wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 09:40 PM EDT

PDB ID	:	3IT8
Title	:	Crystal structure of TNF alpha complexed with a poxvirus MHC-related TNF binding protein
Authors	:	Yang, Z.; West Jr., A.P.; Bjorkman, P.J.
Deposited on	:	2009-08-27
Resolution	:	2.80 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 (i) 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 (1)) were used in the production of this report:

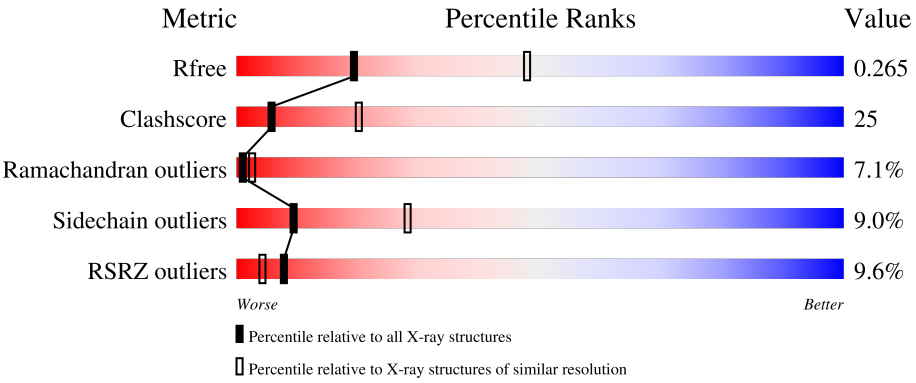
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	161	11% 51% 29% 14% • 6%
1	B	161	10% 53% 29% 12% • 6%
1	C	161	9% 51% 30% 12% • 6%
1	G	161	13% 48% 32% 13% • 6%
1	H	161	12% 52% 29% 13% • 6%

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Mol	Chain	Length	Quality of chain
1	I	161	11% 49% 33% 12% • 6%
2	D	324	6% 55% 31% 5% • 8%
2	E	324	6% 54% 31% 6% • 8%
2	F	324	9% 54% 32% 5% • 8%
2	J	324	6% 54% 31% 6% • 8%
2	K	324	6% 56% 30% 6% • 8%
2	L	324	15% 54% 32% 5% • 8%

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
3	NAG	F	327	-	-	-	X
3	NAG	J	327	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22002 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	B	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	C	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	G	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	H	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			
1	I	152	Total	C	N	O	S	0	0	0
			1190	760	207	221	2			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP P01375
A	-2	GLY	-	expression tag	UNP P01375
A	-1	SER	-	expression tag	UNP P01375
A	0	HIS	-	expression tag	UNP P01375
A	1	HIS	-	expression tag	UNP P01375
A	2	HIS	-	expression tag	UNP P01375
A	3	HIS	-	expression tag	UNP P01375
A	4	HIS	-	expression tag	UNP P01375
A	5	HIS	-	expression tag	UNP P01375
A	143	LEU	ASP	conflict	UNP P01375
B	-3	MET	-	expression tag	UNP P01375
B	-2	GLY	-	expression tag	UNP P01375
B	-1	SER	-	expression tag	UNP P01375
B	0	HIS	-	expression tag	UNP P01375
B	1	HIS	-	expression tag	UNP P01375
B	2	HIS	-	expression tag	UNP P01375
B	3	HIS	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
B	4	HIS	-	expression tag	UNP P01375
B	5	HIS	-	expression tag	UNP P01375
B	143	LEU	ASP	conflict	UNP P01375
C	-3	MET	-	expression tag	UNP P01375
C	-2	GLY	-	expression tag	UNP P01375
C	-1	SER	-	expression tag	UNP P01375
C	0	HIS	-	expression tag	UNP P01375
C	1	HIS	-	expression tag	UNP P01375
C	2	HIS	-	expression tag	UNP P01375
C	3	HIS	-	expression tag	UNP P01375
C	4	HIS	-	expression tag	UNP P01375
C	5	HIS	-	expression tag	UNP P01375
C	143	LEU	ASP	conflict	UNP P01375
G	-3	MET	-	expression tag	UNP P01375
G	-2	GLY	-	expression tag	UNP P01375
G	-1	SER	-	expression tag	UNP P01375
G	0	HIS	-	expression tag	UNP P01375
G	1	HIS	-	expression tag	UNP P01375
G	2	HIS	-	expression tag	UNP P01375
G	3	HIS	-	expression tag	UNP P01375
G	4	HIS	-	expression tag	UNP P01375
G	5	HIS	-	expression tag	UNP P01375
G	143	LEU	ASP	conflict	UNP P01375
H	-3	MET	-	expression tag	UNP P01375
H	-2	GLY	-	expression tag	UNP P01375
H	-1	SER	-	expression tag	UNP P01375
H	0	HIS	-	expression tag	UNP P01375
H	1	HIS	-	expression tag	UNP P01375
H	2	HIS	-	expression tag	UNP P01375
H	3	HIS	-	expression tag	UNP P01375
H	4	HIS	-	expression tag	UNP P01375
H	5	HIS	-	expression tag	UNP P01375
H	143	LEU	ASP	conflict	UNP P01375
I	-3	MET	-	expression tag	UNP P01375
I	-2	GLY	-	expression tag	UNP P01375
I	-1	SER	-	expression tag	UNP P01375
I	0	HIS	-	expression tag	UNP P01375
I	1	HIS	-	expression tag	UNP P01375
I	2	HIS	-	expression tag	UNP P01375
I	3	HIS	-	expression tag	UNP P01375
I	4	HIS	-	expression tag	UNP P01375
I	5	HIS	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
I	143	LEU	ASP	conflict	UNP P01375

