Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:51 PM GMT

PDB ID	:	1HKN
Title	:	A COMPLEX BETWEEN ACIDIC FIBROBLAST GROWTH FACTOR AND 5-AMINO-2-NAPHTHALENESULFONATE
Authors	:	Fernandez-Tornero, C.; Lozano, R.M.; Gimenez-Gallego, G.; Romero, A.
Deposited on	:	2003-03-10
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

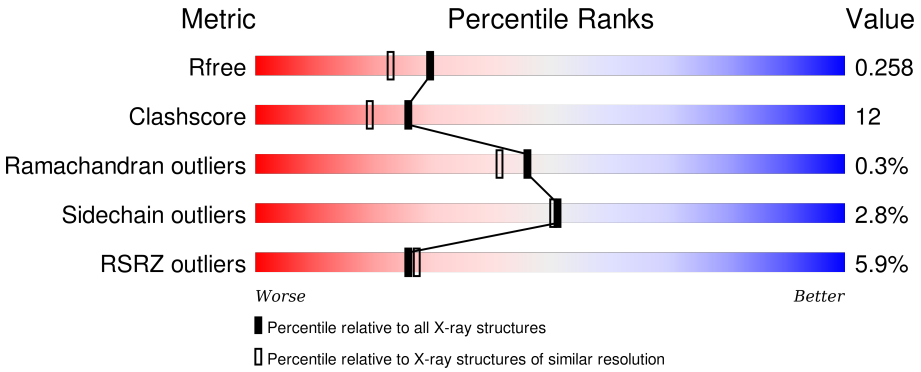
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	139	4% 71% 21% • 7%
1	B	139	3% 71% 21% • 7%
1	C	139	2% 73% 19% • 6%
1	D	139	6% 65% 25% • 6%
1	E	139	4% 73% 19% • 6%

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Mol	Chain	Length	Quality of chain
1	F	139	14% 64% 29% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	N2M	C	4138	-	-	-	X
2	N2M	D	5139	-	-	-	X

2 Entry composition

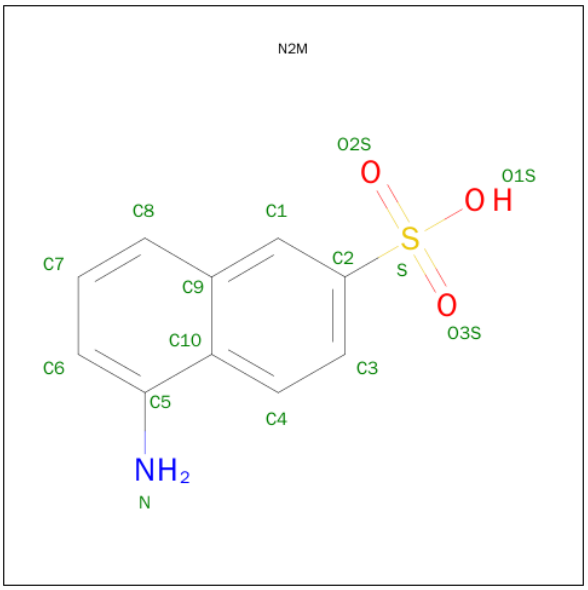
There are 3 unique types of molecules in this entry. The entry contains 6301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEPARIN-BINDING GROWTH FACTOR 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	129	Total	C	N	O	S	0	0	1
			1023	646	180	193	4			
1	B	129	Total	C	N	O	S	0	0	1
			1023	646	180	193	4			
1	C	130	Total	C	N	O	S	0	0	1
			1032	652	182	194	4			
1	D	130	Total	C	N	O	S	0	0	1
			1029	649	181	195	4			
1	E	131	Total	C	N	O	S	0	0	1
			1038	655	183	196	4			
1	F	129	Total	C	N	O	S	5	0	1
			1023	646	180	193	4			

- Molecule 2 is 5-AMINO-NAPHTALENE-2-MONOSULFONATE (three-letter code: N2M) (formula: $C_{10}H_9NO_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			15	10	1	3	1		
2	D	1	Total	C	N	O	S	0	0
			15	10	1	3	1		

- Molecule 3 is water.

