Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 10:31 AM EDT

PDB ID	:	4NGF
Title	:	Structure of human Dicer Platform-PAZ-Connector Helix cassette in complex with 17-mer siRNA having 5'-p and UU-3' ends (3.1 Angstrom resolution)
Authors	:	Simanshu, D.K.; Tian, Y.; Patel, D.J.
Deposited on	:	2013-11-01
Resolution	:	3.10 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:

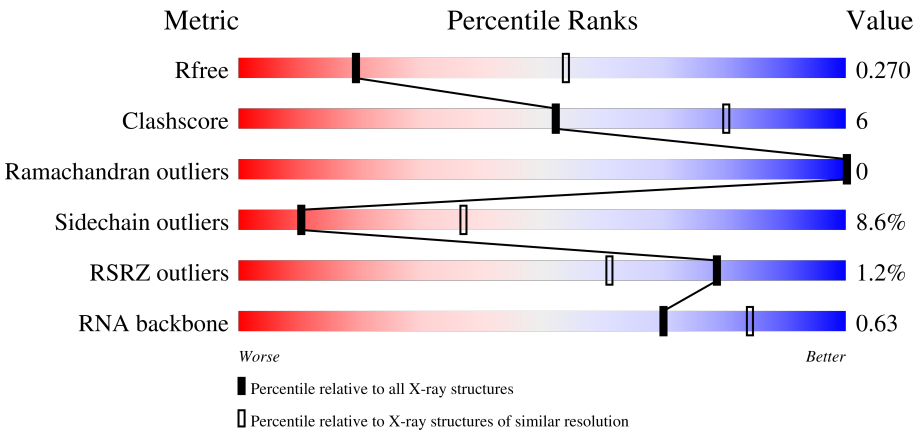
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)
RNA backbone	3102	1116 (3.40-2.80)

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	302	2% 71% 13% • 14%
1	B	302	% 72% 12% • 14%
1	C	302	% 62% 22% • 15%
1	D	302	% 69% 16% • 14%

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Mol	Chain	Length	Quality of chain
2	E	17	94% 6%
2	F	17	71% 29%
2	G	17	94% 6%
2	H	17	94% 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9701 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 Endoribonuclease Dicer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	260	2049	1343	330	367	9	0	0	0
1	B	259	2065	1345	336	375	9	0	0	0
1	C	258	2103	1374	348	372	9	0	0	0
1	D	260	2056	1344	339	365	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	754	SER	-	expression tag	UNP Q9UPY3
B	754	SER	-	expression tag	UNP Q9UPY3
C	754	SER	-	expression tag	UNP Q9UPY3
D	754	SER	-	expression tag	UNP Q9UPY3

- Molecule 2 is a RNA chain called 5'-R(P*UP*CP*GP*AP*AP*GP*GP*UP*CP*CP*UP*UP*CP*GP*UP*UP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	E	17	357	159	56	125	17	0	0	0
2	F	17	357	159	56	125	17	0	0	0
2	G	17	357	159	56	125	17	0	0	0
2	H	17	357	159	56	125	17	0	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: Endoribonuclease Dicer

Chain A: 2% 71% 13% • 14%

SER ASP Q756 L760 L771 P772 D773 E774 L775 P784 P785 T788 T796 I803 P804 H805 S812 T816 L828 L835 Q841 S845 R849 LEU GLU LYS PRO ALA LEU GLU PHE LYS PRO THR ASP ALA ASP SER ALA Y866 C867 V874 ASN ASP SER S878

T879 F886 M887 E888 D889 I890 E891 K892 S893 E894 ALA ARG ILE GLY ILE PRO SER THR LYS TYR T905 K906 V911 I923 Y926 R934 F935 D943 L944 T945 P946 E956 K963 L968 D969 L970 Q975 P976 L977 V980 L987 N988 L989 L990 T991 P992 R993 HIS

LEU ASN GLN LYS GLY LYS ALA LEU P1003 H1031 P1032 R1050 C1053 LEU LEU

• Molecule 1: Endoribonuclease Dicer

Chain B: % 72% 12% • 14%

SER ASP Q756 V762 L767 L771 P772 N776 F777 R778 R779 R780 R790 T796 I803 P804 H805 E814 V815 T816 F826 M827 L828 Q831 M832 L833 E834 L835 L839 I843 L850 GLU LYS PRO ALA LEU GLU PHE LYS PRO THR ASP ALA ASP SER ALA Y866

