



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:57 PM GMT

PDB ID : 4DYA
Title : Crystal Structure of WSN/A Influenza Nucleoprotein with BMS-885986 Lig-
and Bound
Authors : Lewis, H.A.; Baldwin, E.T.; Steinbacher, S.; Maskos, K.; Mortl, M.; Kiefer-
sauer, R.; Edavettal, S.; McDonnell, P.A.; Pearce, B.C.; Langley, D.R.
Deposited on : 2012-02-28
Resolution : 2.75 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

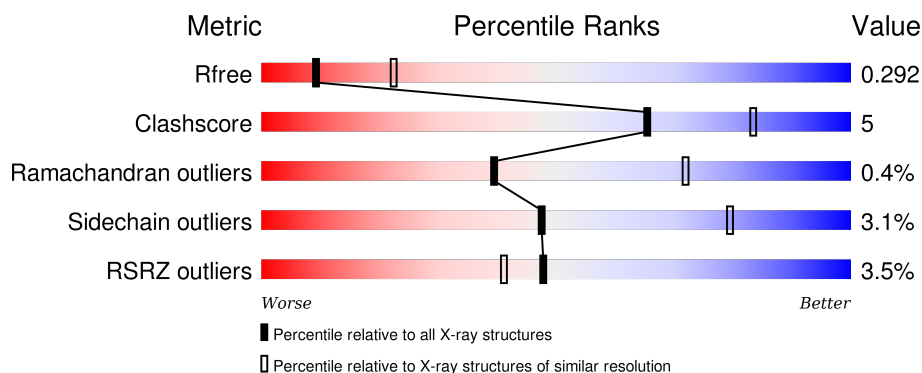
1 Overall quality at a glance

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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 $\leq 5\%$. 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	499	<div> <div></div> <div>75%</div> <div>10%</div> <div>14%</div> </div>
1	B	499	<div> <div>5%</div> <div>76%</div> <div>9%</div> <div>15%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6273 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.

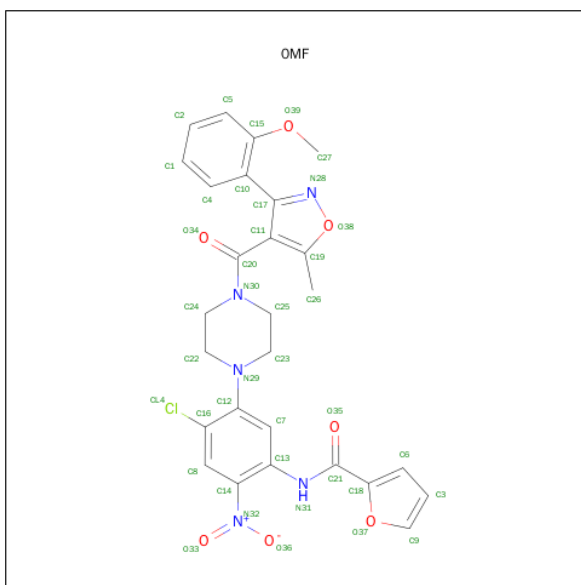
- Molecule 1 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3201	2015	558	603	25			
1	B	422	Total	C	N	O	S	0	0	0
			2969	1863	511	571	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	LEU	-	EXPRESSION TAG	UNP B4URF1
A	500	GLU	-	EXPRESSION TAG	UNP B4URF1
A	501	HIS	-	EXPRESSION TAG	UNP B4URF1
A	502	HIS	-	EXPRESSION TAG	UNP B4URF1
A	503	HIS	-	EXPRESSION TAG	UNP B4URF1
A	504	HIS	-	EXPRESSION TAG	UNP B4URF1
A	505	HIS	-	EXPRESSION TAG	UNP B4URF1
A	506	HIS	-	EXPRESSION TAG	UNP B4URF1
B	499	LEU	-	EXPRESSION TAG	UNP B4URF1
B	500	GLU	-	EXPRESSION TAG	UNP B4URF1
B	501	HIS	-	EXPRESSION TAG	UNP B4URF1
B	502	HIS	-	EXPRESSION TAG	UNP B4URF1
B	503	HIS	-	EXPRESSION TAG	UNP B4URF1
B	504	HIS	-	EXPRESSION TAG	UNP B4URF1
B	505	HIS	-	EXPRESSION TAG	UNP B4URF1
B	506	HIS	-	EXPRESSION TAG	UNP B4URF1

