



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 07:55 AM UTC

PDB ID : 3RMX / pdb_00003rmx
Title : Crystal structure of HCR/D F1240A mutant
Authors : Fu, Z.; Karalewitz, A.; Kroken, A.; Kim, J.-J.P.; Barbieri, J.T.
Deposited on : 2011-04-21
Resolution : 2.75 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
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

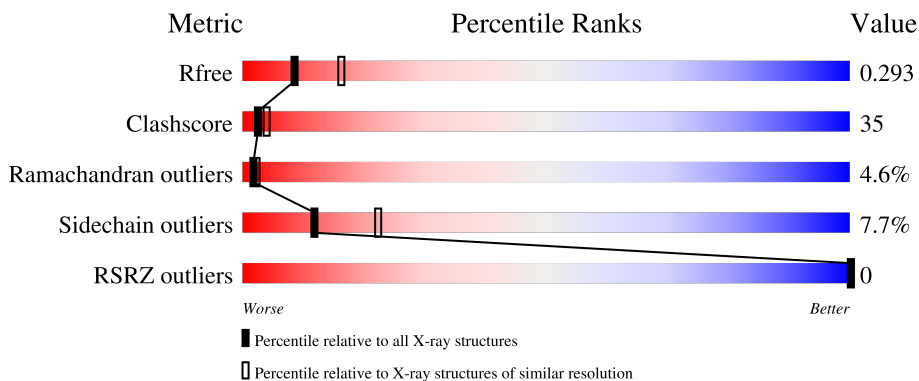
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


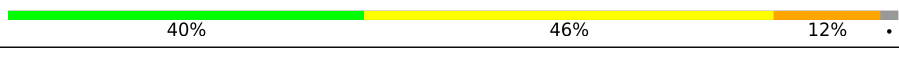
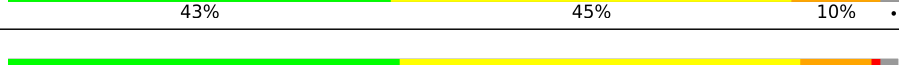

The reported resolution of this entry is 2.75 Å.

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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	415	
1	B	415	
1	C	415	
1	D	415	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 13363 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 Botulinum neurotoxin type D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	404	3317	2119	548	640	10	0	0	0
1	B	407	3336	2131	551	644	10	0	0	0
1	C	403	3304	2111	547	636	10	0	0	0
1	D	406	3333	2131	550	642	10	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1240	ALA	PHE	engineered mutation	UNP P19321
B	1240	ALA	PHE	engineered mutation	UNP P19321
C	1240	ALA	PHE	engineered mutation	UNP P19321
D	1240	ALA	PHE	engineered mutation	UNP P19321

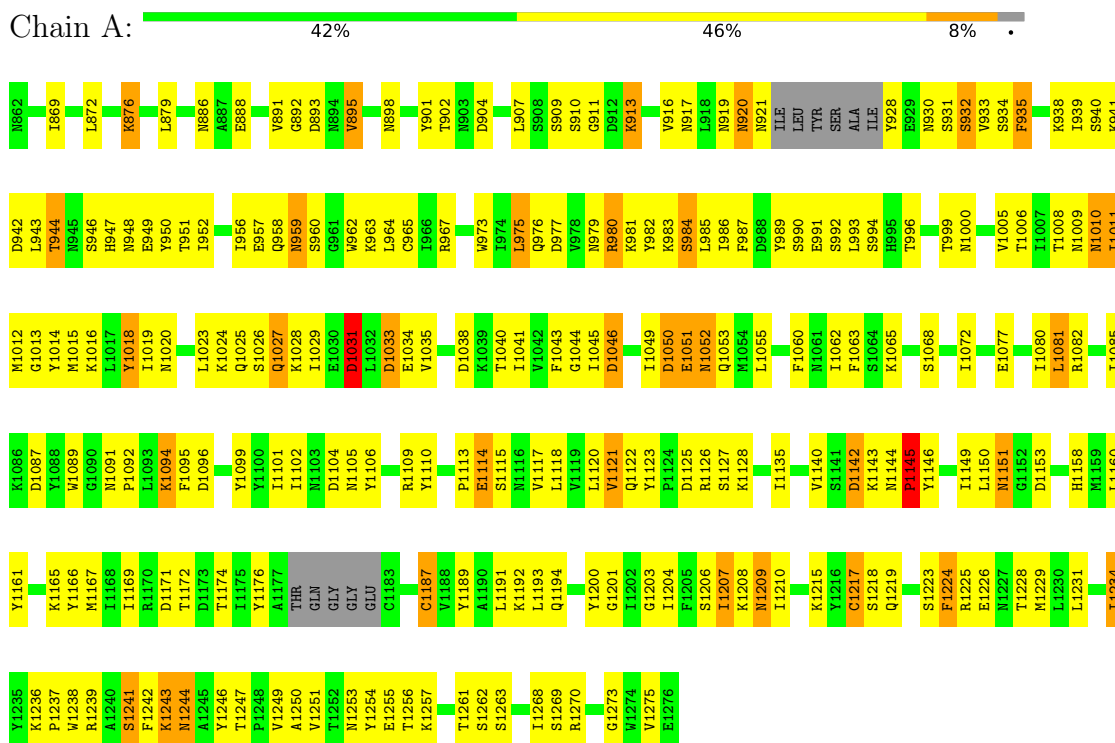
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	18	Total	O	0	0
			18	18		
2	C	17	Total	O	0	0
			17	17		
2	D	19	Total	O	0	0
			19	19		

