (182) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1330	THR	6.4
1	A	643	PHE	5.6
1	A	1312	LEU	5.3
1	D	1116	SER	5.2
1	D	552	LEU	5.2
1	D	1256	GLN	5.1
1	A	806	LEU	5.1
1	D	564	LEU	4.7
1	A	1309	ILE	4.7
1	D	607	LEU	4.6
1	A	852	ILE	4.6
1	D	231	GLY	4.5
1	D	648	MET	4.4
1	A	1292	SER	4.4
1	A	390	LEU	4.2
1	A	1251	ASP	4.2
1	A	833	LEU	4.2
1	A	1046	PHE	4.2
1	A	1063	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	335	LEU	4.1
1	A	1331	ILE	4.0
1	D	1045	PHE	4.0
1	A	1310	ILE	3.9
1	A	812	TYR	3.9
1	D	597	LEU	3.9
1	A	895	ARG	3.9
1	A	1267	ASP	3.7
1	D	568	TYR	3.7
1	A	1266	LEU	3.7
1	D	651	LEU	3.7
1	A	1042	ILE	3.6
1	D	575	PHE	3.6
1	D	1242	TYR	3.5
1	D	569	PHE	3.5
1	A	811	LEU	3.5
1	A	1041	ASN	3.5
1	A	888	ASN	3.4
1	A	1256	GLN	3.4
1	D	1062	LEU	3.3
1	A	1328	ASP	3.3
1	D	203	ALA	3.3
1	D	577	SER	3.3
1	A	1242	TYR	3.3
1	A	569	PHE	3.3
1	D	225	LEU	3.3
1	D	573	GLU	3.3
1	D	1157	LEU	3.2
1	A	841	ILE	3.2
1	D	204	SER	3.2
1	A	784	ILE	3.2
1	A	552	LEU	3.2
1	A	1291	LEU	3.2
1	A	891	LEU	3.2
1	D	229	LEU	3.2
1	A	900	LEU	3.1
1	A	1329	THR	3.1
1	D	615	ILE	3.1
1	A	853	ASP	3.1
1	A	1270	ILE	3.1
1	A	1189	GLU	3.1
1	A	791	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	1301	PRO	3.0
1	D	189	VAL	2.9
1	A	950	ILE	2.9
1	D	1046	PHE	2.9
1	A	433	LEU	2.9
1	D	601	ILE	2.9
1	A	1327	PHE	2.9
2	E	36	A	2.9
1	A	815	TYR	2.9
1	D	352	PHE	2.8
1	A	186	ILE	2.8
1	A	781	MET	2.8
1	A	808	ASN	2.8
1	A	334	LEU	2.7
1	A	1154	SER	2.7
2	B	74	A	2.7
1	D	559	VAL	2.7
1	A	804	THR	2.7
1	A	814	TYR	2.7
1	A	816	LEU	2.7
1	A	1260	GLU	2.7
1	A	106	LEU	2.7
1	A	1285	ALA	2.6
1	A	338	LEU	2.6
1	A	899	ASN	2.6
1	D	1115	ASN	2.6
1	A	1070	GLY	2.6
1	A	1299	ASP	2.6
1	A	1236	LEU	2.6
1	A	830	ILE	2.6
1	A	882	TYR	2.6
1	A	1010	TYR	2.6
1	A	339	VAL	2.6
1	D	205	GLY	2.6
1	A	1322	ALA	2.5
1	A	1072	ILE	2.5
3	C	0	DA	2.5
1	A	1033	THR	2.5
3	F	-1	DC	2.5
1	A	782	LYS	2.5
1	A	350	ILE	2.5
1	A	468	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	1036	TYR	2.5
1	A	1029	ILE	2.5
1	D	519	THR	2.5
1	A	847	LEU	2.5
1	A	876	VAL	2.4
1	D	941	THR	2.4
1	A	892	ILE	2.4
1	D	670	ILE	2.4
1	D	1074	TRP	2.4
1	A	638	THR	2.4
1	A	838	VAL	2.4
1	A	379	ILE	2.4
1	D	539	PHE	2.4
1	A	651	LEU	2.4
1	A	154	ILE	2.3
1	D	182	ASP	2.3
1	A	1232	TYR	2.3
1	D	184	LEU	2.3
1	D	1009	VAL	2.3
1	A	376	ILE	2.3
1	D	201	ILE	2.3
1	A	792	GLY	2.3
1	D	264	LEU	2.3
1	D	514	LEU	2.3
2	E	97	U	2.3
1	D	572	ILE	2.3
1	D	224	ASN	2.3
1	A	1069	THR	2.3
1	D	1065	THR	2.3
2	E	34	A	2.3
1	A	343	LEU	2.3
1	D	551	LEU	2.3
1	D	1117	ASP	2.3
1	A	670	ILE	2.3
1	A	337	ALA	2.3
1	D	1254	GLN	2.3
1	A	831	ASN	2.3
1	A	1269	ILE	2.3
1	D	376	ILE	2.3
1	A	273	ASP	2.3
1	A	1283	ALA	2.3
2	B	76	A	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	764	ALA	2.2
1	D	195	LEU	2.2
1	D	631	MET	2.2
1	D	632	ILE	2.2
1	A	803	ASN	2.2
1	A	898	ASP	2.2
1	D	605	ASP	2.2
1	A	3	LYS	2.2
1	A	428	ASP	2.2
1	A	1235	PHE	2.2
1	A	997	LEU	2.2
1	A	998	ILE	2.2
1	A	423	LEU	2.2
1	A	648	MET	2.1
1	A	551	LEU	2.1
1	A	394	ASN	2.1
1	A	809	GLU	2.1
1	A	1065	THR	2.1
1	A	908	LEU	2.1
1	D	636	LEU	2.1
1	D	1149	VAL	2.1
1	A	601	ILE	2.1
1	D	278	LEU	2.1
1	D	638	THR	2.1
1	A	1119	LEU	2.1
1	A	457	ARG	2.1
1	D	1356	TYR	2.0
1	D	1003	LYS	2.0
1	D	1044	ASN	2.0
1	A	1133	GLY	2.0
1	D	997	LEU	2.0
1	A	1288	ASP	2.0
1	A	822	MET	2.0
1	D	1001	TYR	2.0
1	D	566	GLU	2.0
1	D	234	LYS	2.0
1	D	1261	GLN	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 monosaccharides 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.