



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:55 am GMT

PDB ID : 3RO5
Title : Crystal structure of influenza A virus nucleoprotein with ligand
Authors : Pearce, B.C.; Edavettal, S.; McDonnell, P.A.; Lewis, H.A.; Steinbacher, S.; Baldwin, E.T.; Langley, D.R.; Maskos, K.; Mortl, M.; Kiefersauer, R.
Deposited on : 2011-04-25
Resolution : 2.66 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

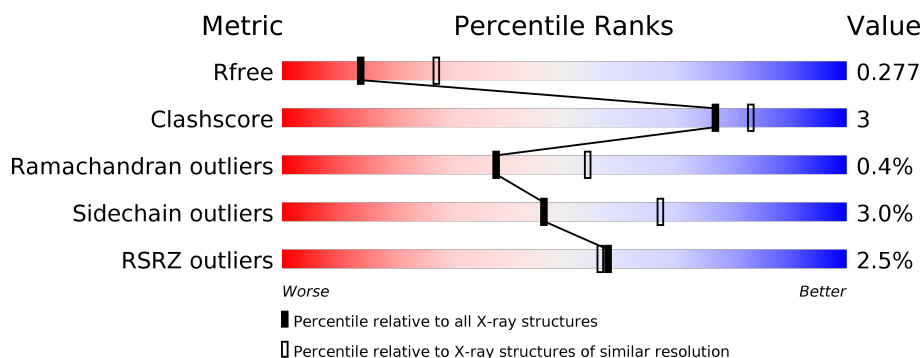
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.66 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}	100719	3491 (2.70-2.62)
Clashscore	112137	1026 (2.68-2.64)
Ramachandran outliers	110173	1010 (2.68-2.64)
Sidechain outliers	110143	1010 (2.68-2.64)
RSRZ outliers	101464	3511 (2.70-2.62)

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 style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 10%, yellow 20%, green 79%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">79% 7% 14%</div> </div> </div>
1	B	499	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0;">3%</div> <div style="position: absolute; top: 0; left: 0; width: 100%; height: 100%; background: linear-gradient(to right, red 0%, orange 3%, yellow 5%, green 79%, grey 100%);"></div> <div style="position: absolute; bottom: -10px; left: 0;">79% 5% 15%</div> </div> </div>

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	LGH	B	1	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6341 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.

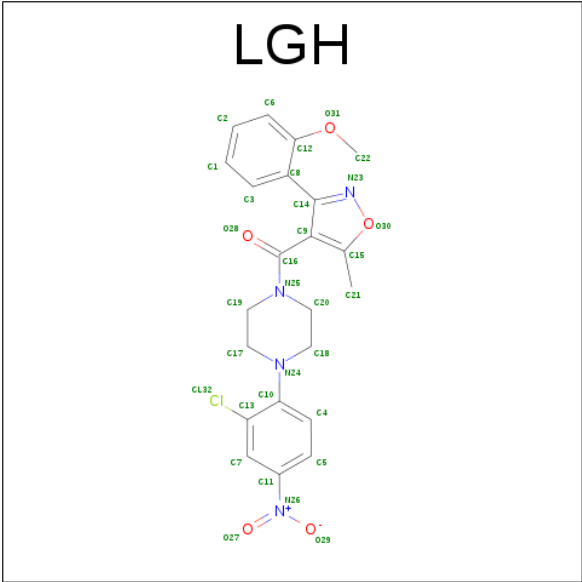
- Molecule 1 is a protein called Nucleocapsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3224	2030	561	608	25			
1	B	423	Total	C	N	O	S	0	0	0
			3023	1899	521	579	24			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	499	LEU	-	EXPRESSION TAG	UNP Q1K9H2
A	500	GLU	-	EXPRESSION TAG	UNP Q1K9H2
A	501	HIS	-	EXPRESSION TAG	UNP Q1K9H2
A	502	HIS	-	EXPRESSION TAG	UNP Q1K9H2
A	503	HIS	-	EXPRESSION TAG	UNP Q1K9H2
A	504	HIS	-	EXPRESSION TAG	UNP Q1K9H2
A	505	HIS	-	EXPRESSION TAG	UNP Q1K9H2
A	506	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	499	LEU	-	EXPRESSION TAG	UNP Q1K9H2
B	500	GLU	-	EXPRESSION TAG	UNP Q1K9H2
B	501	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	502	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	503	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	504	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	505	HIS	-	EXPRESSION TAG	UNP Q1K9H2
B	506	HIS	-	EXPRESSION TAG	UNP Q1K9H2

