wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:08 PM GMT

PDB ID	:	4NQX
Title	:	Crystal Structure of HLA A*0101 in complex with NP44-S7N, an 9-mer influenza epitope
Authors	:	Rossjohn, J.; Gras, S.
Deposited on	:	2013-11-26
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

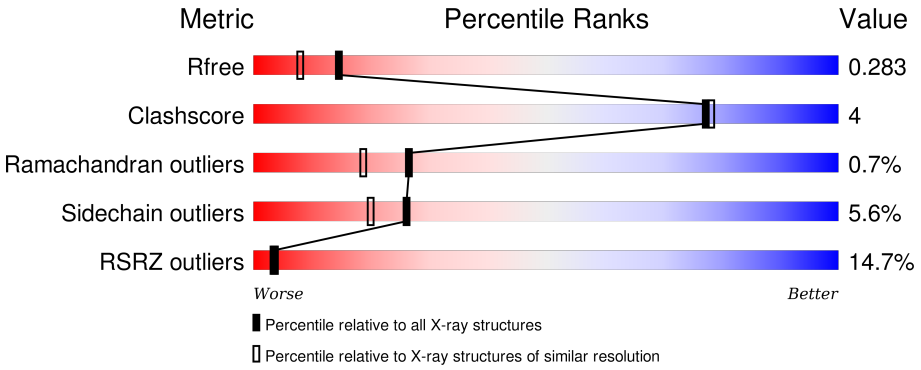
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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 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 <=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	284	4% 87% 8%
1	C	284	11% 87% 9%
1	E	284	10% 83% 12%
1	G	284	13% 85% 10%
1	I	284	11% 85% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	284	19% 86% 10%
2	B	100	9% 86% 14%
2	D	100	8% 91% 8%
2	F	100	36% 63% 28% 6%
2	H	100	10% 92% 8%
2	J	100	45% 87% 11%
2	L	100	29% 86% 13%
3	M	9	89% 11%
3	N	9	22% 78% 22%
3	O	9	11% 78% 22%
3	P	9	11% 67% 33%
3	Q	9	78% 22%
3	R	9	33% 78% 22%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19771 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 HLA class I histocompatibility antigen, A-1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	3	0
			2255	1399	416	430	10			
1	C	275	Total	C	N	O	S	0	1	0
			2245	1394	411	430	10			
1	E	275	Total	C	N	O	S	0	2	0
			2256	1399	415	432	10			
1	G	274	Total	C	N	O	S	0	2	0
			2248	1395	415	428	10			
1	I	274	Total	C	N	O	S	0	2	0
			2247	1394	413	430	10			
1	K	275	Total	C	N	O	S	0	1	0
			2243	1392	410	431	10			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	1	0
			845	539	142	160	4			
2	D	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	F	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
2	H	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	J	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			
2	L	100	Total	C	N	O	S	0	0	0
			837	533	141	159	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	EXPRESSION TAG	UNP P61769

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	0	MET	-	EXPRESSION TAG	UNP P61769
F	0	MET	-	EXPRESSION TAG	UNP P61769
H	0	MET	-	EXPRESSION TAG	UNP P61769
J	0	MET	-	EXPRESSION TAG	UNP P61769
L	0	MET	-	EXPRESSION TAG	UNP P61769

- Molecule 3 is a protein called NP44-S7N mutant peptide, CTELKLNDY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	N	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	O	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	P	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	Q	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			
3	R	9	Total	C	N	O	S	0	0	0
			76	47	11	17	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	116	Total	O	0	0
			116	116		
4	B	49	Total	O	0	0
			49	49		
4	C	110	Total	O	0	0
			110	110		
4	D	51	Total	O	0	0
			51	51		
4	E	90	Total	O	0	0
			90	90		
4	F	43	Total	O	0	0
			43	43		
4	G	70	Total	O	0	0
			70	70		
4	H	34	Total	O	0	0
			34	34		
4	I	55	Total	O	0	0
			55	55		

Continued on next page...

