Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:07 PM GMT

PDB ID	:	4NQV
Title	:	Crystal Structure of HLA A*0101 in complex with NP44, an 9-mer influenza epitope
Authors	:	Rossjohn, J.; Gras, S.
Deposited on	:	2013-11-25
Resolution	:	2.39 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 (i) symbol.

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

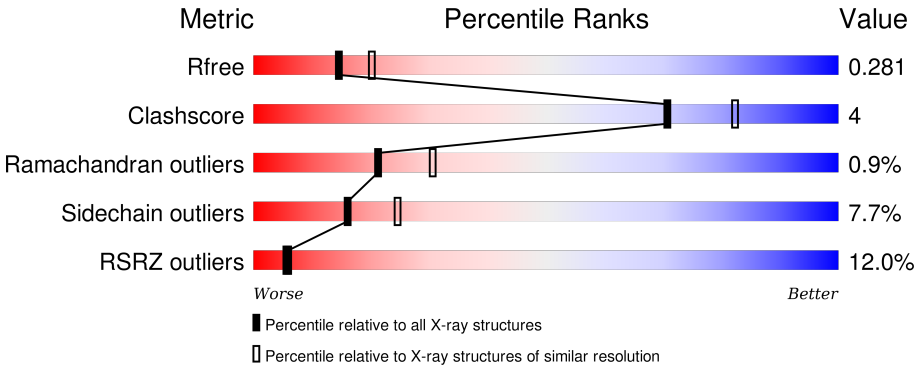
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.39 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	274	86% 14%
1	C	274	7% 86% 12%
1	E	274	14% 81% 17%
1	G	274	12% 86% 13%
1	I	274	5% 86% 13%

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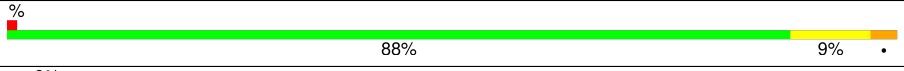
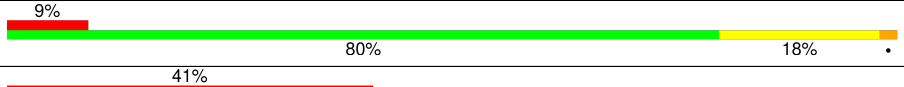
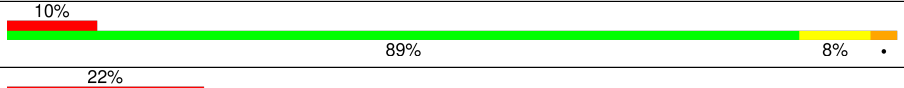
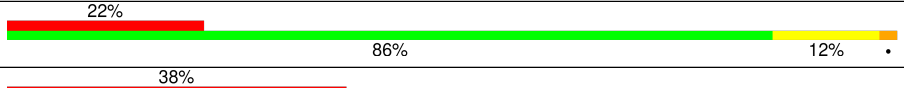
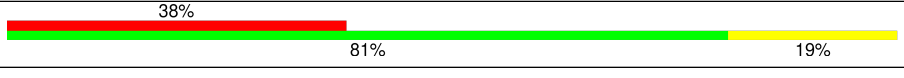
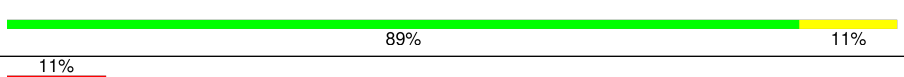
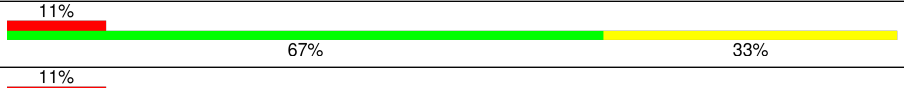
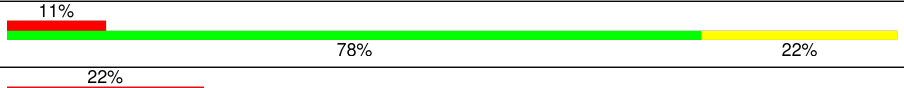
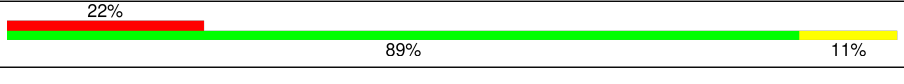
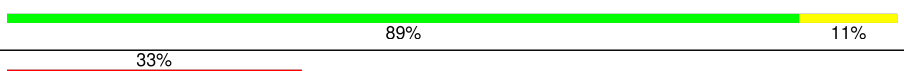
Mol	Chain	Length	Quality of chain
1	K	274	
2	B	100	
2	D	100	
2	F	100	
2	H	100	
2	J	100	
2	L	100	
3	M	9	
3	N	9	
3	O	9	
3	P	9	
3	Q	9	
3	R	9	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19628 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	0	0
			2227	1383	408	426	10			
1	C	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
1	E	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
1	G	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
1	I	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	10			
1	K	274	Total	C	N	O	S	0	0	0
			2227	1383	408	426	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	0	0
			837	533	141	159	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