- Molecule 2 is [4-(2-CHLORO-4-NITROPHENYL)PIPERAZIN-1-YL][3-(2-METHOXY-PHENYL)-5-METHYL-1,2-OXAZOL-4-YL]METHANONE (three-letter code: LGH) (formula: C₂₂H₂₁ClN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total 32	C 22	Cl 1	N 4	O 5	0	0
2	B	1	Total 32	C 22	Cl 1	N 4	O 5	0	0

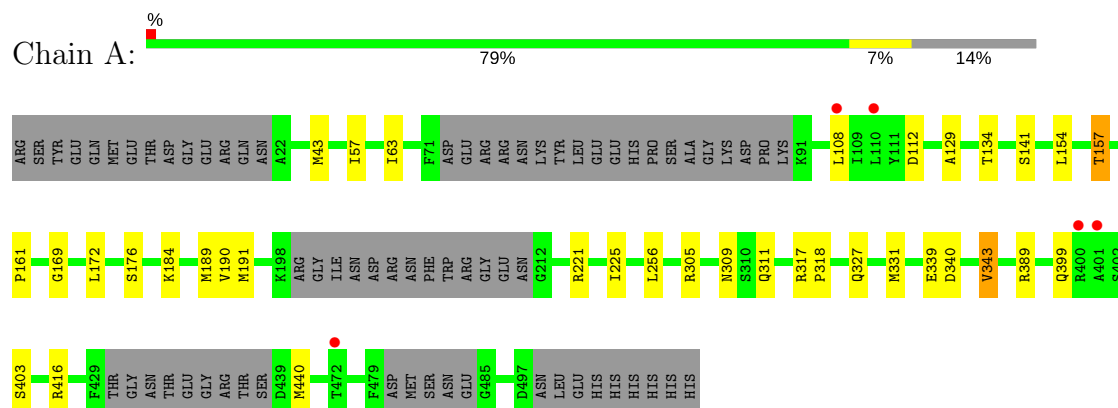
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	7	Total	O	0	0
			7	7		

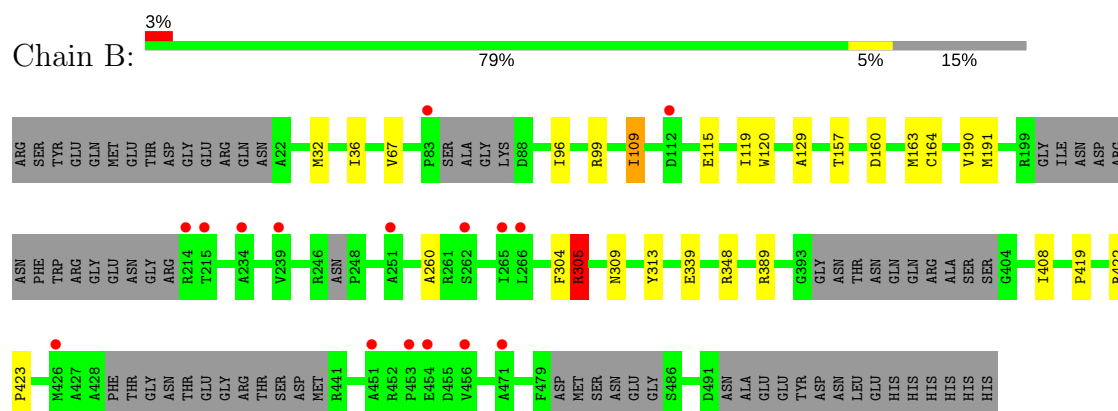
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: 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	146.20Å 146.20Å 146.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.70 – 2.66 48.73 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.70-2.66) 99.9 (48.73-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.245 , 0.280 0.244 , 0.277	Depositor DCC
R_{free} test set	1527 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	54.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6341	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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, 0.333 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: LGH

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	0.34	0/3279	0.48	0/4433
1	B	0.33	0/3075	0.46	0/4178
All	All	0.33	0/6354	0.47	0/8611

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	305	ARG	Sidechain

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	3224	0	3082	23	0
1	B	3023	0	2731	16	0
2	B	64	0	42	16	0
3	A	23	0	0	0	0
3	B	7	0	0	0	0
All	All	6341	0	5855	42	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 3.