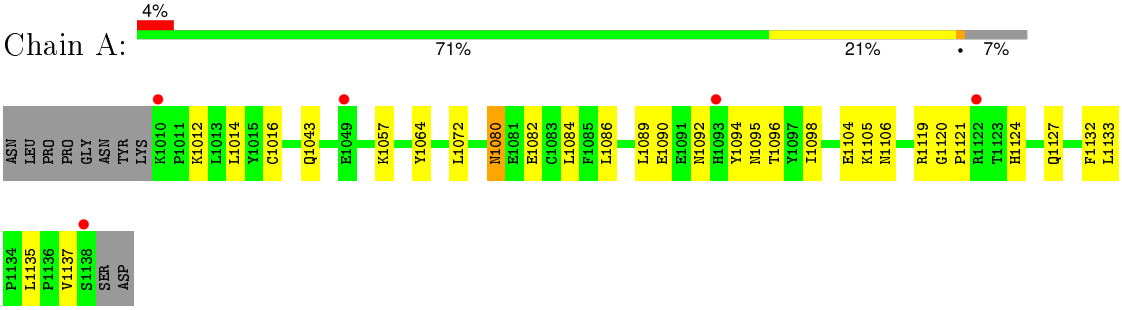
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	23	Total	O	0	0
			23	23		
3	C	27	Total	O	0	0
			27	27		
3	D	17	Total	O	0	0
			17	17		
3	E	13	Total	O	0	0
			13	13		
3	F	5	Total	O	0	0
			5	5		

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 errors 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.

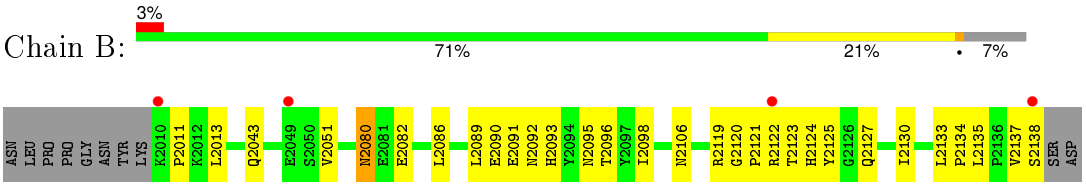
- Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain A:



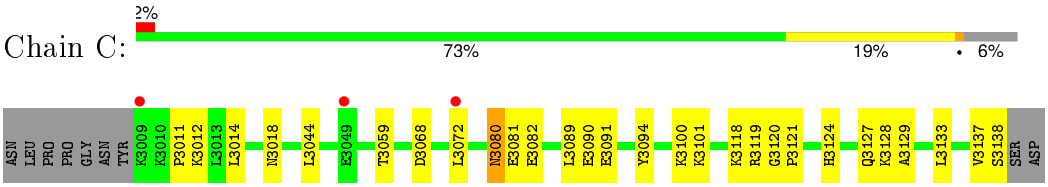
- Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain B:



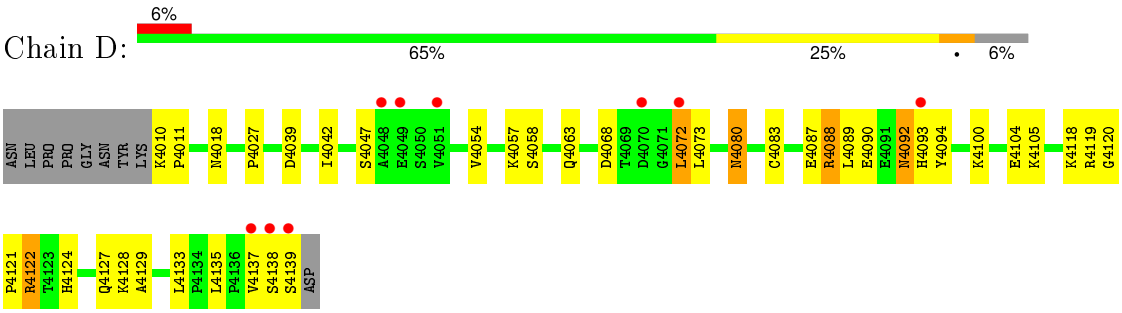
- Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain C:



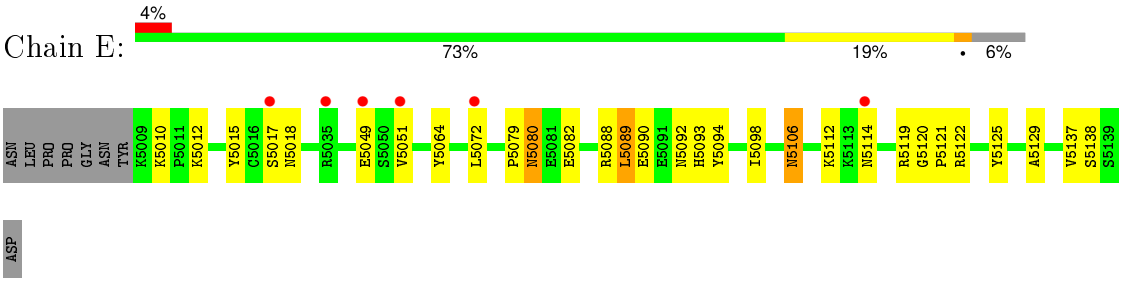
- Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain D:



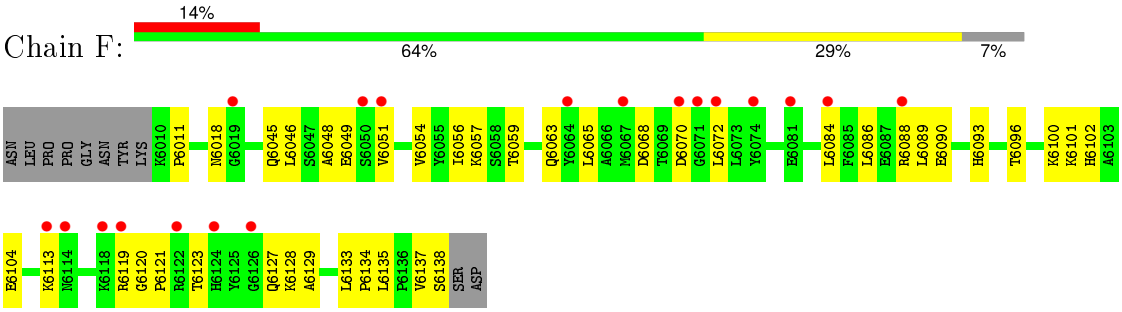
- Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain E:



• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.53Å 47.21Å 97.84Å 90.00° 107.04° 90.00°	Depositor
Resolution (Å)	33.57 – 2.00 33.57 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (33.57-2.00) 98.9 (33.57-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.64 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.259 0.226 , 0.258	Depositor DCC
R_{free} test set	5786 reflections (11.31%)	DCC
Wilson B-factor (Å^2)	27.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 48.7	EDS
Estimated twinning fraction	0.012 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 56956 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6301	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 66.10 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.3756e-06.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: N2M

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	0.35	0/1046	0.62	0/1412
1	B	0.35	0/1046	0.62	0/1412
1	C	0.37	0/1055	0.64	0/1423
1	D	0.34	0/1052	0.61	0/1420
1	E	0.32	0/1061	0.60	0/1431
1	F	0.31	0/1046	0.56	0/1412
All	All	0.34	0/6306	0.61	0/8510