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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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			
3	N	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			
3	O	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			
3	P	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			
3	Q	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			
3	R	9	Total	C	N	O	S	0	0	0
			74	46	10	17	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	44	Total	O	0	0
			44	44		
4	C	106	Total	O	0	0
			106	106		
4	D	40	Total	O	0	0
			40	40		
4	E	107	Total	O	0	0
			107	107		
4	F	28	Total	O	0	0
			28	28		
4	G	86	Total	O	0	0
			86	86		
4	H	33	Total	O	0	0
			33	33		
4	I	94	Total	O	0	0
			94	94		

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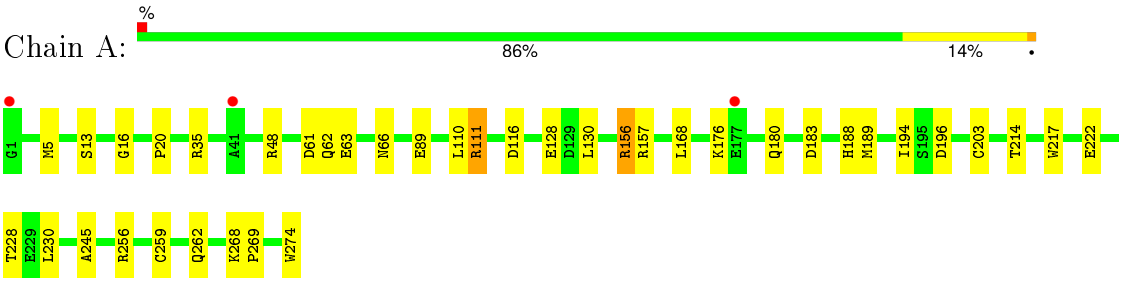
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	28	Total O 28 28	0	0
4	K	84	Total O 84 84	0	0
4	L	27	Total O 27 27	0	0
4	M	4	Total O 4 4	0	0
4	N	3	Total O 3 3	0	0
4	O	2	Total O 2 2	0	0
4	P	3	Total O 3 3	0	0
4	Q	2	Total O 2 2	0	0
4	R	3	Total O 3 3	0	0

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.

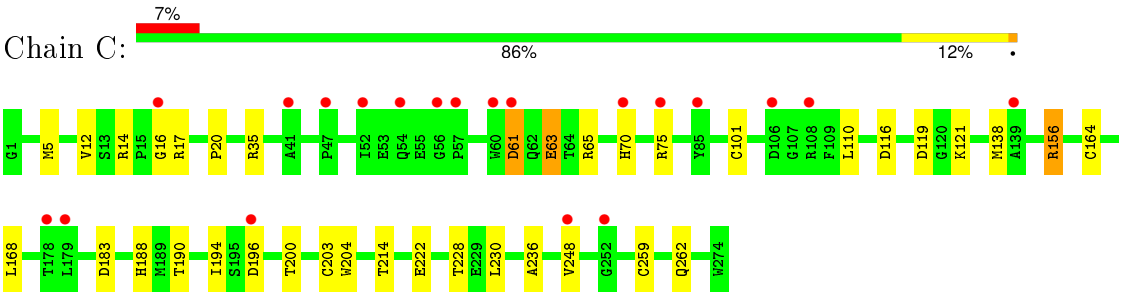
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain A:



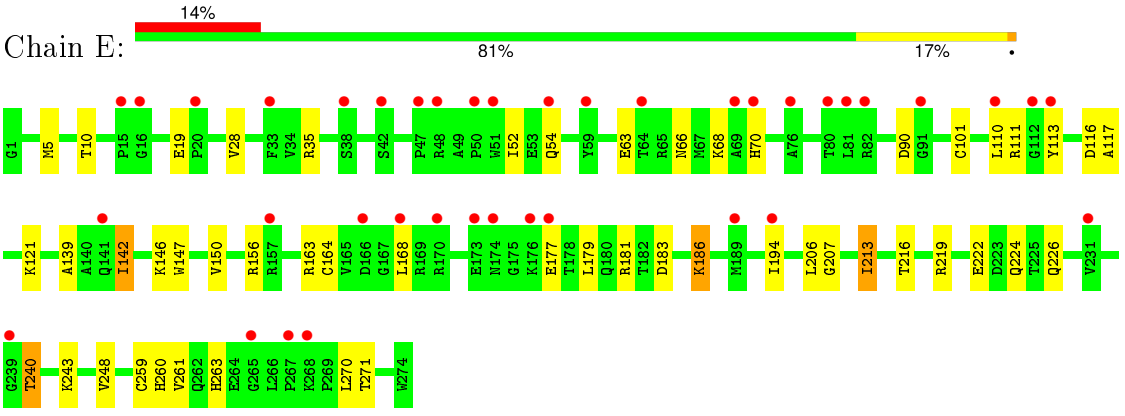
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