C867 V873 VAL ASN ASP SER S878 D883 F884 M887 E888 E894 ALA ARG ILE GLY ILE PRO SER THR LYS Y904 F910 D919 I923 D943 L970 D981 N988 T991 P992 ARG HIS LEU ASN GLN LYS GLY LYS ALA LEU PRO L1004 S1005 S1006 A1007 E1008

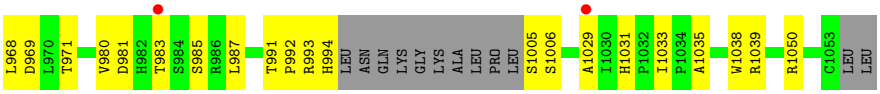
H1031 P1032 I1033 P1034 A1035 S1036 L1037 I1047 C1053 LEU LEU

• Molecule 1: Endoribonuclease Dicer

Chain C: % 62% 22% • 15%

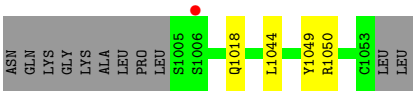
SER ASP Q756 Y759 E774 L775 N776 R779 R780 P784 P785 R790 T796 P799 I800 P801 Q802 I803 P804 H805 F806 Y809 T810 R811 E820 M827 Q831 M832 L833 E834 L835 I836 T837 R838 L839 H840 Q841 Y842 I843 I847 L848 R849 L850 GLU LYS PRO ALA LEU

GLU PHE LYS PRO THR ASP ALA ASP SER ALA Y866 C867 V873 V874 ASN ASP SER SER T879 L880 D883 F886 M887 E888 D889 I890 E894 ALA ARG ILE GLY ILE PRO SER THR LYS TYR THR K906 I923 P924 R925 Y926 R927 N928 R934 F935 T942 K963 Y966 N967



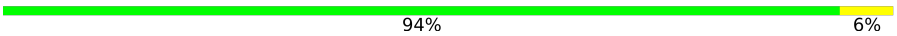
• Molecule 1: Endoribonuclease Dicer

Chain D:



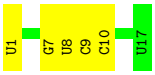
• Molecule 2: 5'-R(P*UP*CP*GP*AP*AP*GP*GP*UP*CP*CP*UP*UP*CP*GP*UP*UP*U)-3'

Chain E:



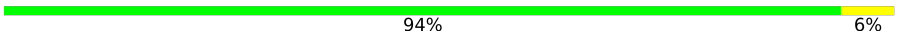
• Molecule 2: 5'-R(P*UP*CP*GP*AP*AP*GP*GP*UP*CP*CP*UP*UP*CP*GP*UP*UP*U)-3'

Chain F:



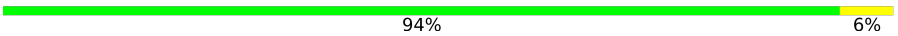
• Molecule 2: 5'-R(P*UP*CP*GP*AP*AP*GP*GP*UP*CP*CP*UP*UP*CP*GP*UP*UP*U)-3'

Chain G:



• Molecule 2: 5'-R(P*UP*CP*GP*AP*AP*GP*GP*UP*CP*CP*UP*UP*CP*GP*UP*UP*U)-3'

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.25Å 104.19Å 368.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.48 – 3.10 47.96 – 3.10	Depositor EDS
% Data completeness (in resolution range)	91.1 (42.48-3.10) 88.6 (47.96-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.99 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.223 , 0.270 0.223 , 0.270	Depositor DCC
R_{free} test set	1591 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	74.4	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 34.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.049 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9701	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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	0.30	0/2105	0.58	1/2875 (0.0%)
1	B	0.33	0/2120	0.61	0/2891
1	C	0.36	0/2160	0.61	0/2939
1	D	0.30	0/2112	0.58	0/2887
2	E	0.61	1/396 (0.3%)	0.77	0/612
2	F	0.62	1/396 (0.3%)	0.77	0/612
2	G	0.59	1/396 (0.3%)	0.75	0/612
2	H	0.66	1/396 (0.3%)	0.76	0/612
All	All	0.39	4/10081 (0.0%)	0.63	1/14040 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-11.17	1.47	1.61
2	E	1	U	OP3-P	-10.49	1.48	1.61
2	F	1	U	OP3-P	-10.32	1.48	1.61
2	G	1	U	OP3-P	-10.21	1.48	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	889	ASP	N-CA-C	-5.01	97.48	111.00

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	2049	0	1994	19	0
1	B	2065	0	2006	18	0
1	C	2103	0	2096	35	0
1	D	2056	0	1989	26	0
2	E	357	0	181	0	0
2	F	357	0	181	3	0
2	G	357	0	181	0	0
2	H	357	0	181	0	0
All	All	9701	0	8809	101	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 6.