Continued from previous page...

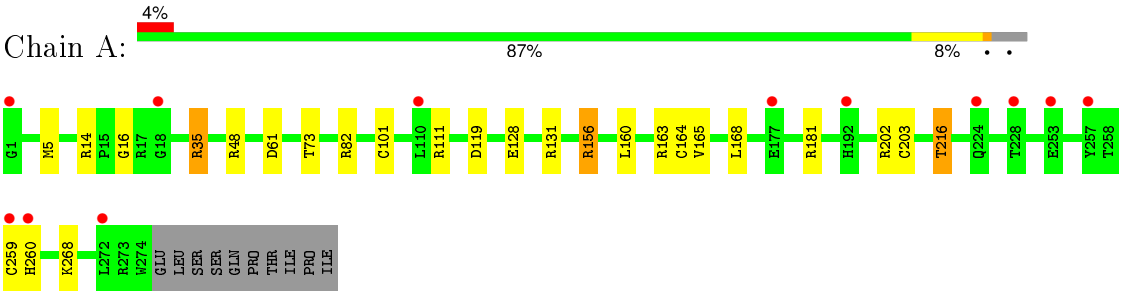
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	27	Total O 27 27	0	0
4	K	97	Total O 97 97	0	0
4	L	32	Total O 32 32	0	0
4	M	7	Total O 7 7	0	0
4	N	5	Total O 5 5	0	0
4	O	2	Total O 2 2	0	0
4	P	4	Total O 4 4	0	0
4	Q	3	Total O 3 3	0	0
4	R	4	Total O 4 4	0	0

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.

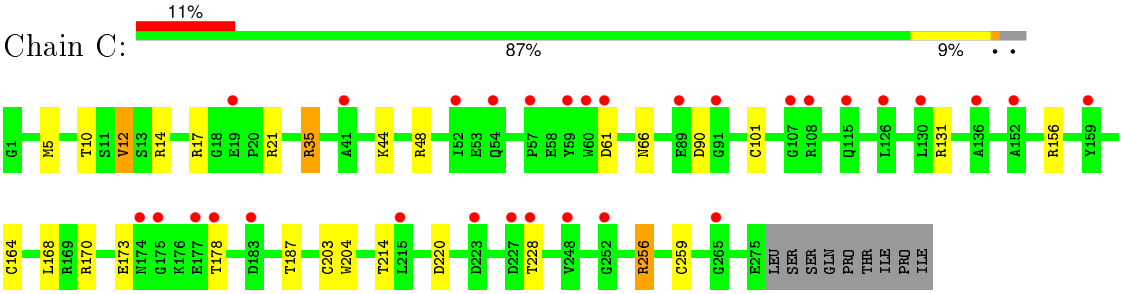
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A:



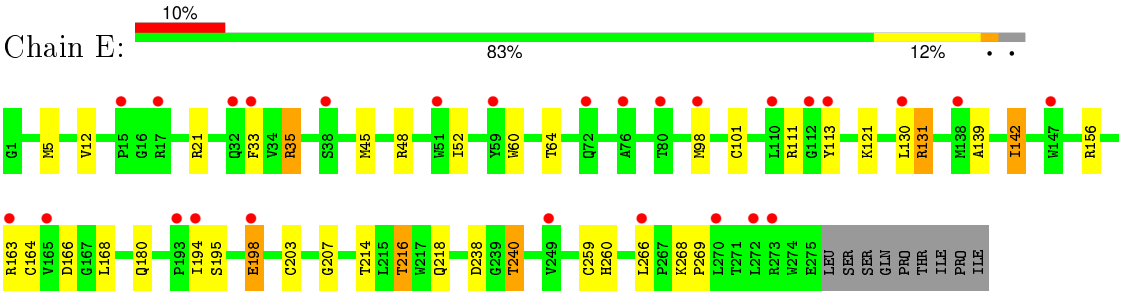
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain C:



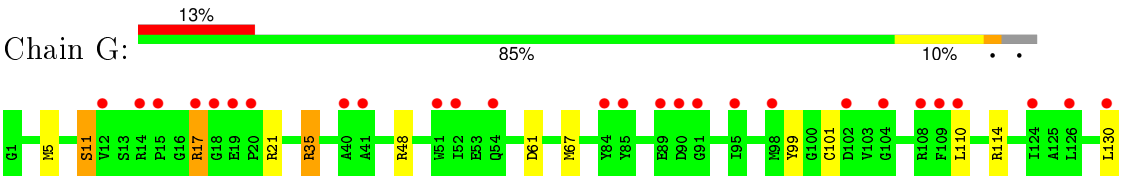
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

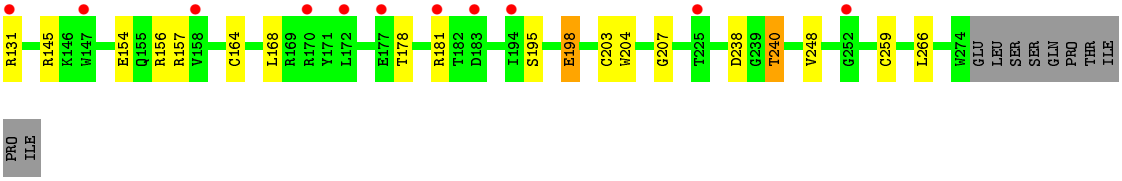
Chain E:



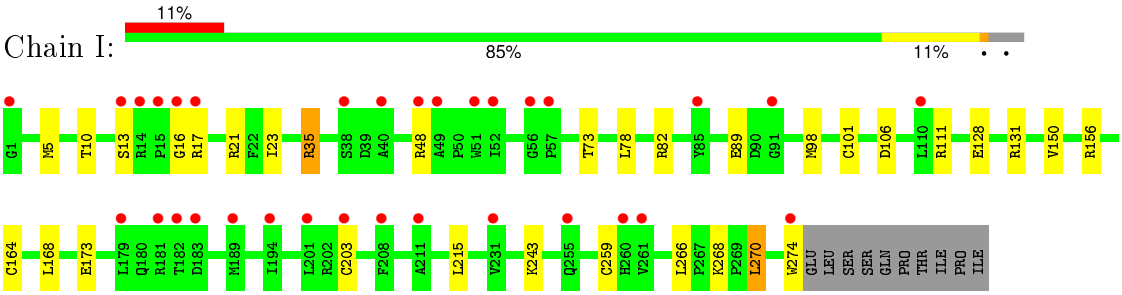
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain G:

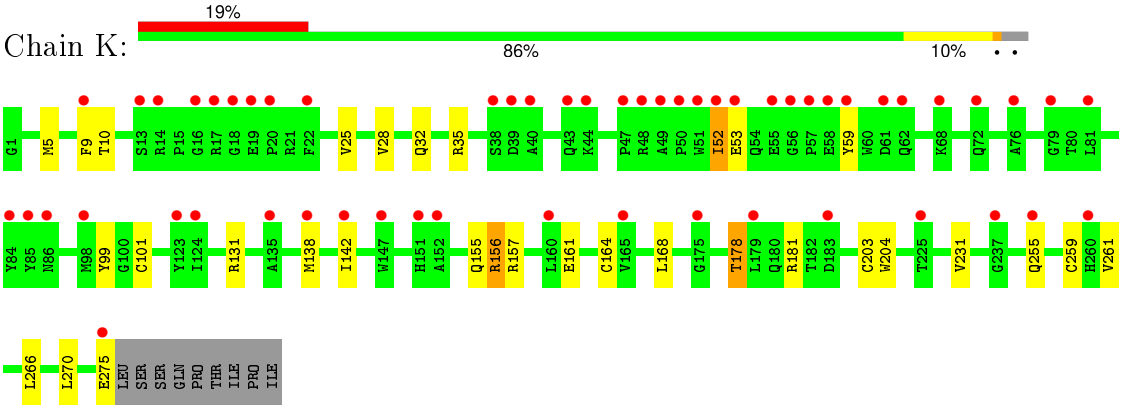




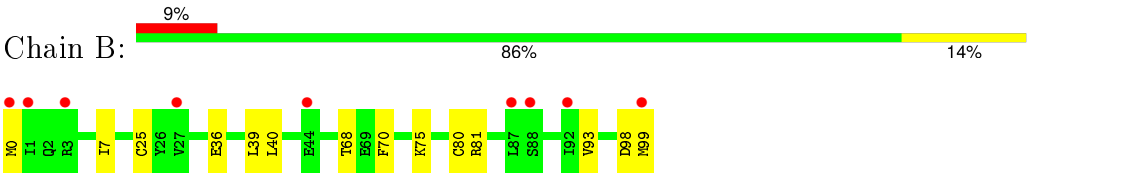
• Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



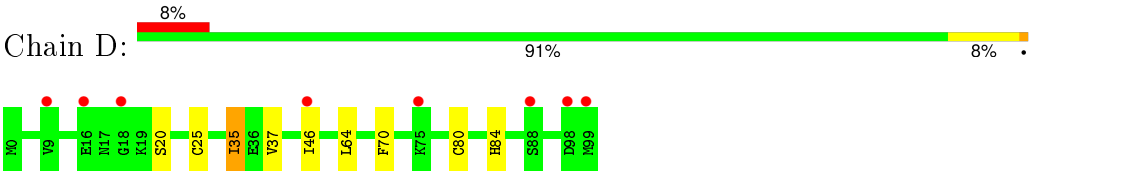
• Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