- Molecule 2 is N-[4-CHLORANYL-5-[4-[[3-(2-METHOXYPHENYL)-5-METHYL-1,2-OXAZOL-4-YL]CARBONYL]PIPERAZIN-1-YL]-2-NITRO-PHENYL]FURAN-2-CARBOXAMIDE (three-letter code: 0MF) (formula: C₂₇H₂₄ClN₅O₇).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 39	C 26	Cl 1	N 5	O 7	0	0
2	B	1	Total 40	C 27	Cl 1	N 5	O 7	0	0

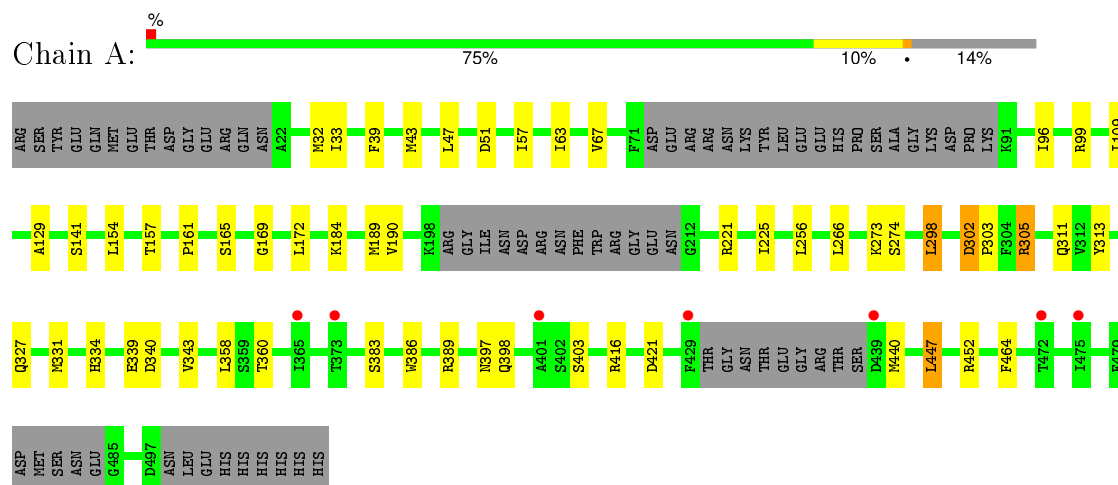
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	17	Total O 17 17	0	0
3	B	7	Total O 7 7	0	0

