



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:06 PM UTC

PDB ID : 1HKN / pdb_00001hkn
Title : A complex between acidic fibroblast growth factor and 5-amino-2-naphthalen
esulfonate
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 wwPDB X-ray Structure Validation Summary 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

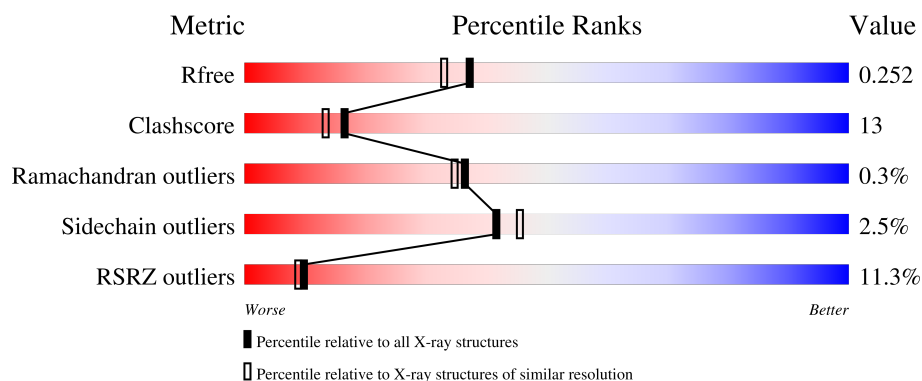
1 Overall quality at a glance

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	139	7% 68% 22% • 7%
1	B	139	6% 69% 22% • 7%
1	C	139	3% 69% 23% • 6%
1	D	139	9% 63% 26% • 6%
1	E	139	11% 71% 22% • 6%

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Mol	Chain	Length	Quality of chain
1	F	139	27% 63% 29% • 7%

2 Entry composition [i](#)

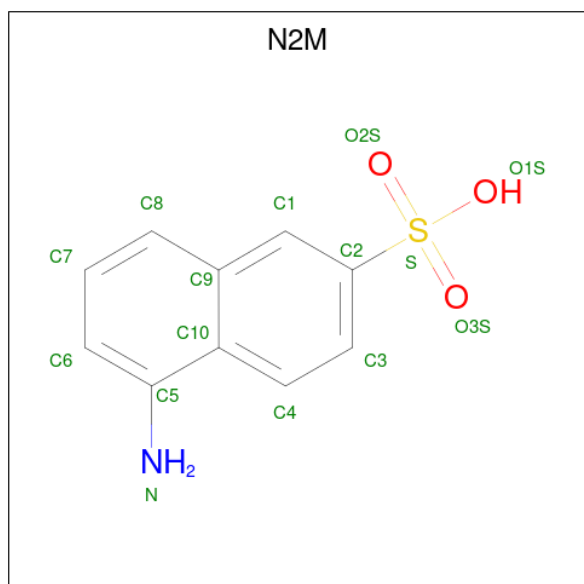
There are 3 unique types of molecules in this entry. The entry contains 6301 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-NAPHTHALENE-2-MONOSULFONATE (CCD ID: 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.

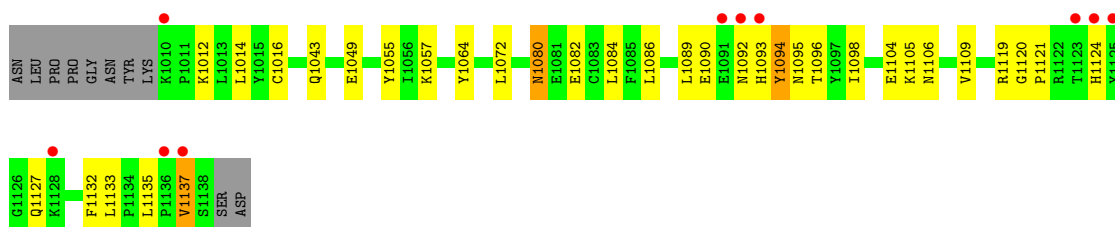
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	23	Total	O	0	0
			23	23		
3	C	27	Total	O	0	0
			27	27		
3	D	17	Total	O	0	0
			17	17		
3	E	13	Total	O	0	0
			13	13		
3	F	5	Total	O	0	0
			5	5		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