All (101) 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:904:TYR:HA	1:B:910:PHE:HB2	1.72	0.71
1:D:795:LEU:O	1:D:866:TYR:N	2.23	0.71
1:A:803:ILE:HG13	1:A:1050:ARG:HH22	1.58	0.68
1:B:1005:SER:HB3	1:B:1008:GLU:HB2	1.76	0.68
1:C:925:ARG:HD3	1:C:1029:ALA:HB2	1.76	0.67
1:C:886:PHE:O	1:C:890:ILE:HG12	1.95	0.66
1:D:847:ILE:O	1:D:934:ARG:NH1	2.30	0.64
1:A:987:LEU:HD22	1:A:990:LEU:HD23	1.82	0.62
1:D:926:TYR:HB3	1:D:968:LEU:HD11	1.85	0.58
1:A:943:ASP:OD1	1:A:943:ASP:N	2.29	0.58
1:C:776:ASN:HD21	1:C:780:ARG:N	2.03	0.57
1:B:839:LEU:O	1:B:843:ILE:HG12	2.05	0.57
1:B:826:PHE:HE2	1:B:828:LEU:HD22	1.68	0.57
1:D:762:VAL:HG23	1:D:871:LEU:HD12	1.89	0.55
1:D:947:LEU:HD21	1:D:973:LEU:HD13	1.91	0.53
1:D:769:THR:HB	1:D:814:GLU:HB3	1.90	0.53
1:C:927:ARG:NH1	1:C:928:ASN:OD1	2.40	0.52
1:C:803:ILE:HD12	1:C:804:PRO:HD2	1.92	0.52
1:A:990:LEU:HG	1:A:992:PRO:HD3	1.91	0.52
1:A:889:ASP:O	1:A:892:LYS:HB2	2.09	0.52
1:A:946:PRO:HD3	1:A:975:GLN:O	2.09	0.51
1:B:790:ARG:NE	1:B:883:ASP:OD2	2.43	0.51
1:B:1033:ILE:HG23	1:B:1037:LEU:HD23	1.93	0.51
1:D:963:LYS:HE3	1:D:969:ASP:OD1	2.11	0.50
1:B:1005:SER:OG	1:B:1006:SER:N	2.45	0.50
1:C:1005:SER:OG	1:C:1006:SER:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:847:ILE:HD11	1:C:1033:ILE:HD12	1.93	0.50
1:C:992:PRO:HG2	1:C:993:ARG:HG3	1.94	0.50
1:D:990:LEU:HD13	1:D:991:THR:H	1.77	0.49
1:D:832:MET:HG3	1:D:835:LEU:HD23	1.93	0.49
1:B:1031:HIS:CG	1:B:1032:PRO:HD2	2.48	0.48
1:C:790:ARG:NE	1:C:883:ASP:OD2	2.41	0.48
1:C:832:MET:O	1:C:836:ILE:HG12	2.14	0.48
2:F:8:U:H2'	2:F:9:C:C6	2.48	0.48
1:A:1031:HIS:CG	1:A:1032:PRO:HD2	2.49	0.48
1:A:944:LEU:HB3	1:A:977:LEU:HD12	1.96	0.47
1:B:777:PHE:HB2	1:B:778:ARG:NH1	2.30	0.47
1:B:833:LEU:HD12	1:B:833:LEU:HA	1.70	0.47
1:C:809:TYR:O	1:C:993:ARG:NH2	2.48	0.47
1:C:963:LYS:O	1:C:967:ASN:HA	2.15	0.47
1:C:847:ILE:HD11	1:C:1033:ILE:CD1	2.45	0.46
1:A:926:TYR:HB3	1:A:968:LEU:HD11	1.96	0.46
1:B:884:PHE:HA	1:B:887:MET:HE2	1.97	0.46
1:A:887:MET:O	1:A:891:GLU:HG2	2.15	0.46
1:C:836:ILE:HG22	1:C:867:CYS:SG	2.56	0.46
1:C:843:ILE:O	1:C:847:ILE:HB	2.16	0.46
1:D:847:ILE:HG22	1:D:848:LEU:HD23	1.98	0.46
1:D:784:PRO:HA	1:D:785:PRO:HD3	1.86	0.46
1:D:771:LEU:HA	1:D:772:PRO:HD3	1.55	0.46
1:D:908:THR:O	1:D:971:THR:HB	2.15	0.45
1:D:936:TYR:HE2	1:D:983:THR:HG23	1.82	0.45
1:C:906:LYS:O	1:C:971:THR:HG21	2.17	0.45
1:A:771:LEU:HA	1:A:772:PRO:HD3	1.70	0.45
1:A:987:LEU:HD21	1:A:989:LEU:HB2	1.98	0.45
1:C:774:GLU:HG2	1:C:775:LEU:N	2.32	0.45
1:D:963:LYS:O	1:D:967:ASN:HA	2.18	0.44