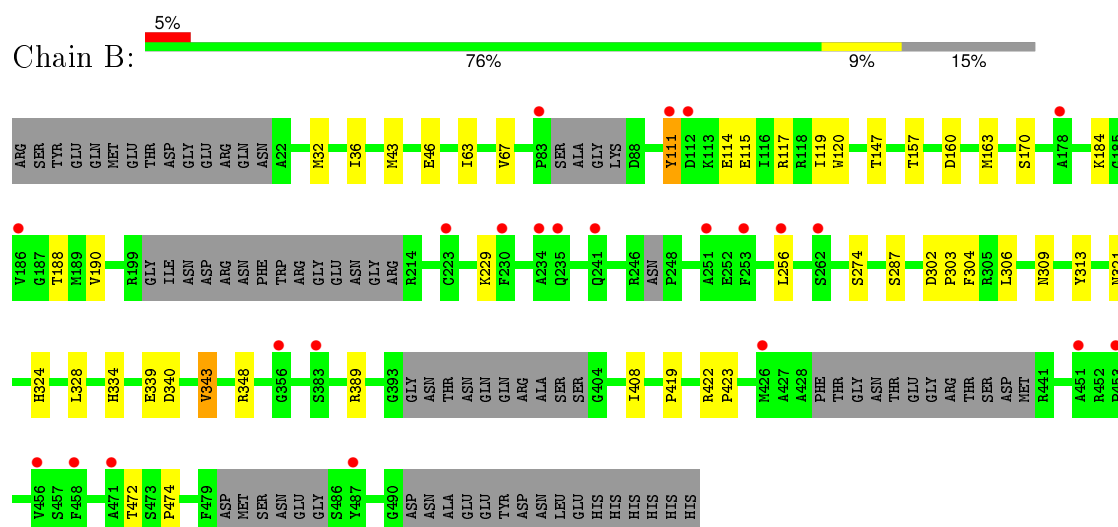
3 Residue-property plots [i](#)

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: Nucleocapsid protein



• Molecule 1: Nucleocapsid protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	145.50Å 145.50Å 145.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.51 – 2.75 48.50 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.51-2.75) 99.8 (48.50-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.252 , 0.298 0.249 , 0.292	Depositor DCC
R_{free} test set	1062 reflections (4.12%)	DCC
Wilson B-factor (Å ²)	55.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.5	EDS
Estimated twinning fraction	0.036 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 26867 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6273	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% 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, 0.375 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: 0MF

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	0.33	0/3256	0.48	0/4404
1	B	0.32	0/3021	0.46	0/4108
All	All	0.32	0/6277	0.47	0/8512

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	3201	0	3031	30	0
1	B	2969	0	2612	27	0
2	A	39	0	21	7	0
2	B	40	0	24	7	0
3	A	17	0	0	1	0
3	B	7	0	0	0	0
All	All	6273	0	5688	60	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 5.