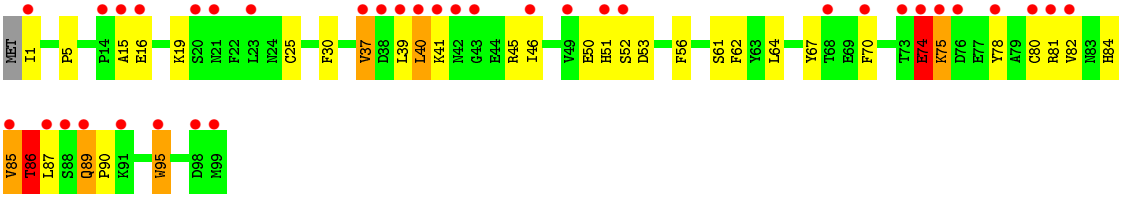
• Molecule 2: Beta-2-microglobulin



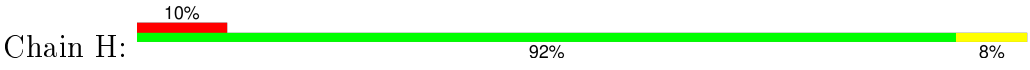
• Molecule 2: Beta-2-microglobulin



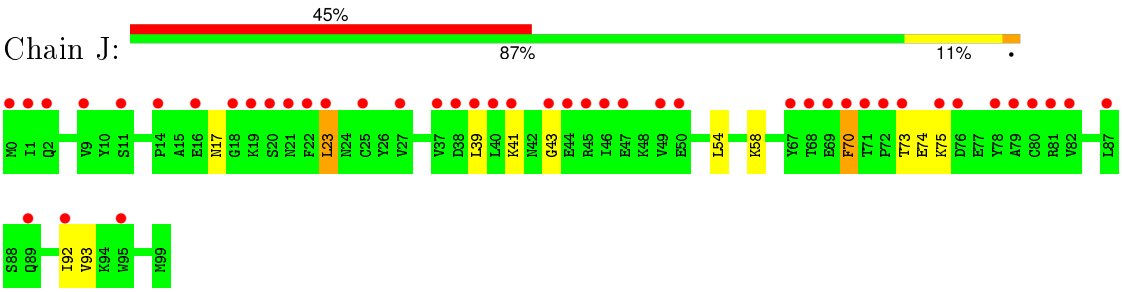
• Molecule 2: Beta-2-microglobulin



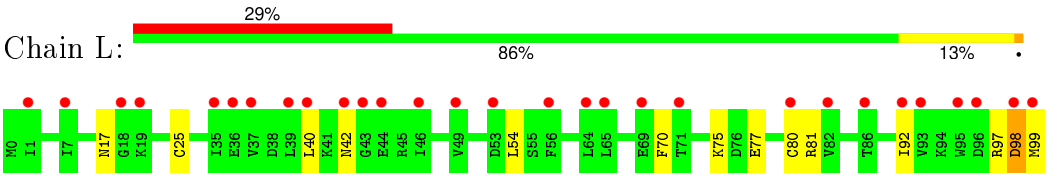
• Molecule 2: Beta-2-microglobulin



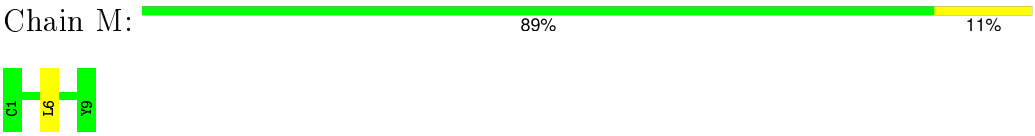
• Molecule 2: Beta-2-microglobulin



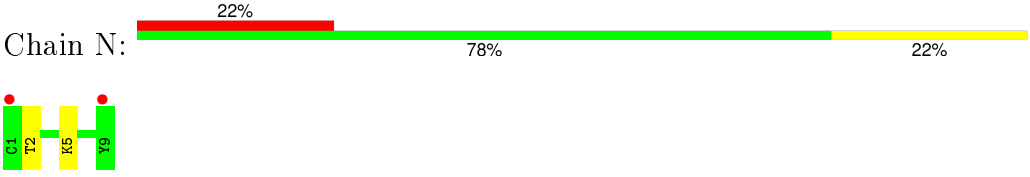
• Molecule 2: Beta-2-microglobulin



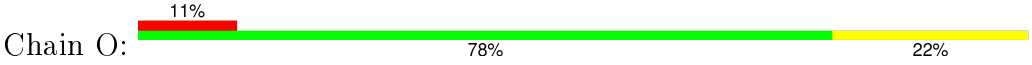
• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY

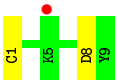


• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY



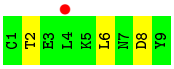
• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY





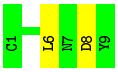
• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY

Chain P:



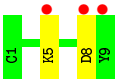
• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY

Chain Q:



• Molecule 3: NP44-S7N mutant peptide, CTELKLNDY

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	264.61Å 81.41Å 140.29Å 90.00° 121.82° 90.00°	Depositor
Resolution (Å)	45.75 – 2.00 45.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.75-2.00) 96.2 (45.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.00Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.270 , 0.283 0.275 , 0.283	Depositor DCC
R_{free} test set	8305 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	36.0	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.0	EDS
Estimated twinning fraction	0.077 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 165610 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19771	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 47.67 % 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 9.6027e-05.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.37	0/2316	0.58	0/3140
1	C	0.38	0/2305	0.58	0/3125
1	E	0.39	0/2316	0.61	0/3139
1	G	0.37	0/2309	0.59	0/3131
1	I	0.35	0/2307	0.58	0/3127
1	K	0.38	0/2303	0.61	0/3123
2	B	0.38	0/868	0.64	0/1173
2	D	0.37	0/860	0.63	0/1162
2	F	0.45	0/852	0.83	2/1152 (0.2%)
2	H	0.39	0/860	0.63	0/1162
2	J	0.40	0/860	0.61	0/1162
2	L	0.37	0/860	0.63	0/1162
3	M	0.35	0/76	0.63	0/100
3	N	0.35	0/76	0.57	0/100
3	O	0.33	0/76	0.54	0/100
3	P	0.38	0/76	0.83	0/100
3	Q	0.31	0/76	0.61	0/100
3	R	0.36	0/76	0.51	0/100
All	All	0.38	0/19472	0.61	2/26358 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	85	VAL	C-N-CA	9.21	144.74	121.70
2	F	74	GLU	C-N-CA	5.33	135.03	121.70