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1023	0	1007	23	0
1	B	1023	0	1007	23	0
1	C	1032	0	1020	25	0
1	D	1029	0	1012	39	0
1	E	1038	0	1025	24	0
1	F	1023	0	1007	28	0
2	C	15	0	9	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	15	0	9	4	0
3	A	18	0	0	0	0
3	B	23	0	0	0	0
3	C	27	0	0	0	0
3	D	17	0	0	0	0
3	E	13	0	0	0	0
3	F	5	0	0	0	0
All	All	6301	0	6096	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (152) 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)
2:D:5139:N2M:C5	2:D:5139:N2M:N	1.79	1.44
2:C:4138:N2M:C5	2:C:4138:N2M:N	1.79	1.44
1:C:3128:LYS:H	2:C:4138:N2M:H4	1.40	0.83
1:B:2119:ARG:NH1	1:B:2122:ARG:HE	1.79	0.81
1:C:3080:ASN:HD22	1:C:3082:GLU:H	1.33	0.77
1:B:2091:GLU:HA	1:E:5012:LYS:NZ	2.02	0.75
1:C:3072:LEU:HD23	1:C:3119:ARG:HG2	1.70	0.72
1:B:2091:GLU:HA	1:E:5012:LYS:HZ3	1.57	0.69
1:D:4088:ARG:HH12	1:F:6086:LEU:HD13	1.58	0.69
1:B:2080:ASN:C	1:B:2080:ASN:HD22	1.95	0.68
1:D:4119:ARG:HH21	1:D:4122:ARG:NH2	1.92	0.68
1:A:1098:ILE:HD11	1:A:1106:ASN:HA	1.77	0.66
1:D:4092:ASN:H	1:D:4092:ASN:HD22	1.43	0.66
1:E:5089:LEU:HD22	1:E:5093:HIS:HA	1.77	0.66
1:E:5098:ILE:HD13	1:E:5106:ASN:HD22	1.61	0.65
1:D:4092:ASN:ND2	1:D:4092:ASN:H	1.96	0.63
1:A:1080:ASN:HD22	1:A:1080:ASN:C	2.01	0.63
1:F:6088:ARG:HG3	1:F:6096:THR:OG1	2.00	0.62
1:C:3128:LYS:HG3	2:C:4138:N2M:HN2	1.65	0.62
1:A:1133:LEU:O	1:A:1135:LEU:HD22	2.01	0.61
1:F:6072:LEU:HD23	1:F:6119:ARG:HG2	1.83	0.61
1:C:3072:LEU:CD2	1:C:3119:ARG:HG2	2.31	0.61
1:B:2093:HIS:CE1	1:E:5010:LYS:HB2	2.36	0.61
1:C:3128:LYS:H	2:C:4138:N2M:C4	2.13	0.59
1:F:6011:PRO:HB3	1:F:6059:THR:HG21	1.84	0.59
1:A:1086:LEU:HB2	1:A:1098:ILE:CG2	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2119:ARG:HH11	1:B:2122:ARG:HE	1.51	0.58
1:B:2089:LEU:HD11	1:B:2093:HIS:HA	1.84	0.58
1:A:1124:HIS:CE1	1:A:1127:GLN:HE21	2.20	0.58
1:B:2013:LEU:HD21	1:B:2043:GLN:OE1	2.02	0.58
1:F:6048:ALA:HB2	1:F:6054:VAL:HG12	1.86	0.58
1:D:4092:ASN:HD22	1:D:4092:ASN:N	2.01	0.58