All (60) 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:A:311:GLN:HE22	1:B:309:ASN:HA	1.56	0.70
1:A:96:ILE:HD12	1:A:109:ILE:HG12	1.77	0.67
2:A:601:0MF:O35	2:A:601:0MF:H7	1.94	0.66
2:A:601:0MF:H20	1:B:313:TYR:CG	2.32	0.65
1:B:304:PHE:HE2	1:B:389:ARG:HH12	1.44	0.65
2:A:601:0MF:C10	2:A:601:0MF:H17	2.28	0.63
2:A:601:0MF:C17	2:A:601:0MF:H17	2.29	0.61
1:B:408:ILE:HD12	1:B:419:PRO:HG2	1.84	0.59
1:A:273:LYS:HD3	1:A:298:LEU:HD23	1.86	0.58
1:B:472:THR:O	1:B:474:PRO:HD3	2.04	0.56
1:A:311:GLN:NE2	1:B:309:ASN:HA	2.20	0.56
1:A:302:ASP:HB2	1:A:303:PRO:HD3	1.85	0.56
1:B:36:ILE:HD13	1:B:120:TRP:HH2	1.71	0.54
1:B:306:LEU:HD13	2:B:601:0MF:H8	1.89	0.54
2:B:601:0MF:O35	2:B:601:0MF:H7	2.08	0.54
2:B:601:0MF:C10	2:B:601:0MF:H17	2.37	0.53
1:A:184:LYS:HD3	1:A:189:MET:CE	2.38	0.53
1:A:340:ASP:HB3	1:A:343:VAL:HG13	1.90	0.52
1:A:43:MET:HG2	1:A:63:ILE:HG23	1.91	0.52
2:B:601:0MF:H17	2:B:601:0MF:C17	2.40	0.51
1:A:221:ARG:O	1:A:225:ILE:HG12	2.10	0.51
1:B:302:ASP:HB2	1:B:303:PRO:HD3	1.92	0.49
1:A:274:SER:OG	1:A:334:HIS:HD2	1.95	0.49
1:A:305:ARG:HE	2:A:601:0MF:C21	2.25	0.49
1:A:141:SER:OG	1:A:169:GLY:HA2	2.13	0.49
1:A:358:LEU:HB3	1:A:360:THR:HG22	1.95	0.48
1:A:190:VAL:HG13	1:A:256:LEU:HB3	1.95	0.48
1:B:43:MET:HG2	1:B:63:ILE:HG23	1.96	0.48
1:B:114:GLU:HA	1:B:117:ARG:HE	1.79	0.47
1:A:397:ASN:HA	3:A:714:HOH:O	2.15	0.47
1:B:147:THR:HA	1:B:328:LEU:HD11	1.97	0.46
1:B:321:ASN:HD22	1:B:324:HIS:CE1	2.34	0.46
1:A:266:LEU:HD11	1:A:447:LEU:HB3	1.97	0.46
1:A:184:LYS:HD3	1:A:189:MET:HE1	1.97	0.46
1:B:184:LYS:O	1:B:229:LYS:NZ	2.42	0.46
1:A:32:MET:HG3	1:A:33:ILE:HD12	1.98	0.46
1:B:32:MET:O	1:B:36:ILE:HG12	2.15	0.46
1:A:313:TYR:CG	2:B:601:0MF:H20	2.51	0.45
2:A:601:0MF:H20	1:B:313:TYR:CD2	2.52	0.45
1:B:190:VAL:HG13	1:B:256:LEU:HB3	1.98	0.45
1:B:422:ARG:N	1:B:423:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ASP:HB3	1:B:287:SER:HA	1.99	0.45
1:A:327:GLN:O	1:A:331:MET:HG3	2.17	0.45
1:B:46:GLU:HB3	1:B:111:TYR:OH	2.17	0.44
1:A:141:SER:HB2	1:A:172:LEU:HD13	1.99	0.44
1:B:160:ASP:HB3	1:B:163:MET:HG3	1.99	0.44
1:A:154:LEU:HD13	1:A:161:PRO:HA	1.98	0.44
1:B:115:GLU:O	1:B:119:ILE:HG12	2.19	0.43
1:B:170:SER:HA	1:B:188:THR:HG23	2.01	0.43
1:A:386:TRP:NE1	1:A:464:PHE:HB2	2.33	0.43
1:A:47:LEU:HD13	1:A:96:ILE:HD13	1.99	0.42
1:A:421:ASP:OD2	1:A:452:ARG:NH2	2.52	0.42
1:A:39:PHE:CZ	1:A:67:VAL:HB	2.55	0.41
1:A:305:ARG:HD3	2:A:601:OMF:C18	2.50	0.41
1:B:274:SER:OG	1:B:334:HIS:HD2	2.03	0.41
1:B:309:ASN:OD1	2:B:601:OMF:H15	2.21	0.41
1:B:340:ASP:HB3	1:B:343:VAL:HG13	2.02	0.41
1:A:99:ARG:CZ	2:B:601:OMF:H22	2.51	0.40
1:B:36:ILE:HD13	1:B:120:TRP:CH2	2.55	0.40
1:A:184:LYS:HD3	1:A:189:MET:HE3	2.02	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	420/499 (84%)	404 (96%)	13 (3%)	3 (1%)	26	59
1	B	408/499 (82%)	394 (97%)	14 (3%)	0	100	100
All	All	828/998 (83%)	798 (96%)	27 (3%)	3 (0%)	39	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ALA
1	A	403	SER
1	A	398	GLN

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	313/425 (74%)	301 (96%)	12 (4%)	40	73
1	B	265/425 (62%)	259 (98%)	6 (2%)	58	87
All	All	578/850 (68%)	560 (97%)	18 (3%)	47	79