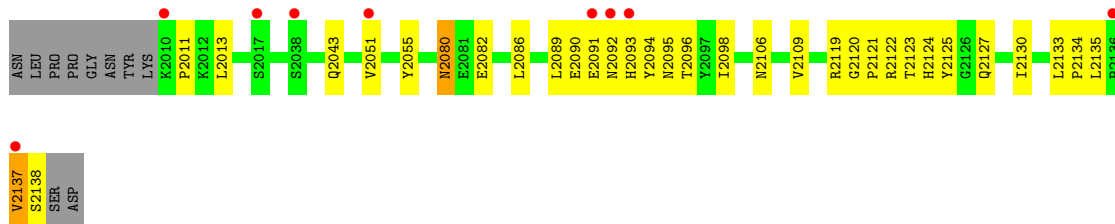
• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain A: 



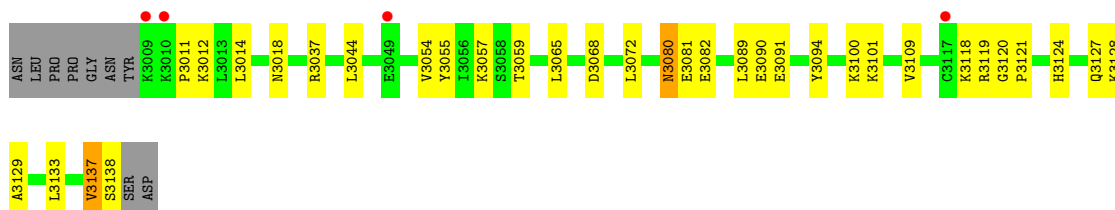
• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain B: 



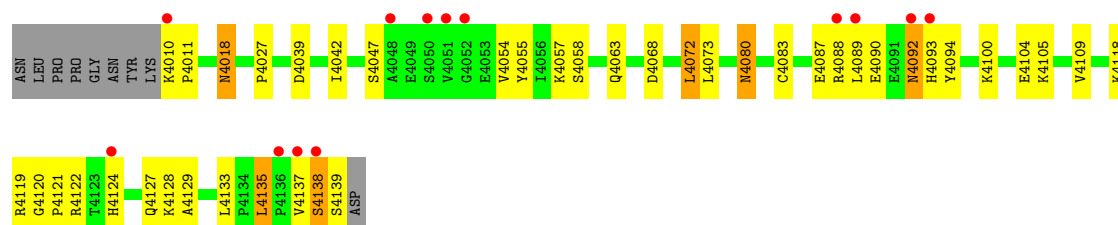
• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

Chain C: 



• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1

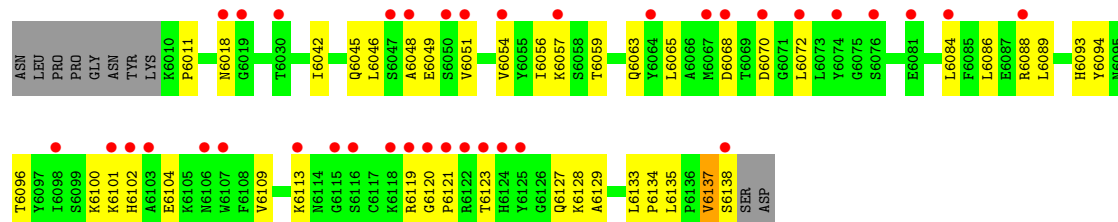
Chain D: 



• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1



• Molecule 1: HEPARIN-BINDING GROWTH FACTOR 1



4 Data and refinement statistics

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) 98.8 (33.57-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.64 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.259 0.221 , 0.252	Depositor DCC
R_{free} test set	5786 reflections (10.16%)	wwPDB-VP
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 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for l,-k,h	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.*

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](#)

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	0.40	1/1046 (0.1%)	0.86	4/1412 (0.3%)
1	B	0.40	1/1046 (0.1%)	0.88	3/1412 (0.2%)
1	C	0.43	1/1055 (0.1%)	0.90	5/1423 (0.4%)
1	D	0.39	1/1052 (0.1%)	0.86	3/1420 (0.2%)
1	E	0.38	1/1061 (0.1%)	0.85	3/1431 (0.2%)
1	F	0.35	1/1046 (0.1%)	0.81	3/1412 (0.2%)
All	All	0.39	6/6306 (0.1%)	0.86	21/8510 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	3137	VAL	C-N	-5.82	1.25	1.33
1	A	1137	VAL	C-N	-5.71	1.25	1.33
1	F	6137	VAL	C-N	-5.66	1.25	1.33
1	E	5138	SER	C-N	-5.58	1.25	1.33
1	D	4138	SER	C-N	-5.56	1.25	1.33