- Molecule 2 is a protein called 2L protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	E	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	F	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	J	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	K	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			
2	L	299	Total	C	N	O	S	0	0	0
			2419	1545	395	466	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	317	GLY	-	expression tag	UNP Q9DHW0
D	318	SER	-	expression tag	UNP Q9DHW0
D	319	HIS	-	expression tag	UNP Q9DHW0
D	320	HIS	-	expression tag	UNP Q9DHW0
D	321	HIS	-	expression tag	UNP Q9DHW0
D	322	HIS	-	expression tag	UNP Q9DHW0
D	323	HIS	-	expression tag	UNP Q9DHW0
D	324	HIS	-	expression tag	UNP Q9DHW0
E	317	GLY	-	expression tag	UNP Q9DHW0
E	318	SER	-	expression tag	UNP Q9DHW0
E	319	HIS	-	expression tag	UNP Q9DHW0
E	320	HIS	-	expression tag	UNP Q9DHW0
E	321	HIS	-	expression tag	UNP Q9DHW0
E	322	HIS	-	expression tag	UNP Q9DHW0
E	323	HIS	-	expression tag	UNP Q9DHW0
E	324	HIS	-	expression tag	UNP Q9DHW0
F	317	GLY	-	expression tag	UNP Q9DHW0
F	318	SER	-	expression tag	UNP Q9DHW0
F	319	HIS	-	expression tag	UNP Q9DHW0
F	320	HIS	-	expression tag	UNP Q9DHW0
F	321	HIS	-	expression tag	UNP Q9DHW0

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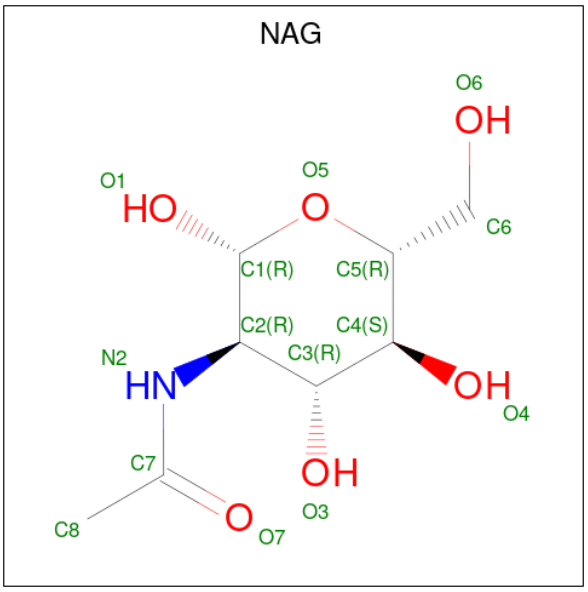
Chain	Residue	Modelled	Actual	Comment	Reference
F	322	HIS	-	expression tag	UNP Q9DHW0
F	323	HIS	-	expression tag	UNP Q9DHW0
F	324	HIS	-	expression tag	UNP Q9DHW0
J	317	GLY	-	expression tag	UNP Q9DHW0
J	318	SER	-	expression tag	UNP Q9DHW0
J	319	HIS	-	expression tag	UNP Q9DHW0
J	320	HIS	-	expression tag	UNP Q9DHW0
J	321	HIS	-	expression tag	UNP Q9DHW0
J	322	HIS	-	expression tag	UNP Q9DHW0
J	323	HIS	-	expression tag	UNP Q9DHW0
J	324	HIS	-	expression tag	UNP Q9DHW0
K	317	GLY	-	expression tag	UNP Q9DHW0
K	318	SER	-	expression tag	UNP Q9DHW0
K	319	HIS	-	expression tag	UNP Q9DHW0
K	320	HIS	-	expression tag	UNP Q9DHW0
K	321	HIS	-	expression tag	UNP Q9DHW0
K	322	HIS	-	expression tag	UNP Q9DHW0
K	323	HIS	-	expression tag	UNP Q9DHW0
K	324	HIS	-	expression tag	UNP Q9DHW0
L	317	GLY	-	expression tag	UNP Q9DHW0
L	318	SER	-	expression tag	UNP Q9DHW0
L	319	HIS	-	expression tag	UNP Q9DHW0
L	320	HIS	-	expression tag	UNP Q9DHW0
L	321	HIS	-	expression tag	UNP Q9DHW0
L	322	HIS	-	expression tag	UNP Q9DHW0
L	323	HIS	-	expression tag	UNP Q9DHW0
L	324	HIS	-	expression tag	UNP Q9DHW0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	E	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	F	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 14 8 1 5	0	0
3	J	1	Total C N O 14 8 1 5	0	0
3	K	1	Total C N O 14 8 1 5	0	0
3	K	1	Total C N O 14 8 1 5	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	1	Total C N O 14 8 1 5	0	0
3	L	1	Total C N O 14 8 1 5	0	0
3	L	1	Total C N O 14 8 1 5	0	0
3	L	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is water.