All (42) 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:305:ARG:HD2	2:B:1:LGH:C5	1.82	1.08
1:A:305:ARG:HD2	2:B:1:LGH:H5	1.59	0.84
1:A:305:ARG:CD	2:B:1:LGH:C5	2.67	0.72
1:B:96:ILE:HD12	1:B:109:ILE:HG21	1.82	0.60
1:B:304:PHE:HE2	1:B:389:ARG:HH12	1.48	0.59
1:A:311:GLN:HE22	1:B:309:ASN:HA	1.68	0.58
2:B:1:LGH:C8	2:B:1:LGH:H19A	2.33	0.58
1:B:99:ARG:CZ	2:B:1:LGH:H22A	2.33	0.58
2:B:1:LGH:H19A	2:B:1:LGH:C14	2.34	0.57
1:B:408:ILE:HD12	1:B:419:PRO:HG2	1.87	0.56
1:A:141:SER:HB2	1:A:172:LEU:HD13	1.87	0.56
1:B:99:ARG:NE	2:B:1:LGH:H22A	2.21	0.55
1:A:305:ARG:CD	2:B:1:LGH:C4	2.85	0.55
1:B:305:ARG:NH1	2:B:2:LGH:H5	2.23	0.53
1:A:305:ARG:HD2	2:B:1:LGH:C4	2.38	0.53
1:A:189:MET:HE2	1:A:189:MET:HA	1.90	0.53
1:A:184:LYS:HD3	1:A:189:MET:HE1	1.90	0.52
2:B:2:LGH:C14	2:B:2:LGH:H19A	2.40	0.52
1:A:141:SER:OG	1:A:169:GLY:HA2	2.10	0.52
2:B:2:LGH:H19A	2:B:2:LGH:C8	2.42	0.49
1:A:309:ASN:ND2	2:B:1:LGH:H20A	2.28	0.49
1:A:305:ARG:HD3	2:B:1:LGH:C4	2.43	0.49
1:B:157:THR:HG21	1:B:191:MET:HG3	1.95	0.48
1:B:115:GLU:O	1:B:119:ILE:HG12	2.13	0.48
1:A:43:MET:HG2	1:A:63:ILE:HG23	1.94	0.48
1:A:221:ARG:O	1:A:225:ILE:HG12	2.14	0.48
1:A:311:GLN:NE2	1:B:309:ASN:HA	2.29	0.48
1:A:184:LYS:HD3	1:A:189:MET:CE	2.44	0.47
1:B:32:MET:O	1:B:36:ILE:HG12	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:ARG:N	1:B:423:PRO:HD2	2.31	0.45
1:A:189:MET:HA	1:A:189:MET:CE	2.47	0.44
1:A:340:ASP:HB3	1:A:343:VAL:HG13	1.99	0.44
1:B:313:TYR:CG	2:B:1:LGH:H21B	2.53	0.44
1:A:190:VAL:HG13	1:A:256:LEU:HB3	2.00	0.43
1:B:190:VAL:HG21	1:B:260:ALA:HB2	2.00	0.43
1:A:154:LEU:HD13	1:A:161:PRO:HA	1.99	0.43
1:A:327:GLN:O	1:A:331:MET:HG3	2.20	0.42
1:B:160:ASP:HB3	1:B:163:MET:HG3	2.02	0.42
2:B:2:LGH:H17A	2:B:2:LGH:CL32	2.57	0.41
1:B:36:ILE:HD13	1:B:120:TRP:HH2	1.85	0.41
1:A:317:ARG:HB3	1:A:318:PRO:HD2	2.03	0.41
1:A:157:THR:HG21	1:A:191:MET:HG3	2.03	0.40