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	2255	0	2114	14	0
1	C	2245	0	2109	13	0
1	E	2256	0	2115	24	0
1	G	2248	0	2109	18	0
1	I	2247	0	2107	14	0
1	K	2243	0	2102	16	0
2	B	845	0	815	8	0
2	D	837	0	805	5	0
2	F	829	0	796	18	0
2	H	837	0	805	3	0
2	J	837	0	805	4	0
2	L	837	0	805	9	0
3	M	76	0	74	1	0
3	N	76	0	74	2	0
3	O	76	0	74	1	0
3	P	76	0	74	3	0
3	Q	76	0	74	1	0
3	R	76	0	74	0	0
4	A	116	0	0	2	0
4	B	49	0	0	0	0
4	C	110	0	0	0	0
4	D	51	0	0	1	0
4	E	90	0	0	0	0
4	F	43	0	0	0	0
4	G	70	0	0	0	0
4	H	34	0	0	0	0
4	I	55	0	0	0	0
4	J	27	0	0	0	0
4	K	97	0	0	2	0
4	L	32	0	0	0	0
4	M	7	0	0	0	0
4	N	5	0	0	0	0
4	O	2	0	0	0	0
4	P	4	0	0	0	0
4	Q	3	0	0	0	0
4	R	4	0	0	0	0
All	All	19771	0	17931	132	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 4.

The worst 5 of 132 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:B:7:ILE:HD11	2:B:25:CYS:SG	2.05	0.96
1:E:45:MET:H	1:E:64:THR:HG22	1.38	0.87
1:G:67:MET:CE	3:P:2:THR:HG21	2.15	0.77
1:A:216:THR:HG23	1:A:260[A]:HIS:HB3	1.66	0.76
2:D:35:ILE:HD11	2:D:64:LEU:HD12	1.67	0.76

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	275/284 (97%)	270 (98%)	4 (2%)	1 (0%)	39 33
1	C	274/284 (96%)	268 (98%)	6 (2%)	0	100 100
1	E	275/284 (97%)	269 (98%)	6 (2%)	0	100 100
1	G	274/284 (96%)	269 (98%)	4 (2%)	1 (0%)	39 33
1	I	274/284 (96%)	270 (98%)	3 (1%)	1 (0%)	39 33
1	K	274/284 (96%)	262 (96%)	11 (4%)	1 (0%)	39 33
2	B	99/100 (99%)	98 (99%)	0	1 (1%)	19 11
2	D	98/100 (98%)	97 (99%)	1 (1%)	0	100 100
2	F	97/100 (97%)	79 (81%)	8 (8%)	10 (10%)	1 0
2	H	98/100 (98%)	94 (96%)	3 (3%)	1 (1%)	19 11
2	J	98/100 (98%)	94 (96%)	4 (4%)	0	100 100
2	L	98/100 (98%)	92 (94%)	6 (6%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	7/9 (78%)	7 (100%)	0	0	100	100
3	N	7/9 (78%)	7 (100%)	0	0	100	100
3	O	7/9 (78%)	7 (100%)	0	0	100	100
3	P	7/9 (78%)	7 (100%)	0	0	100	100
3	Q	7/9 (78%)	7 (100%)	0	0	100	100
3	R	7/9 (78%)	7 (100%)	0	0	100	100
All	All	2276/2358 (96%)	2204 (97%)	56 (2%)	16 (1%)	26	19