1:D:830:LEU:HD12	1:D:833:LEU:HD12	1.98	0.44
1:B:767:LEU:HD12	1:B:814:GLU:O	2.17	0.44
1:C:1031:HIS:ND1	1:C:1038:TRP:HZ3	2.16	0.44
1:C:756:GLN:N	1:C:827:MET:SD	2.91	0.44
1:C:963:LYS:HE3	1:C:969:ASP:OD1	2.18	0.44
1:C:935:PHE:HB3	1:C:980:VAL:HB	2.00	0.44
1:A:991:THR:O	1:A:991:THR:OG1	2.19	0.43
1:B:771:LEU:HA	1:B:772:PRO:HD3	1.86	0.43
1:B:919:ASP:OD1	1:B:1035:ALA:HB3	2.18	0.43
1:C:967:ASN:ND2	1:C:967:ASN:O	2.51	0.43
1:A:935:PHE:HB3	1:A:980:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:ASN:HD21	1:B:780:ARG:HG2	1.84	0.43
1:C:842:TYR:CZ	1:C:890:ILE:HD12	2.53	0.43
1:D:803:ILE:HD12	1:D:804:PRO:HD2	2.00	0.43
1:C:806:PHE:CD2	1:C:1050:ARG:HG2	2.53	0.43
1:D:809:TYR:CD1	1:D:809:TYR:N	2.86	0.43
1:C:759:TYR:HE2	1:C:799:PRO:HD3	1.84	0.43
1:C:834:GLU:O	1:C:838:ARG:HD3	2.19	0.43
1:D:963:LYS:NZ	1:D:969:ASP:HA	2.34	0.43
1:B:777:PHE:HB2	1:B:778:ARG:HH11	1.84	0.42
1:C:811:ARG:HD2	1:C:983:THR:HG21	2.01	0.42
2:F:9:C:H2'	2:F:10:C:H6	1.84	0.42
1:A:772:PRO:HD2	1:A:775:LEU:CB	2.49	0.42
1:C:784:PRO:HA	1:C:785:PRO:HD3	1.88	0.42
1:C:780:ARG:NH1	1:C:811:ARG:O	2.52	0.42
1:D:935:PHE:HE2	1:D:1018:GLN:HG2	1.84	0.42
1:A:905:THR:HA	1:A:906:LYS:HA	1.75	0.42
1:C:1035:ALA:O	1:C:1039:ARG:HG3	2.20	0.41
1:D:926:TYR:CB	1:D:968:LEU:HD11	2.50	0.41
1:C:803:ILE:HA	1:C:804:PRO:HD3	1.96	0.41
1:A:828:LEU:HD13	1:A:828:LEU:HA	1.88	0.41
1:B:828:LEU:HD12	1:B:828:LEU:HA	1.77	0.41
1:A:923:ILE:HG22	1:A:934:ARG:HG2	2.02	0.41
1:A:784:PRO:HA	1:A:785:PRO:HD3	1.83	0.41
1:D:955:TYR:CD2	1:D:961:TYR:HA	2.56	0.41
1:C:966:TYR:HB2	1:C:968:LEU:HG	2.03	0.41
1:D:780:ARG:HG2	1:D:781:LYS:N	2.36	0.41
2:F:7:G:C6	2:F:8:U:C4	3.09	0.41
1:D:983:THR:OG1	1:D:984:SER:N	2.54	0.40
1:D:1044:LEU:HA	1:D:1044:LEU:HD23	1.87	0.40
1:C:776:ASN:HD21	1:C:780:ARG:H	1.69	0.40
1:C:831:GLN:HG3	1:C:832:MET:N	2.37	0.40
1:D:990:LEU:HD22	1:D:990:LEU:HA	1.87	0.40
1:B:943:ASP:OD1	1:B:943:ASP:N	2.52	0.40
1:C:800:ILE:HA	1:C:801:PRO:HD3	1.90	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	250/302 (83%)	238 (95%)	12 (5%)	0	100	100
1	B	249/302 (82%)	237 (95%)	12 (5%)	0	100	100
1	C	248/302 (82%)	240 (97%)	8 (3%)	0	100	100
1	D	250/302 (83%)	238 (95%)	12 (5%)	0	100	100
All	All	997/1208 (82%)	953 (96%)	44 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	222/282 (79%)	201 (90%)	21 (10%)	8	31
1	B	226/282 (80%)	207 (92%)	19 (8%)	11	38
1	C	235/282 (83%)	212 (90%)	23 (10%)	8	29
1	D	220/282 (78%)	205 (93%)	15 (7%)	16	45
All	All	903/1128 (80%)	825 (91%)	78 (9%)	10	37