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3109	VAL	N-CA-C	-8.02	98.30	108.89
1	B	2094	TYR	N-CA-C	-7.92	99.10	110.59
1	E	5109	VAL	N-CA-C	-7.76	98.66	109.21
1	B	2109	VAL	N-CA-C	-7.45	99.06	108.89
1	F	6109	VAL	N-CA-C	-7.17	99.42	108.89

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	24	0
1	B	1023	0	1007	25	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	31	0
2	C	15	0	9	4	0
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	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 13.

The worst 5 of 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)
2:D:5139:N2M:N	2:D:5139:N2M:C5	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

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	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%)	16	11
1	F	127/139 (91%)	119 (94%)	7 (6%)	1 (1%)	16	11
All	All	766/834 (92%)	742 (97%)	22 (3%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

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

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	112/122 (92%)	109 (97%)	3 (3%)	39	42
1	B	112/122 (92%)	110 (98%)	2 (2%)	51	58
1	C	113/122 (93%)	110 (97%)	3 (3%)	39	42
1	D	113/122 (93%)	109 (96%)	4 (4%)	32	32
1	E	114/122 (93%)	110 (96%)	4 (4%)	32	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	112/122 (92%)	111 (99%)	1 (1%)	70	78
All	All	676/732 (92%)	659 (98%)	17 (2%)	42	45

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	5089	LEU
1	F	6045	GLN
1	C	3090	GLU
1	D	4072	LEU
1	D	4080	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	4063	GLN
1	F	6045	GLN
1	D	4092	ASN
1	E	5095	ASN
1	D	4080	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	5139	-	16,16,16	4.41	7 (43%)	23,24,24	2.23	5 (21%)
2	N2M	C	4138	-	16,16,16	4.39	7 (43%)	23,24,24	2.14	5 (21%)

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	D	5139	-	-	0/6/6/6	0/2/2/2
2	N2M	C	4138	-	-	0/6/6/6	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5139	N2M	C5-N	11.42	1.79	1.38
2	C	4138	N2M	C5-N	11.32	1.79	1.38
2	D	5139	N2M	O3S-S	6.80	1.76	1.43
2	C	4138	N2M	O3S-S	6.79	1.76	1.43
2	D	5139	N2M	O2S-S	6.35	1.74	1.43

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	5139	N2M	O1S-S-C2	8.07	127.48	106.64
2	C	4138	N2M	O1S-S-C2	7.61	126.29	106.64
2	C	4138	N2M	C6-C5-C10	2.75	123.03	119.38
2	D	5139	N2M	C6-C5-C10	2.73	122.99	119.38
2	D	5139	N2M	C3-C2-C1	-2.57	117.63	121.14

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	D	5139	N2M	4	0
2	C	4138	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 [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	129/139 (92%)	0.59	10 (7%) 19 18	17, 32, 47, 55	6 (4%)
1	B	129/139 (92%)	0.49	9 (6%) 22 21	19, 30, 46, 54	5 (3%)
1	C	130/139 (93%)	0.16	4 (3%) 51 50	17, 26, 42, 51	3 (2%)
1	D	130/139 (93%)	0.77	13 (10%) 12 11	17, 31, 51, 61	7 (5%)
1	E	131/139 (94%)	0.76	15 (11%) 9 8	22, 35, 49, 61	7 (5%)
1	F	129/139 (92%)	1.52	37 (28%) 1 1	27, 43, 61, 65	11 (8%)
All	All	778/834 (93%)	0.71	88 (11%) 10 9	17, 33, 52, 65	39 (5%)

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4051	VAL	4.9
1	D	4010	LYS	4.4
1	F	6048	ALA	4.2
1	D	4092	ASN	3.9
1	A	1093	HIS	3.8

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors($\text{\AA}^2$)	Q<0.9
2	N2M	D	5139	15/15	0.55	0.28	68,68,69,69	0
2	N2M	C	4138	15/15	0.64	0.27	63,64,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.