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	420/499 (84%)	402 (96%)	16 (4%)	2 (0%)	32	49
1	B	409/499 (82%)	397 (97%)	11 (3%)	1 (0%)	51	69
All	All	829/998 (83%)	799 (96%)	27 (3%)	3 (0%)	38	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	ALA
1	A	129	ALA
1	A	403	SER

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	321/425 (76%)	309 (96%)	12 (4%)	39	59
1	B	282/425 (66%)	276 (98%)	6 (2%)	59	78
All	All	603/850 (71%)	585 (97%)	18 (3%)	46	67

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

Mol	Chain	Res	Type
1	A	57	ILE
1	A	108	LEU
1	A	112	ASP
1	A	134	THR
1	A	157	THR
1	A	176	SER
1	A	339	GLU
1	A	343	VAL
1	A	389	ARG
1	A	399	GLN
1	A	416	ARG
1	A	440	MET
1	B	67	VAL
1	B	109	ILE
1	B	164	CYS
1	B	305	ARG
1	B	339	GLU
1	B	348	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	309	ASN
1	A	334	HIS
1	A	409	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	334	HIS
1	B	370	ASN

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	LGH	B	1	-	31,35,35	1.27	4 (12%)	37,50,50	1.58	8 (21%)
2	LGH	B	2	-	31,35,35	1.29	3 (9%)	37,50,50	1.38	5 (13%)

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	LGH	B	1	-	-	0/14/32/32	0/3/4/4
2	LGH	B	2	-	-	0/14/32/32	0/3/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	LGH	C8-C14	-5.08	1.44	1.49
2	B	1	LGH	C8-C14	-4.83	1.44	1.49
2	B	1	LGH	C9-C16	-2.89	1.47	1.51
2	B	2	LGH	C9-C16	-2.53	1.47	1.51
2	B	1	LGH	C11-N26	-2.02	1.41	1.45
2	B	1	LGH	C16-N25	2.33	1.39	1.34
2	B	2	LGH	C16-N25	2.55	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	LGH	O31-C12-C6	-3.60	118.32	124.37
2	B	2	LGH	O31-C12-C6	-3.34	118.77	124.37
2	B	2	LGH	C4-C10-N24	-3.08	117.44	122.28
2	B	1	LGH	C4-C10-N24	-2.94	117.67	122.28
2	B	1	LGH	O28-C16-C9	-2.09	115.24	119.11
2	B	1	LGH	C14-C9-C16	2.04	131.01	126.08
2	B	1	LGH	C9-C16-N25	2.19	120.07	117.80
2	B	2	LGH	C18-N24-C17	2.33	116.50	111.57
2	B	2	LGH	C9-C16-N25	2.46	120.35	117.80
2	B	1	LGH	C5-C11-N26	2.75	121.50	119.41
2	B	2	LGH	O31-C12-C8	3.24	121.23	116.27
2	B	1	LGH	C10-C13-CL32	3.45	123.96	120.23
2	B	1	LGH	O31-C12-C8	3.65	121.86	116.27

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	LGH	12	0
2	B	2	LGH	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	0.10	5 (1%) 79 79	31, 44, 61, 69	0
1	B	423/499 (84%)	0.30	16 (3%) 41 39	33, 55, 82, 86	0
All	All	853/998 (85%)	0.20	21 (2%) 58 56	31, 49, 79, 86	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	83	PRO	3.9
1	B	453	PRO	3.9
1	A	401	ALA	3.6
1	A	472	THR	2.9
1	A	108	LEU	2.8
1	B	262	SER	2.7
1	B	426	MET	2.7
1	A	110	LEU	2.7
1	B	266	LEU	2.7
1	B	234	ALA	2.7
1	B	454	GLU	2.6
1	B	239	VAL	2.4
1	B	215	THR	2.4
1	B	214	ARG	2.3
1	B	456	VAL	2.3
1	B	265	ILE	2.2
1	A	400	ARG	2.2
1	B	112	ASP	2.1
1	B	251	ALA	2.1
1	B	471	ALA	2.1
1	B	451	ALA	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	LGH	B	1	32/32	0.95	0.17	0.01	33,34,36,36	0
2	LGH	B	2	32/32	0.93	0.16	-0.28	38,41,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.