1:A:1104:GLU:OE2	1:A:1105:LYS:HG3	2.05	0.57
1:C:3089:LEU:N	1:C:3089:LEU:HD22	2.20	0.57
1:D:4089:LEU:HD23	1:D:4090:GLU:N	2.20	0.57
1:D:4011:PRO:O	1:D:4137:VAL:HG12	2.06	0.56
1:B:2086:LEU:HB2	1:B:2098:ILE:HG22	1.87	0.55
1:F:6072:LEU:CD2	1:F:6119:ARG:HG2	2.36	0.55
1:F:6120:GLY:N	1:F:6121:PRO:HD2	2.20	0.55
1:B:2080:ASN:ND2	1:B:2082:GLU:H	2.04	0.55
1:F:6134:PRO:O	1:F:6135:LEU:HD12	2.07	0.55
1:F:6113:LYS:O	1:F:6113:LYS:HD2	2.07	0.54
1:B:2124:HIS:HD2	1:B:2125:TYR:O	1.91	0.54
1:A:1057:LYS:HD3	1:A:1064:TYR:CZ	2.42	0.54
1:C:3011:PRO:HB3	1:C:3059:THR:HG21	1.90	0.54
1:C:3018:ASN:HB2	1:C:3129:ALA:HA	1.89	0.54
1:A:1072:LEU:HD23	1:A:1119:ARG:HG2	1.90	0.54
1:F:6137:VAL:HG23	1:F:6138:SER:N	2.23	0.54
1:C:3100:LYS:HG3	1:E:5051:VAL:HG21	1.90	0.54
1:A:1016:CYS:HB2	1:A:1132:PHE:CE1	2.43	0.53
1:C:3091:GLU:HG2	1:E:5125:TYR:CD2	2.43	0.53
1:D:4080:ASN:C	1:D:4080:ASN:HD22	2.11	0.53
1:E:5098:ILE:HD13	1:E:5106:ASN:ND2	2.22	0.53
1:A:1012:LYS:HA	1:A:1137:VAL:HG23	1.91	0.53
1:A:1092:ASN:HD21	1:A:1094:TYR:HB2	1.74	0.53
1:B:2092:ASN:O	1:B:2093:HIS:HB2	2.10	0.52
1:E:5018:ASN:HB2	1:E:5129:ALA:HA	1.90	0.52
1:B:2095:ASN:ND2	1:B:2134:PRO:HG2	2.24	0.52
1:D:4119:ARG:HE	1:D:4122:ARG:NH2	2.08	0.52
1:C:3137:VAL:HG12	1:C:3138:SER:N	2.25	0.52
1:A:1080:ASN:ND2	1:A:1082:GLU:H	2.07	0.52
1:E:5080:ASN:C	1:E:5080:ASN:HD22	2.12	0.52
1:F:6133:LEU:O	1:F:6135:LEU:HD13	2.10	0.51
1:D:4089:LEU:HD23	1:D:4090:GLU:H	1.76	0.51
1:C:3012:LYS:HA	1:C:3137:VAL:HG23	1.93	0.51
1:D:4080:ASN:ND2	1:D:4083:CYS:SG	2.84	0.51
1:D:4057:LYS:HE3	1:D:4058:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3080:ASN:HD22	1:C:3082:GLU:N	2.04	0.51
1:D:4119:ARG:HH21	1:D:4122:ARG:HH21	1.56	0.51
1:E:5072:LEU:HD23	1:E:5119:ARG:HG2	1.94	0.50
1:D:4018:ASN:HB2	1:D:4129:ALA:HA	1.93	0.50
1:E:5137:VAL:HG23	1:E:5138:SER:N	2.26	0.50
1:B:2120:GLY:N	1:B:2121:PRO:HD2	2.27	0.50
1:F:6046:LEU:N	1:F:6046:LEU:HD12	2.26	0.50
1:A:1106:ASN:ND2	1:D:4124:HIS:HD2	2.10	0.50