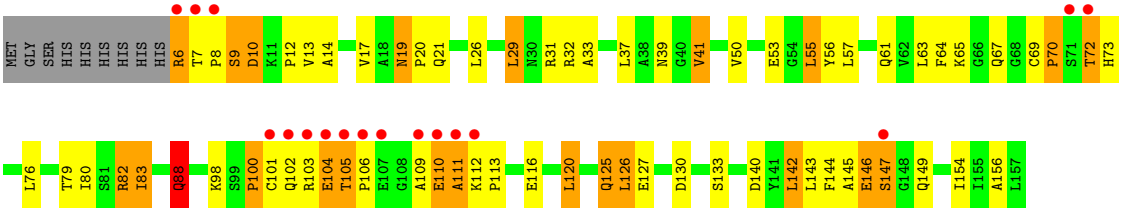
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	10	Total O 10 10	0	0
4	B	9	Total O 9 9	0	0
4	C	10	Total O 10 10	0	0
4	D	6	Total O 6 6	0	0
4	E	7	Total O 7 7	0	0
4	F	6	Total O 6 6	0	0
4	G	10	Total O 10 10	0	0
4	H	9	Total O 9 9	0	0
4	I	11	Total O 11 11	0	0
4	J	6	Total O 6 6	0	0
4	K	6	Total O 6 6	0	0
4	L	6	Total O 6 6	0	0

3 Residue-property plots

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.

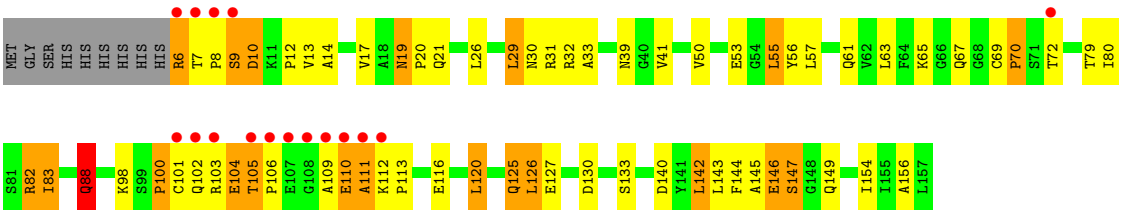
• Molecule 1: Tumor necrosis factor

Chain A:



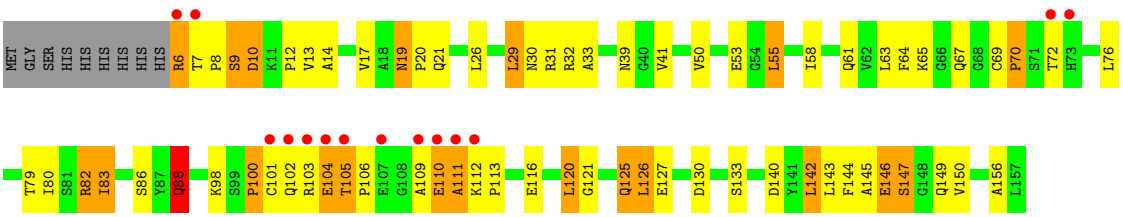
• Molecule 1: Tumor necrosis factor

Chain B:



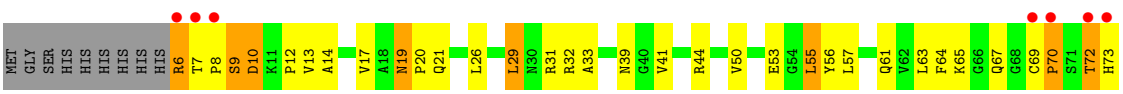
• Molecule 1: Tumor necrosis factor

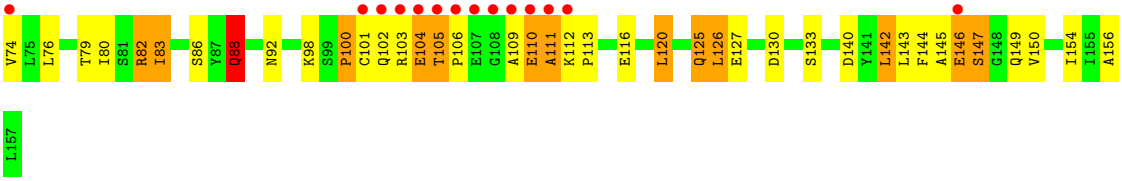
Chain C:



• Molecule 1: Tumor necrosis factor

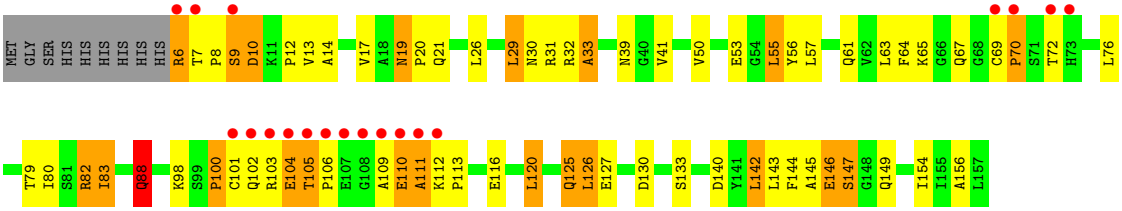
Chain G:





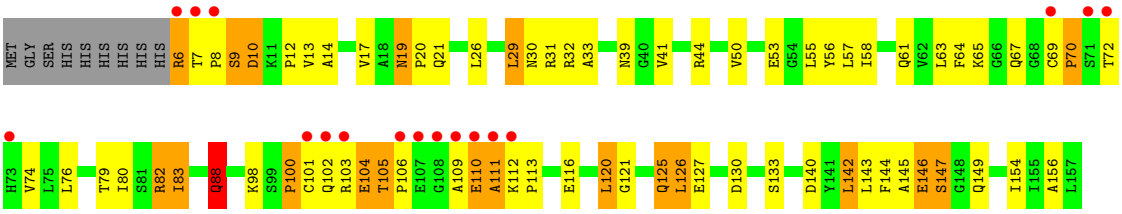
• Molecule 1: Tumor necrosis factor

Chain H:



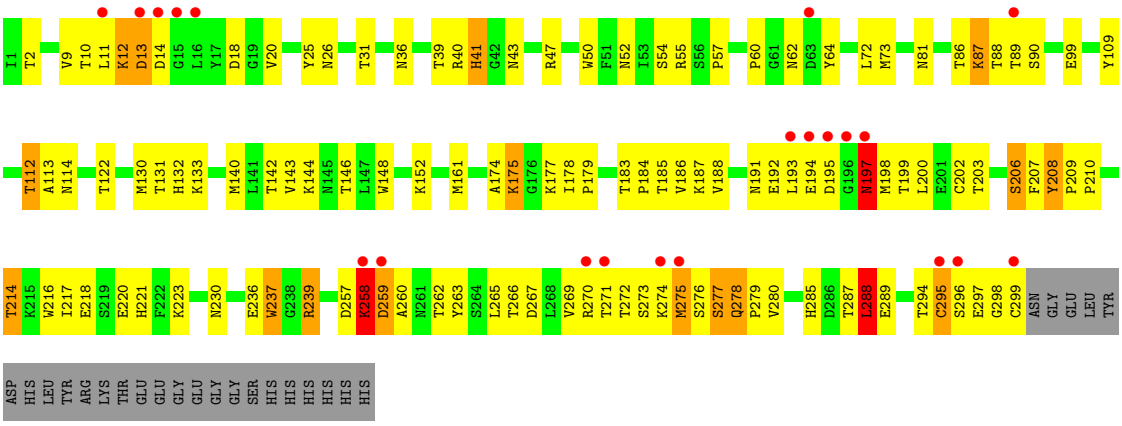
• Molecule 1: Tumor necrosis factor

Chain I:



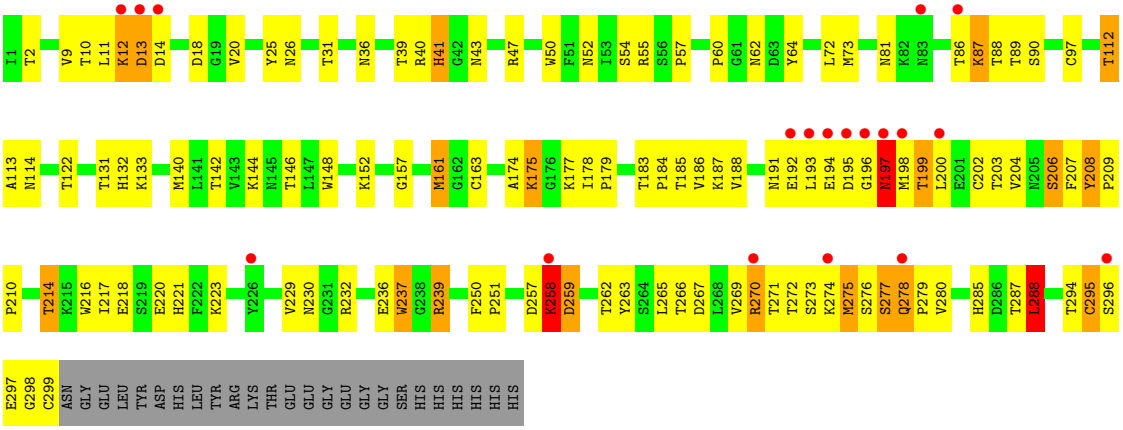
• Molecule 2: 2L protein

Chain D:



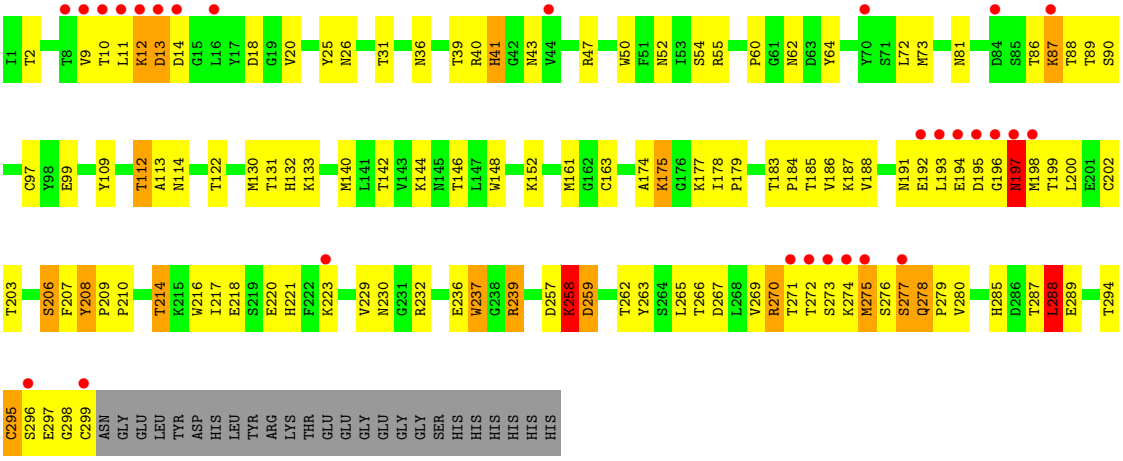
• Molecule 2: 2L protein

Chain E:



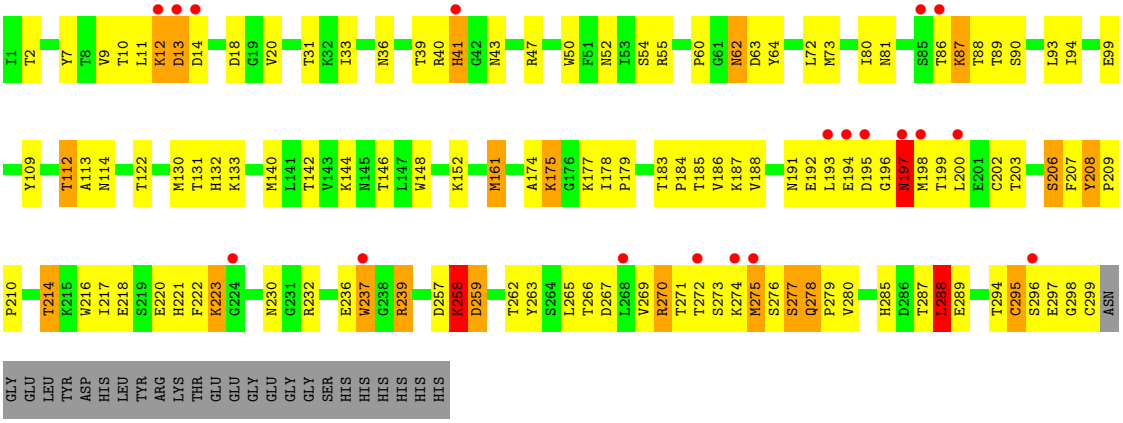
• Molecule 2: 2L protein

Chain F:



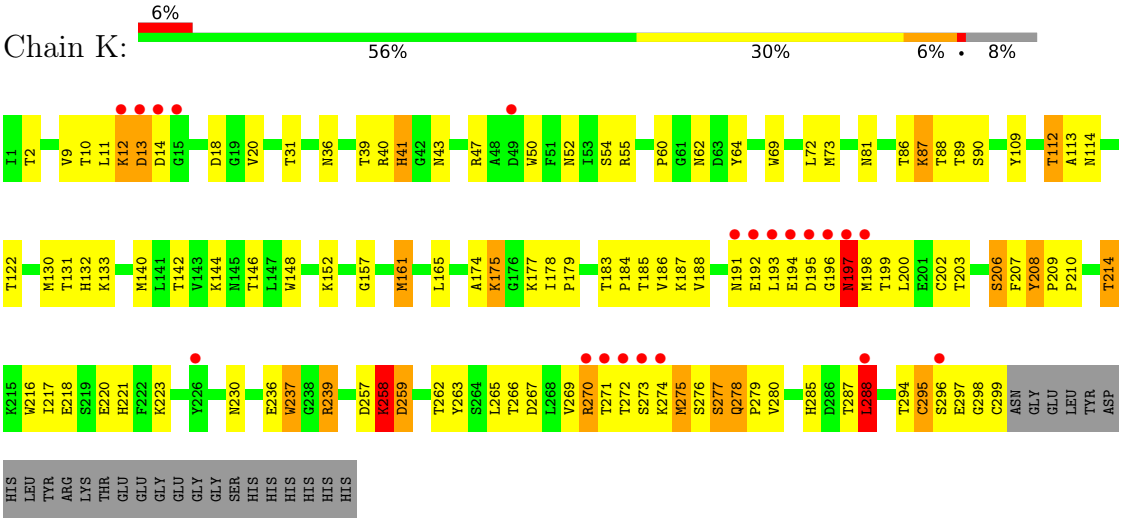
• Molecule 2: 2L protein

Chain J:



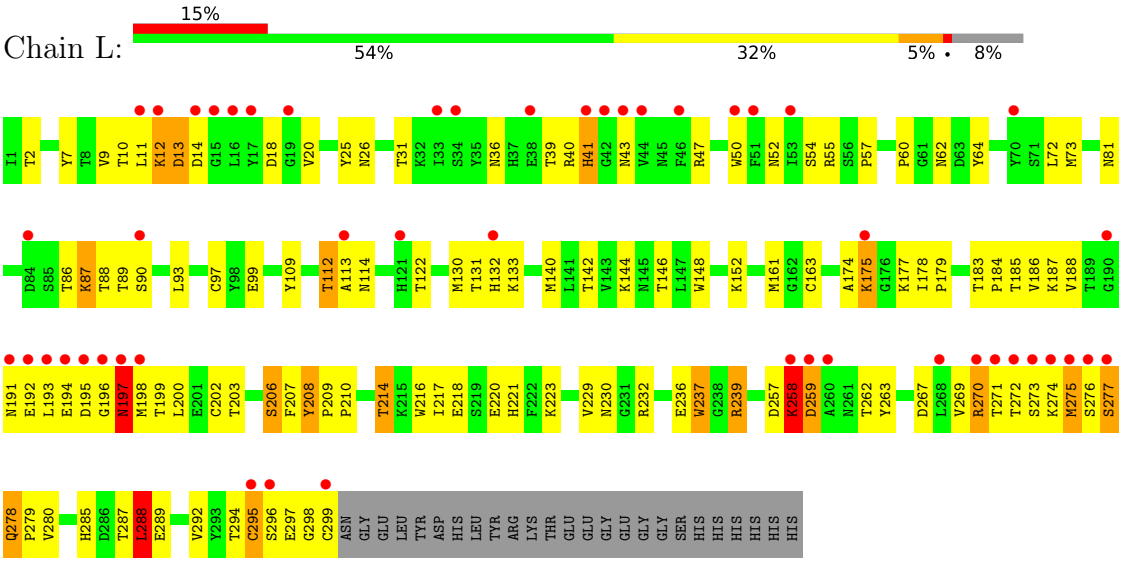
• Molecule 2: 2L protein

Chain K:



• Molecule 2: 2L protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	101.66Å 170.29Å 122.00Å 90.00° 92.04° 90.00°	Depositor
Resolution (Å)	38.77 – 2.80 45.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (38.77-2.80) 96.9 (45.07-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.266 0.239 , 0.265	Depositor DCC
R_{free} test set	5139 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	50.1	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 69.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	22002	wwPDB-VP
Average B, all atoms (Å^2)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.93% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

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	0.39	0/1217	0.68	0/1656
1	B	0.39	0/1217	0.69	0/1656
1	C	0.39	0/1217	0.68	0/1656
1	G	0.39	0/1217	0.69	0/1656
1	H	0.37	0/1217	0.68	0/1656
1	I	0.38	0/1217	0.68	0/1656
2	D	0.43	0/2487	0.69	2/3374 (0.1%)
2	E	0.41	0/2487	0.68	2/3374 (0.1%)
2	F	0.38	0/2487	0.68	2/3374 (0.1%)
2	J	0.43	0/2487	0.68	2/3374 (0.1%)
2	K	0.42	0/2487	0.68	2/3374 (0.1%)
2	L	0.36	0/2487	0.67	2/3374 (0.1%)
All	All	0.40	0/22224	0.68	12/30180 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	288	LEU	CA-CB-CG	9.00	136.00	115.30
2	J	288	LEU	CA-CB-CG	8.99	135.97	115.30
2	E	288	LEU	CA-CB-CG	8.95	135.88	115.30
2	D	288	LEU	CA-CB-CG	8.91	135.80	115.30
2	L	288	LEU	CA-CB-CG	8.75	135.43	115.30

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	1190	0	1192	76	0
1	B	1190	0	1192	71	0
1	C	1190	0	1192	73	0
1	G	1190	0	1192	84	0
1	H	1190	0	1192	74	0
1	I	1190	0	1192	78	0
2	D	2419	0	2309	103	1
2	E	2419	0	2309	115	0
2	F	2419	0	2308	113	0
2	J	2419	0	2308	118	1
2	K	2419	0	2309	113	0
2	L	2419	0	2308	116	0
3	D	42	0	39	3	0
3	E	42	0	39	4	0
3	F	42	0	39	5	0
3	J	42	0	39	3	0
3	K	42	0	39	4	0
3	L	42	0	39	6	0
4	A	10	0	0	0	0
4	B	9	0	0	0	0
4	C	10	0	0	0	0
4	D	6	0	0	0	0
4	E	7	0	0	0	0
4	F	6	0	0	0	0
4	G	10	0	0	0	0
4	H	9	0	0	0	0
4	I	11	0	0	0	0
4	J	6	0	0	0	0
4	K	6	0	0	0	0
4	L	6	0	0	0	0
All	All	22002	0	21237	1094	1

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 25.