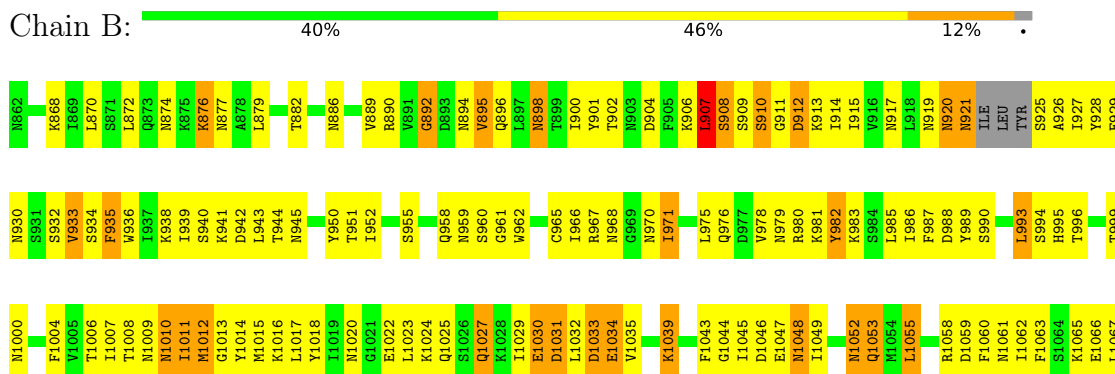
3 Residue-property plots [i](#)

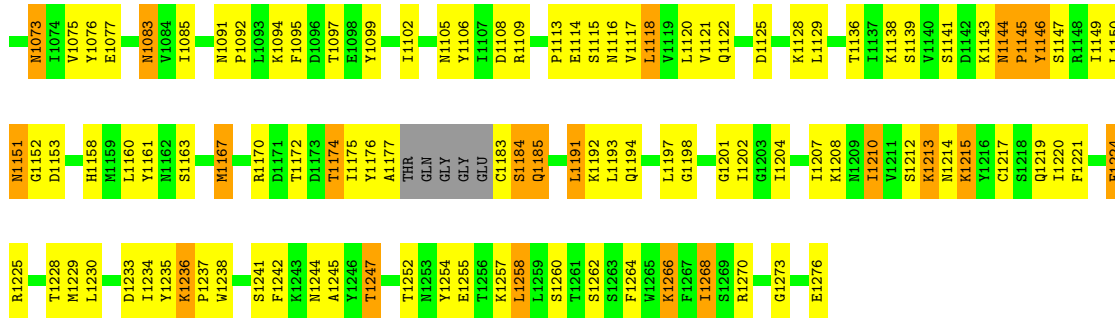
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