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	15	ALA
2	F	61	SER
2	F	62	PHE
2	F	86	THR
1	G	17	ARG

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	234/241 (97%)	226 (97%)	8 (3%)	44	41
1	C	233/241 (97%)	220 (94%)	13 (6%)	26	20
1	E	234/241 (97%)	218 (93%)	16 (7%)	20	13
1	G	233/241 (97%)	220 (94%)	13 (6%)	26	20
1	I	233/241 (97%)	221 (95%)	12 (5%)	29	23
1	K	233/241 (97%)	222 (95%)	11 (5%)	32	27
2	B	96/95 (101%)	92 (96%)	4 (4%)	36	31
2	D	95/95 (100%)	91 (96%)	4 (4%)	36	31
2	F	94/95 (99%)	85 (90%)	9 (10%)	10	6
2	H	95/95 (100%)	91 (96%)	4 (4%)	36	31

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	J	95/95 (100%)	87 (92%)	8 (8%)	14 8
2	L	95/95 (100%)	91 (96%)	4 (4%)	36 31
3	M	9/9 (100%)	9 (100%)	0	100 100
3	N	9/9 (100%)	8 (89%)	1 (11%)	8 4
3	O	9/9 (100%)	8 (89%)	1 (11%)	8 4
3	P	9/9 (100%)	7 (78%)	2 (22%)	1 0
3	Q	9/9 (100%)	8 (89%)	1 (11%)	8 4
3	R	9/9 (100%)	7 (78%)	2 (22%)	1 0
All	All	2024/2070 (98%)	1911 (94%)	113 (6%)	26 20

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	86	THR
1	G	198	GLU
2	L	75	LYS
2	F	87	LEU
1	G	61	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	192	HIS
1	E	96	GLN
1	G	96	GLN
1	C	66	ASN
2	F	2	GLN

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	274/284 (96%)	0.63	12 (4%) 38 39	19, 38, 61, 79	0
1	C	275/284 (96%)	1.01	30 (10%) 7 8	26, 42, 70, 82	0
1	E	275/284 (96%)	0.98	27 (9%) 10 10	27, 41, 64, 93	0
1	G	274/284 (96%)	1.13	38 (13%) 4 4	26, 45, 73, 95	0
1	I	274/284 (96%)	1.04	32 (11%) 6 7	24, 49, 81, 109	0
1	K	275/284 (96%)	1.39	55 (20%) 1 2	28, 47, 90, 119	0
2	B	100/100 (100%)	0.84	9 (9%) 12 12	20, 36, 58, 64	0
2	D	100/100 (100%)	0.75	8 (8%) 15 16	25, 36, 62, 70	0
2	F	99/100 (99%)	2.08	36 (36%) 0 1	25, 53, 89, 99	0
2	H	100/100 (100%)	0.82	10 (10%) 9 10	27, 39, 61, 67	0
2	J	100/100 (100%)	2.28	45 (45%) 0 1	26, 57, 95, 104	0
2	L	100/100 (100%)	1.49	29 (29%) 1 1	32, 49, 77, 84	0
3	M	9/9 (100%)	0.15	0 100 100	21, 27, 30, 43	0
3	N	9/9 (100%)	1.34	2 (22%) 1 1	35, 42, 48, 61	0
3	O	9/9 (100%)	0.99	1 (11%) 7 8	31, 40, 44, 58	0
3	P	9/9 (100%)	1.39	1 (11%) 7 8	38, 43, 45, 60	0
3	Q	9/9 (100%)	0.25	0 100 100	31, 35, 39, 49	0
3	R	9/9 (100%)	1.77	3 (33%) 0 1	40, 47, 62, 63	0
All	All	2300/2358 (97%)	1.12	338 (14%) 3 4	19, 43, 76, 119	0

The worst 5 of 338 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	82	VAL	11.8
2	J	18	GLY	8.8
1	K	53	GLU	8.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	80	CYS	8.2
2	F	40	LEU	8.0

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.