The worst 5 of 1094 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:L:50:TRP:HB3	2:L:177:LYS:HD2	1.30	1.09
2:J:50:TRP:HB3	2:J:177:LYS:HD2	1.32	1.08
2:F:50:TRP:HB3	2:F:177:LYS:HD2	1.31	1.07
2:K:50:TRP:HB3	2:K:177:LYS:HD2	1.32	1.07
2:L:112:THR:HG22	2:L:114:ASN:H	1.18	1.07

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:ASP:O	2:J:62:ASN:OD1[2_545]	2.12	0.08

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	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	B	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	C	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	2
1	G	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	H	150/161 (93%)	127 (85%)	11 (7%)	12 (8%)	1	2
1	I	150/161 (93%)	128 (85%)	10 (7%)	12 (8%)	1	2
2	D	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
2	E	297/324 (92%)	256 (86%)	22 (7%)	19 (6%)	1	3
2	F	297/324 (92%)	257 (86%)	20 (7%)	20 (7%)	1	3
2	J	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
2	K	297/324 (92%)	255 (86%)	23 (8%)	19 (6%)	1	3
2	L	297/324 (92%)	256 (86%)	21 (7%)	20 (7%)	1	3
All	All	2682/2910 (92%)	2300 (86%)	192 (7%)	190 (7%)	1	2

5 of 190 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	33	ALA
1	A	88	GLN
1	A	105	THR
1	A	110	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	128/136 (94%)	111 (87%)	17 (13%)	4	12
1	B	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	C	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	G	128/136 (94%)	111 (87%)	17 (13%)	4	12
1	H	128/136 (94%)	110 (86%)	18 (14%)	3	10
1	I	128/136 (94%)	110 (86%)	18 (14%)	3	10
2	D	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	E	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	F	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	J	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	K	267/288 (93%)	249 (93%)	18 (7%)	16	43
2	L	267/288 (93%)	249 (93%)	18 (7%)	16	43
All	All	2370/2544 (93%)	2156 (91%)	214 (9%)	9	28

5 of 214 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	83	ILE
1	I	19	ASN
2	L	41	HIS
1	G	125	GLN

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Mol	Chain	Res	Type
1	H	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	102	GLN
2	J	121	HIS
1	I	19	ASN
1	I	125	GLN
2	K	41	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	$\#\|Z\| > 2$
3	NAG	F	327	2	14,14,15	0.79	1 (7%)	17,19,21	0.65	0
3	NAG	D	325	2	14,14,15	0.61	0	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	J	325	2	14,14,15	0.54	0	17,19,21	0.93	1 (5%)
3	NAG	L	325	2	14,14,15	0.57	0	17,19,21	0.76	1 (5%)
3	NAG	F	326	2	14,14,15	0.82	1 (7%)	17,19,21	0.66	0
3	NAG	K	325	2	14,14,15	0.58	0	17,19,21	0.73	0
3	NAG	D	327	2	14,14,15	0.85	1 (7%)	17,19,21	0.86	0
3	NAG	D	326	2	14,14,15	1.08	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	F	325	2	14,14,15	0.74	0	17,19,21	0.72	1 (5%)
3	NAG	L	326	2	14,14,15	0.87	1 (7%)	17,19,21	0.80	0
3	NAG	E	325	2	14,14,15	0.55	0	17,19,21	0.82	0
3	NAG	K	326	2	14,14,15	0.85	1 (7%)	17,19,21	0.90	0
3	NAG	E	326	2	14,14,15	1.01	1 (7%)	17,19,21	1.16	1 (5%)
3	NAG	J	326	2	14,14,15	0.86	1 (7%)	17,19,21	0.95	2 (11%)
3	NAG	K	327	2	14,14,15	0.89	1 (7%)	17,19,21	0.63	0
3	NAG	E	327	2	14,14,15	0.75	1 (7%)	17,19,21	0.56	0
3	NAG	L	327	2	14,14,15	0.65	0	17,19,21	0.73	1 (5%)
3	NAG	J	327	2	14,14,15	0.70	0	17,19,21	0.59	0