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ILE
1	A	157	THR
1	A	165	SER
1	A	298	LEU
1	A	302	ASP
1	A	305	ARG
1	A	339	GLU
1	A	383	SER
1	A	389	ARG
1	A	416	ARG
1	A	440	MET
1	A	447	LEU
1	B	67	VAL
1	B	111	TYR
1	B	157	THR
1	B	339	GLU
1	B	343	VAL
1	B	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	144	ASN
1	A	250	ASN
1	A	309	ASN
1	A	311	GLN
1	A	334	HIS
1	A	409	GLN
1	B	144	ASN
1	B	235	GLN
1	B	334	HIS

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 carbohydrates 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	0MF	A	601	-	35,43,44	1.17	3 (8%)	40,62,63	1.30	5 (12%)
2	0MF	B	601	-	36,44,44	1.18	4 (11%)	41,63,63	1.44	8 (19%)

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	OMF	A	601	-	-	0/18/38/40	0/3/5/5
2	OMF	B	601	-	-	0/20/40/40	0/3/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	OMF	C10-C17	-4.85	1.44	1.49
2	A	601	OMF	C10-C17	-4.49	1.44	1.49
2	A	601	OMF	C11-C20	-2.72	1.47	1.51
2	B	601	OMF	C11-C20	-2.20	1.48	1.51
2	B	601	OMF	C21-N31	2.11	1.41	1.35
2	A	601	OMF	C20-N30	2.27	1.39	1.34
2	B	601	OMF	C20-N30	2.57	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	OMF	O39-C15-C5	-3.28	118.83	124.35
2	A	601	OMF	C7-C12-N29	-2.97	118.69	122.72
2	B	601	OMF	C7-C12-N29	-2.54	119.28	122.72
2	A	601	OMF	C8-C14-C13	-2.29	119.67	121.62
2	B	601	OMF	O34-C20-C11	-2.11	115.11	119.19
2	B	601	OMF	C4-C10-C15	2.04	120.05	117.36
2	A	601	OMF	C12-C16-CL4	2.23	122.05	120.18
2	A	601	OMF	C16-C12-N29	2.38	122.01	119.97
2	B	601	OMF	C17-C11-C20	2.55	132.22	126.03
2	B	601	OMF	C7-C13-C14	2.67	120.32	116.57
2	A	601	OMF	C7-C13-C14	2.74	120.42	116.57
2	B	601	OMF	O39-C15-C10	3.10	121.25	116.30
2	B	601	OMF	C11-C20-N30	3.24	121.13	117.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	OMF	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	0MF	7	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, 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	430/499 (86%)	0.21	7 (1%) 74 70	29, 42, 57, 64	0
1	B	422/499 (84%)	0.44	23 (5%) 29 22	33, 54, 78, 84	0
All	All	852/998 (85%)	0.32	30 (3%) 48 41	29, 47, 75, 84	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	230	PHE	2.9
1	A	401	ALA	2.9
1	B	471	ALA	2.9
1	A	373	THR	2.8
1	B	256	LEU	2.8
1	B	251	ALA	2.8
1	B	83	PRO	2.7
1	B	458	PHE	2.7
1	B	223	CYS	2.6
1	B	178	ALA	2.6
1	B	253	PHE	2.6
1	B	456	VAL	2.6
1	A	429	PHE	2.6
1	A	365	ILE	2.5
1	B	426	MET	2.5
1	B	487	TYR	2.3
1	A	439	ASP	2.3
1	B	356	GLY	2.3
1	B	451	ALA	2.3
1	B	234	ALA	2.2
1	A	475	ILE	2.2
1	B	235	GLN	2.1
1	B	262	SER	2.1
1	B	383	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	472	THR	2.1
1	B	241	GLN	2.1
1	B	111	TYR	2.1
1	B	186	VAL	2.0
1	B	453	PRO	2.0
1	B	112	ASP	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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	0MF	A	601	39/40	0.95	0.20	0.37	34,35,36,37	0
2	0MF	B	601	40/40	0.94	0.17	-0.57	36,41,43,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.