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

Mol	Chain	Res	Type
1	A	760	LEU
1	A	788	THR

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Mol	Chain	Res	Type
1	A	796	THR
1	A	803	ILE
1	A	805	HIS
1	A	812	SER
1	A	816	THR
1	A	828	LEU
1	A	835	LEU
1	A	841	GLN
1	A	845	SER
1	A	867	CYS
1	A	879	THR
1	A	911	VAL
1	A	923	ILE
1	A	943	ASP
1	A	956	GLU
1	A	963	LYS
1	A	970	LEU
1	A	990	LEU
1	A	1050	ARG
1	B	762	VAL
1	B	771	LEU
1	B	776	ASN
1	B	778	ARG
1	B	796	THR
1	B	805	HIS
1	B	816	THR
1	B	828	LEU
1	B	831	GLN
1	B	835	LEU
1	B	839	LEU
1	B	866	TYR
1	B	867	CYS
1	B	888	GLU
1	B	923	ILE
1	B	943	ASP
1	B	970	LEU
1	B	981	ASP
1	B	991	THR
1	C	779	ARG
1	C	796	THR
1	C	803	ILE
1	C	820	GLU

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Mol	Chain	Res	Type
1	C	827	MET
1	C	831	GLN
1	C	832	MET
1	C	839	LEU
1	C	841	GLN
1	C	848	LEU
1	C	867	CYS
1	C	873	VAL
1	C	880	LEU
1	C	888	GLU
1	C	906	LYS
1	C	923	ILE
1	C	934	ARG
1	C	942	THR
1	C	981	ASP
1	C	985	SER
1	C	987	LEU
1	C	991	THR
1	C	994	HIS
1	D	788	THR
1	D	796	THR
1	D	820	GLU
1	D	839	LEU
1	D	841	GLN
1	D	879	THR
1	D	894	GLU
1	D	908	THR
1	D	923	ILE
1	D	934	ARG
1	D	963	LYS
1	D	990	LEU
1	D	994	HIS
1	D	1049	TYR
1	D	1050	ARG

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

Mol	Chain	Res	Type
1	A	846	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	16/17 (94%)	0	0
2	F	16/17 (94%)	0	0
2	G	16/17 (94%)	0	0
2	H	16/17 (94%)	0	0
All	All	64/68 (94%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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	260/302 (86%)	-0.16	5 (1%)	66	46	29, 68, 138, 185	0
1	B	259/302 (85%)	-0.08	4 (1%)	73	54	22, 62, 133, 167	0
1	C	258/302 (85%)	-0.11	2 (0%)	86	72	26, 56, 104, 199	0
1	D	260/302 (86%)	-0.06	2 (0%)	86	72	25, 71, 150, 217	0
2	E	17/17 (100%)	-0.43	0	100	100	37, 47, 56, 62	0
2	F	17/17 (100%)	-0.50	0	100	100	36, 44, 52, 58	0
2	G	17/17 (100%)	-0.65	0	100	100	41, 50, 60, 62	0
2	H	17/17 (100%)	-0.49	0	100	100	37, 44, 68, 77	0
All	All	1105/1276 (86%)	-0.13	13 (1%)	79	61	22, 62, 134, 217	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1006	SER	3.1
1	A	774	GLU	3.1
1	A	772	PRO	2.7
1	C	983	THR	2.7
1	A	886	PHE	2.6
1	D	988	ASN	2.6
1	B	805	HIS	2.3
1	B	1047	ILE	2.3
1	B	988	ASN	2.3
1	C	1029	ALA	2.3
1	A	988	ASN	2.2
1	B	803	ILE	2.1
1	A	874	VAL	2.1

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.