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
3	NAG	F	327	2	-	5/6/23/26	0/1/1/1
3	NAG	D	325	2	-	2/6/23/26	0/1/1/1
3	NAG	J	325	2	-	2/6/23/26	0/1/1/1
3	NAG	L	325	2	-	4/6/23/26	0/1/1/1
3	NAG	F	326	2	-	3/6/23/26	0/1/1/1
3	NAG	K	325	2	-	0/6/23/26	0/1/1/1
3	NAG	D	327	2	-	6/6/23/26	0/1/1/1
3	NAG	D	326	2	-	3/6/23/26	0/1/1/1
3	NAG	F	325	2	-	4/6/23/26	0/1/1/1
3	NAG	L	326	2	-	5/6/23/26	0/1/1/1
3	NAG	E	325	2	-	0/6/23/26	0/1/1/1
3	NAG	K	326	2	-	5/6/23/26	0/1/1/1
3	NAG	E	326	2	-	5/6/23/26	0/1/1/1
3	NAG	J	326	2	-	5/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	K	327	2	-	4/6/23/26	0/1/1/1
3	NAG	E	327	2	-	5/6/23/26	0/1/1/1
3	NAG	L	327	2	-	3/6/23/26	0/1/1/1
3	NAG	J	327	2	-	4/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	326	NAG	C1-C2	3.41	1.57	1.52
3	E	326	NAG	C1-C2	3.21	1.57	1.52
3	K	327	NAG	C1-C2	2.81	1.56	1.52
3	J	326	NAG	C1-C2	2.74	1.56	1.52
3	D	327	NAG	C1-C2	2.58	1.56	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	326	NAG	C3-C4-C5	-3.12	104.68	110.24
3	J	325	NAG	C3-C4-C5	-2.55	105.68	110.24
3	L	325	NAG	C2-N2-C7	-2.30	119.63	122.90
3	F	325	NAG	C2-N2-C7	-2.21	119.75	122.90
3	D	326	NAG	C3-C4-C5	-2.18	106.36	110.24

There are no chirality outliers.

5 of 65 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	326	NAG	C3-C2-N2-C7
3	D	326	NAG	C8-C7-N2-C2
3	D	326	NAG	O7-C7-N2-C2
3	D	327	NAG	C8-C7-N2-C2
3	D	327	NAG	O7-C7-N2-C2

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	325	NAG	2	0
3	F	326	NAG	5	0
3	D	327	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	326	NAG	1	0
3	L	326	NAG	5	0
3	K	326	NAG	3	0
3	E	326	NAG	3	0
3	J	326	NAG	1	0
3	K	327	NAG	1	0
3	E	327	NAG	1	0
3	L	327	NAG	1	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	152/161 (94%)	0.64	17 (11%) 5 3	31, 56, 172, 191	0
1	B	152/161 (94%)	0.57	16 (10%) 6 3	28, 53, 170, 200	0
1	C	152/161 (94%)	0.48	14 (9%) 9 5	28, 56, 176, 195	0
1	G	152/161 (94%)	0.78	21 (13%) 2 1	27, 56, 176, 195	0
1	H	152/161 (94%)	0.57	19 (12%) 3 2	33, 65, 169, 194	0
1	I	152/161 (94%)	0.56	17 (11%) 5 3	31, 59, 172, 201	0
2	D	299/324 (92%)	0.45	21 (7%) 16 9	29, 58, 138, 201	0
2	E	299/324 (92%)	0.32	19 (6%) 19 12	32, 59, 134, 199	0
2	F	299/324 (92%)	0.52	28 (9%) 8 4	35, 74, 144, 201	0
2	J	299/324 (92%)	0.27	19 (6%) 19 12	31, 57, 130, 189	0
2	K	299/324 (92%)	0.36	21 (7%) 16 9	26, 59, 136, 201	0
2	L	299/324 (92%)	0.96	49 (16%) 1 1	39, 90, 153, 201	0
All	All	2706/2910 (92%)	0.52	261 (9%) 8 4	26, 63, 159, 201	0

The worst 5 of 261 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	196	GLY	18.1
2	L	193	LEU	16.3
2	E	197	ASN	14.9
2	K	193	LEU	14.8
2	D	193	LEU	14.5

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides 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, 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	B-factors(Å^2)	Q<0.9
3	NAG	F	326	14/15	0.56	0.23	141,141,141,141	0
3	NAG	D	326	14/15	0.66	0.26	112,112,112,112	0
3	NAG	F	327	14/15	0.67	0.47	140,140,140,140	0
3	NAG	J	327	14/15	0.67	0.54	140,140,140,140	0
3	NAG	E	327	14/15	0.70	0.35	140,140,140,140	0
3	NAG	E	326	14/15	0.72	0.21	81,81,81,81	0
3	NAG	K	327	14/15	0.72	0.32	140,140,140,140	0
3	NAG	D	327	14/15	0.73	0.23	140,140,140,140	0
3	NAG	L	327	14/15	0.73	0.30	140,140,140,140	0
3	NAG	L	326	14/15	0.76	0.21	128,128,128,128	0
3	NAG	K	326	14/15	0.76	0.16	122,122,122,122	0
3	NAG	J	326	14/15	0.80	0.20	96,96,96,96	0
3	NAG	L	325	14/15	0.86	0.19	90,90,90,90	0
3	NAG	F	325	14/15	0.87	0.20	79,79,79,79	0
3	NAG	D	325	14/15	0.89	0.21	57,57,57,57	0
3	NAG	J	325	14/15	0.93	0.18	49,49,49,49	0
3	NAG	K	325	14/15	0.94	0.13	54,54,54,54	0
3	NAG	E	325	14/15	0.95	0.16	56,56,56,56	0

6.5 Other polymers (i)

There are no such residues in this entry.