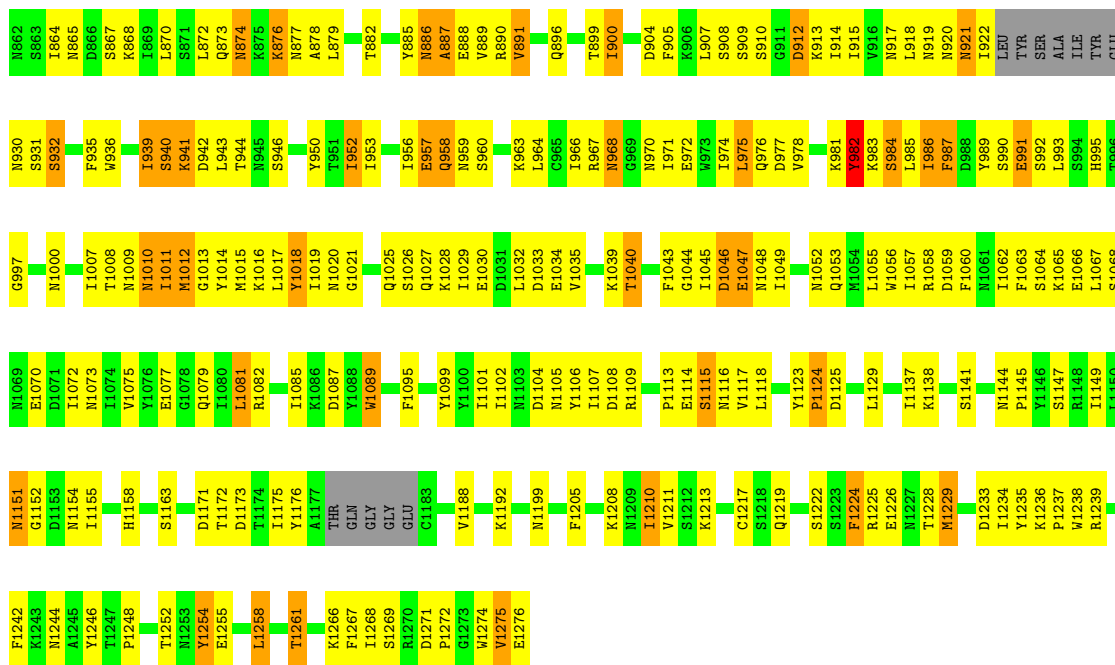
• Molecule 1: Botulinum neurotoxin type D





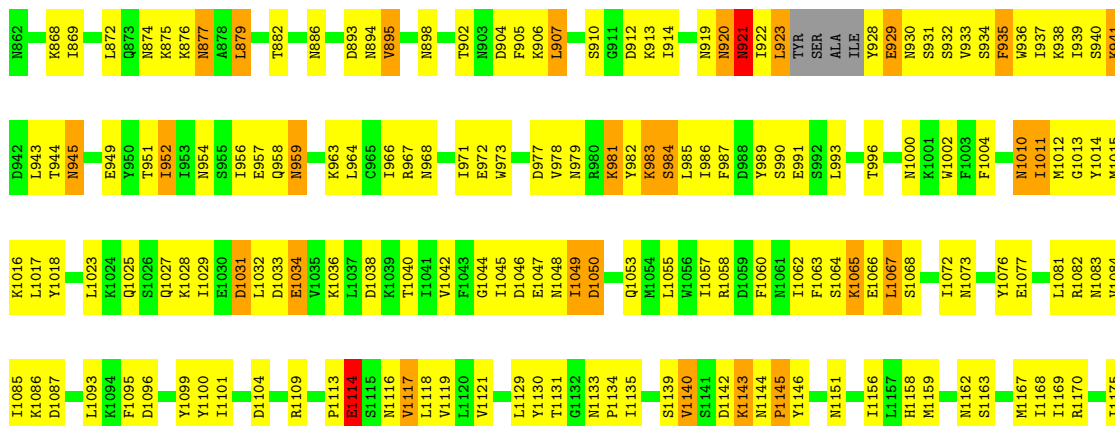
• Molecule 1: Botulinum neurotoxin type D

Chain C: 43% 45% 10%



• Molecule 1: Botulinum neurotoxin type D

Chain D: 44% 45% 8%



Y1176	Y1177	THR	GLN	GLY	GLY	GLU	C1183	S1184	Q1185	N1186	C1187	V1188	Y1189	A1190	L1191	K1192	L1193	Q1194	S1195	N1196	L1197	G1198	N1199	I1202	G1203	I1204	F1205	S1206	N1209	I1210	K1213	N1214	K1215	Y1216	C1217	S1218	Q1219	S1222	S1223	F1224	R1225	E1226	N1227	T1228	M1229	L1230	L1231	K1236	P1237	A1240	S1241	F1242	K1243
M1244	A1245	Y1246	T1247	P1248	V1249	A1250	V1251	T1252	N1253	Y1254	E1255	T1256	K1257	L1258	F1264	F1267	I1268	S1269	R1270	G1273	W1274	Y1275	E1276																														