1:A:1089:LEU:HA	1:A:1095:ASN:HD22	1.77	0.49
1:A:1080:ASN:HD22	1:A:1082:GLU:H	1.61	0.49
1:D:4133:LEU:O	1:D:4135:LEU:HD22	2.11	0.49
1:D:4087:GLU:C	1:D:4088:ARG:HD2	2.33	0.49
1:D:4124:HIS:O	1:D:4127:GLN:HG3	2.13	0.49
1:F:6048:ALA:HA	1:F:6054:VAL:HA	1.94	0.49
1:D:4027:PRO:HA	1:D:4063:GLN:NE2	2.28	0.49
1:C:3080:ASN:HD21	1:C:3082:GLU:HB2	1.78	0.48
1:E:5137:VAL:HG23	1:E:5138:SER:H	1.78	0.48
1:E:5089:LEU:CD2	1:E:5093:HIS:HA	2.43	0.48
1:A:1090:GLU:CG	1:A:1096:THR:HG23	2.44	0.48
1:B:2090:GLU:CG	1:B:2096:THR:HG23	2.44	0.48
1:D:4027:PRO:HA	1:D:4063:GLN:HE22	1.78	0.48
1:C:3080:ASN:ND2	1:C:3082:GLU:H	2.07	0.47
1:F:6104:GLU:H	1:F:6104:GLU:CD	2.18	0.47
1:F:6057:LYS:HG3	1:F:6063:GLN:O	2.15	0.47
1:D:4072:LEU:HD13	1:D:4073:LEU:N	2.30	0.47
1:C:3124:HIS:O	1:C:3127:GLN:HG3	2.15	0.47
1:E:5120:GLY:N	1:E:5121:PRO:HD2	2.30	0.47
1:C:3118:LYS:HE2	1:C:3127:GLN:OE1	2.15	0.47
1:D:4088:ARG:NH1	1:F:6086:LEU:HD13	2.28	0.46
1:A:1092:ASN:ND2	1:A:1094:TYR:HB2	2.31	0.46
1:B:2137:VAL:HG22	1:B:2138:SER:N	2.30	0.46
1:F:6056:ILE:HD12	1:F:6065:LEU:HD23	1.98	0.46
1:D:4120:GLY:N	1:D:4121:PRO:HD2	2.30	0.46
1:B:2123:THR:HA	1:B:2127:GLN:OE1	2.15	0.46
1:B:2127:GLN:O	1:B:2130:ILE:HG12	2.15	0.45
1:D:4127:GLN:HA	2:D:5139:N2M:H4	1.97	0.45
1:D:4092:ASN:O	1:D:4093:HIS:HB2	2.17	0.45
1:C:3081:GLU:HG3	1:C:3101:LYS:HD2	1.98	0.45
1:D:4128:LYS:H	2:D:5139:N2M:H4	1.82	0.45
1:A:1090:GLU:HA	1:A:1090:GLU:OE2	2.16	0.45
1:F:6018:ASN:HB2	1:F:6128:LYS:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4100:LYS:HG3	1:F:6051:VAL:HG21	1.99	0.45
1:E:5112:LYS:HB2	1:E:5114:ASN:OD1	2.17	0.44
1:D:4010:LYS:HB3	1:D:4011:PRO:HD2	2.00	0.44
1:F:6018:ASN:HB2	1:F:6128:LYS:O	2.18	0.44
1:F:6068:ASP:OD2	1:F:6072:LEU:HB2	2.17	0.44
1:E:5072:LEU:CD2	1:E:5119:ARG:HG2	2.47	0.44
1:C:3120:GLY:N	1:C:3121:PRO:HD2	2.33	0.44
1:C:3094:TYR:CE1	1:C:3133:LEU:HB2	2.53	0.44
1:B:2080:ASN:HD22	1:B:2082:GLU:H	1.64	0.44
1:D:4104:GLU:HG2	1:D:4105:LYS:N	2.33	0.43