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.57Å 115.63Å 107.24Å 90.00° 91.91° 90.00°	Depositor
Resolution (Å)	36.61 – 2.75 36.61 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.3 (36.61-2.75) 96.3 (36.61-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.03 (at 2.72Å)	Xtrriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.239 , 0.293 0.238 , 0.293	Depositor DCC
R_{free} test set	5885 reflections (10.15%)	wwPDB-VP
Wilson B-factor (Å ²)	56.7	Xtrriage
Anisotropy	0.174	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.077 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13363	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.49	0/3385	0.99	16/4583 (0.3%)
1	B	0.51	0/3404	1.00	15/4609 (0.3%)
1	C	0.46	0/3371	0.95	12/4564 (0.3%)
1	D	0.50	0/3401	0.96	14/4605 (0.3%)
All	All	0.49	0/13561	0.97	57/18361 (0.3%)

There are no bond length outliers.

The worst 5 of 57 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1252	THR	N-CA-C	9.19	124.03	113.01
1	B	1039	LYS	N-CA-C	-8.63	101.52	114.64
1	C	1152	GLY	N-CA-C	-8.46	103.70	114.37
1	D	1236	LYS	CA-C-N	7.19	127.03	119.05
1	D	1236	LYS	C-N-CA	7.19	127.03	119.05

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	3317	0	3260	210	0
1	B	3336	0	3281	269	0
1	C	3304	0	3256	242	0
1	D	3333	0	3282	199	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	19	0	0	0	0
2	B	18	0	0	2	0
2	C	17	0	0	1	0
2	D	19	0	0	1	0
All	All	13363	0	13079	911	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 35.

The worst 5 of 911 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:910:SER:HB3	1:B:1048:ASN:HA	1.36	1.08
1:B:1114:GLU:HG3	1:B:1115:SER:H	1.10	1.07
1:B:943:LEU:HD13	1:B:1053:GLN:HE22	1.17	1.05
1:B:927:ILE:HG22	1:B:1029:ILE:HD13	1.37	1.05
1:C:958:GLN:HG2	1:C:959:ASN:H	1.19	1.04

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	398/415 (96%)	328 (82%)	53 (13%)	17 (4%)	2	3
1	B	401/415 (97%)	327 (82%)	57 (14%)	17 (4%)	2	3
1	C	397/415 (96%)	326 (82%)	52 (13%)	19 (5%)	2	2
1	D	400/415 (96%)	340 (85%)	39 (10%)	21 (5%)	1	2
All	All	1596/1660 (96%)	1321 (83%)	201 (13%)	74 (5%)	2	2

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	LYS
1	A	920	ASN
1	A	1127	SER
1	A	1142	ASP
1	A	1224	PHE

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	378/386 (98%)	351 (93%)	27 (7%)	13	25
1	B	380/386 (98%)	343 (90%)	37 (10%)	8	15
1	C	377/386 (98%)	356 (94%)	21 (6%)	19	36
1	D	380/386 (98%)	349 (92%)	31 (8%)	10	20
All	All	1515/1544 (98%)	1399 (92%)	116 (8%)	12	22

5 of 116 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1191	LEU
1	D	1206	SER
1	C	1010	ASN
1	D	1185	GLN
1	D	1011	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	958	GLN
1	C	1244	ASN
1	C	995	HIS
1	C	1073	ASN
1	D	919	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](#)

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	404/415 (97%)	-1.35	0 100 100	28, 60, 94, 106	0
1	B	407/415 (98%)	-1.36	0 100 100	29, 55, 91, 104	0
1	C	403/415 (97%)	-1.26	0 100 100	33, 68, 107, 120	0
1	D	406/415 (97%)	-1.35	0 100 100	31, 60, 96, 105	0
All	All	1620/1660 (97%)	-1.33	0 100 100	28, 61, 100, 120	0

There are no RSRZ outliers to report.

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.