1:F:6084:LEU:HD13	1:F:6100:LYS:HD3	2.00	0.43
1:B:2051:VAL:HG11	1:E:5015:TYR:CE2	2.53	0.43
1:D:4119:ARG:HH11	1:D:4119:ARG:HG2	1.83	0.43
1:A:1120:GLY:N	1:A:1121:PRO:HD2	2.33	0.43
1:A:1086:LEU:HB2	1:A:1098:ILE:HG22	1.97	0.43
1:B:2091:GLU:HA	1:E:5012:LYS:HZ1	1.79	0.43
1:F:6018:ASN:HB2	1:F:6129:ALA:HA	2.01	0.43
1:D:4100:LYS:HG3	1:F:6051:VAL:CG2	2.49	0.43
1:C:3089:LEU:HD22	1:C:3089:LEU:H	1.84	0.42
1:B:2133:LEU:O	1:B:2135:LEU:HD22	2.19	0.42
1:D:4039:ASP:O	1:D:4042:ILE:HG12	2.20	0.42
1:D:4138:SER:OG	1:D:4139:SER:N	2.52	0.42
1:A:1098:ILE:CD1	1:A:1106:ASN:HA	2.45	0.42
1:F:6101:LYS:HG3	1:F:6102:HIS:CD2	2.55	0.42
1:D:4128:LYS:H	2:D:5139:N2M:C4	2.32	0.42
1:F:6113:LYS:HD2	1:F:6113:LYS:C	2.40	0.42
1:F:6123:THR:HA	1:F:6127:GLN:OE1	2.20	0.42
1:D:4092:ASN:ND2	1:D:4094:TYR:HB2	2.35	0.42
1:D:4092:ASN:O	1:D:4094:TYR:HD2	2.03	0.42
1:D:4118:LYS:HE2	1:D:4122:ARG:HB3	2.01	0.42
1:E:5080:ASN:HD22	1:E:5082:GLU:H	1.66	0.41
1:B:2011:PRO:HG2	1:B:2137:VAL:CG1	2.50	0.41
1:E:5064:TYR:CE1	1:E:5079:PRO:HD3	2.55	0.41
1:C:3014:LEU:HD13	1:C:3044:LEU:HD12	2.02	0.41
1:D:4047:SER:O	1:D:4054:VAL:HA	2.19	0.41
1:F:6089:LEU:HD21	1:F:6093:HIS:CD2	2.56	0.41
1:E:5088:ARG:HH22	1:E:5125:TYR:HE1	1.68	0.41
1:C:3068:ASP:OD1	1:C:3068:ASP:C	2.58	0.41
1:E:5122:ARG:HD3	1:E:5122:ARG:HA	1.76	0.41
1:A:1014:LEU:HD23	1:A:1014:LEU:HA	1.93	0.41
1:E:5092:ASN:HB2	1:E:5094:TYR:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1084:LEU:HD23	1:A:1084:LEU:HA	1.95	0.40
1:D:4068:ASP:OD1	1:D:4068:ASP:C	2.60	0.40
1:C:3080:ASN:ND2	1:C:3082:GLU:HB2	2.37	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	127/139 (91%)	123 (97%)	4 (3%)	0	100	100
1	B	127/139 (91%)	123 (97%)	4 (3%)	0	100	100
1	C	128/139 (92%)	127 (99%)	1 (1%)	0	100	100
1	D	128/139 (92%)	124 (97%)	4 (3%)	0	100	100
1	E	129/139 (93%)	126 (98%)	2 (2%)	1 (1%)	24	15
1	F	127/139 (91%)	119 (94%)	7 (6%)	1 (1%)	24	15
All	All	766/834 (92%)	742 (97%)	22 (3%)	2 (0%)	46	41

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	5049	GLU
1	F	6049	GLU

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	112/122 (92%)	110 (98%)	2 (2%)	66	69
1	B	112/122 (92%)	110 (98%)	2 (2%)	66	69
1	C	113/122 (93%)	111 (98%)	2 (2%)	66	69
1	D	113/122 (93%)	108 (96%)	5 (4%)	35	30
1	E	114/122 (93%)	109 (96%)	5 (4%)	35	30
1	F	112/122 (92%)	109 (97%)	3 (3%)	52	52
All	All	676/732 (92%)	657 (97%)	19 (3%)	51	50

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1043	GLN
1	A	1080	ASN
1	B	2080	ASN
1	B	2106	ASN
1	C	3080	ASN
1	C	3090	GLU
1	D	4072	LEU
1	D	4080	ASN
1	D	4088	ARG
1	D	4092	ASN
1	D	4122	ARG
1	E	5017	SER
1	E	5080	ASN
1	E	5089	LEU
1	E	5090	GLU
1	E	5106	ASN
1	F	6045	GLN
1	F	6070	ASP
1	F	6090	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1043	GLN
1	A	1080	ASN
1	A	1095	ASN
1	A	1106	ASN

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Mol	Chain	Res	Type
1	A	1124	HIS
1	A	1127	GLN
1	B	2080	ASN
1	B	2106	ASN
1	B	2124	HIS
1	C	3063	GLN
1	C	3077	GLN
1	C	3080	ASN
1	D	4043	GLN
1	D	4063	GLN
1	D	4077	GLN
1	D	4080	ASN
1	D	4092	ASN
1	E	5021	HIS
1	E	5043	GLN
1	E	5045	GLN
1	E	5080	ASN
1	E	5093	HIS
1	E	5095	ASN
1	F	6043	GLN
1	F	6045	GLN
1	F	6063	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	N2M	C	4138	-	16,16,16	4.71	7 (43%)	24,24,24	1.94	4 (16%)
2	N2M	D	5139	-	16,16,16	4.73	7 (43%)	24,24,24	2.02	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	N2M	C	4138	-	-	0/6/6/6	0/2/2/2
2	N2M	D	5139	-	-	0/6/6/6	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4138	N2M	C4-C10	-4.28	1.33	1.42
2	D	5139	N2M	C4-C10	-4.27	1.33	1.42
2	D	5139	N2M	C4-C3	3.96	1.45	1.36
2	C	4138	N2M	C7-C8	4.01	1.45	1.36
2	D	5139	N2M	C7-C8	4.03	1.45	1.36
2	C	4138	N2M	C4-C3	4.04	1.45	1.36
2	D	5139	N2M	O1S-S	5.96	1.77	1.44
2	C	4138	N2M	O1S-S	6.01	1.77	1.44
2	C	4138	N2M	O2S-S	6.26	1.73	1.43
2	D	5139	N2M	O2S-S	6.33	1.74	1.43
2	C	4138	N2M	O3S-S	6.77	1.76	1.43
2	D	5139	N2M	O3S-S	6.77	1.76	1.43
2	C	4138	N2M	C5-N	13.41	1.79	1.38
2	D	5139	N2M	C5-N	13.54	1.79	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	5139	N2M	C3-C2-C1	-2.75	117.63	121.01
2	C	4138	N2M	C3-C2-C1	-2.56	117.87	121.01
2	D	5139	N2M	C8-C9-C10	-2.15	116.19	119.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	4138	N2M	C8-C9-C10	-2.13	116.21	119.10
2	D	5139	N2M	C6-C5-C10	2.13	122.99	119.65
2	C	4138	N2M	C6-C5-C10	2.15	123.03	119.65
2	C	4138	N2M	O1S-S-C2	6.86	126.29	106.94
2	D	5139	N2M	O1S-S-C2	7.28	127.48	106.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4138	N2M	4	0
2	D	5139	N2M	4	0

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, 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	129/139 (92%)	0.24	5 (3%) 43 45	17, 32, 49, 55	6 (4%)
1	B	129/139 (92%)	0.22	4 (3%) 52 53	19, 31, 47, 54	5 (3%)
1	C	130/139 (93%)	0.06	3 (2%) 64 64	17, 26, 43, 51	3 (2%)
1	D	130/139 (93%)	0.47	9 (6%) 20 21	17, 32, 52, 63	7 (5%)
1	E	131/139 (94%)	0.26	6 (4%) 36 38	22, 35, 49, 61	7 (5%)
1	F	129/139 (92%)	0.88	19 (14%) 3 4	27, 44, 61, 65	11 (8%)
All	All	778/834 (93%)	0.35	46 (5%) 26 27	17, 33, 54, 65	39 (5%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4138	SER	6.4
1	D	4139	SER	6.3
1	F	6019	GLY	4.7
1	F	6113	LYS	4.7
1	D	4051	VAL	4.4
1	B	2138	SER	4.4
1	F	6050	SER	4.2
1	E	5049	GLU	3.7
1	F	6126	GLY	3.7
1	D	4048	ALA	3.6
1	F	6081	GLU	3.5
1	F	6051	VAL	3.4
1	F	6070	ASP	3.0
1	F	6072	LEU	3.0
1	F	6071	GLY	2.9
1	E	5114	ASN	2.9
1	E	5051	VAL	2.8
1	F	6064	TYR	2.8
1	D	4137	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1010	LYS	2.7
1	D	4070	ASP	2.6
1	C	3009	LYS	2.6
1	C	3049	GLU	2.6
1	F	6114	ASN	2.5
1	F	6074	TYR	2.5
1	E	5017	SER	2.5
1	A	1049	GLU	2.4
1	B	2122	ARG	2.4
1	A	1138	SER	2.4
1	E	5035	ARG	2.3
1	F	6084	LEU	2.3
1	C	3072	LEU	2.3
1	F	6119	ARG	2.3
1	D	4072	LEU	2.3
1	B	2049	GLU	2.2
1	A	1093	HIS	2.2
1	F	6124	HIS	2.2
1	B	2010	LYS	2.2
1	D	4093	HIS	2.1
1	F	6118	LYS	2.1
1	F	6088	ARG	2.1
1	F	6122	ARG	2.1
1	A	1122	ARG	2.1
1	D	4049	GLU	2.1
1	E	5072	LEU	2.0
1	F	6067	MET	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	N2M	D	5139	15/15	0.59	0.36	8.05	68,68,69,69	0
2	N2M	C	4138	15/15	0.66	0.36	8.00	63,64,66,67	0

6.5 Other polymers (i)

There are no such residues in this entry.