Chain C:



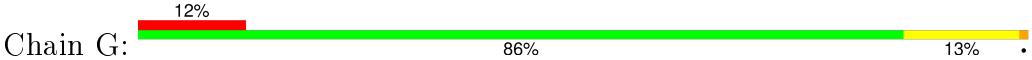
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

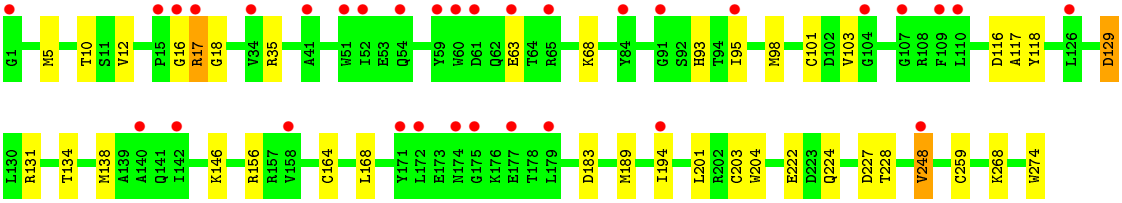
Chain E:



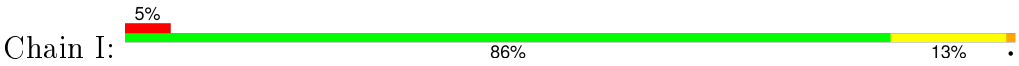
- Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

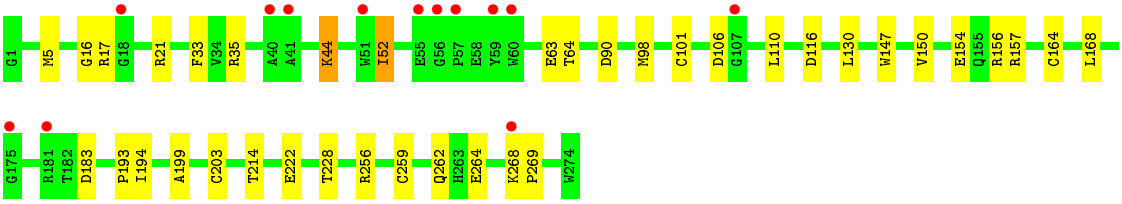
Chain G:



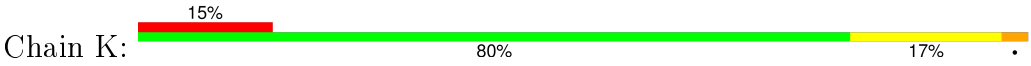


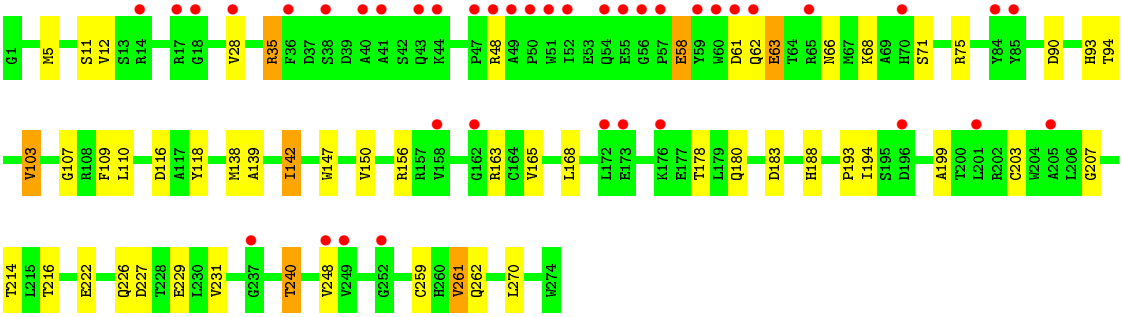
• Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain



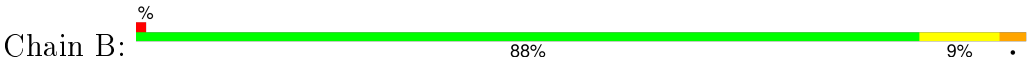


• Molecule 1: HLA class I histocompatibility antigen, A-1 alpha chain

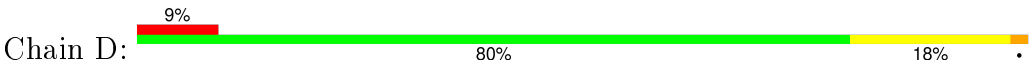




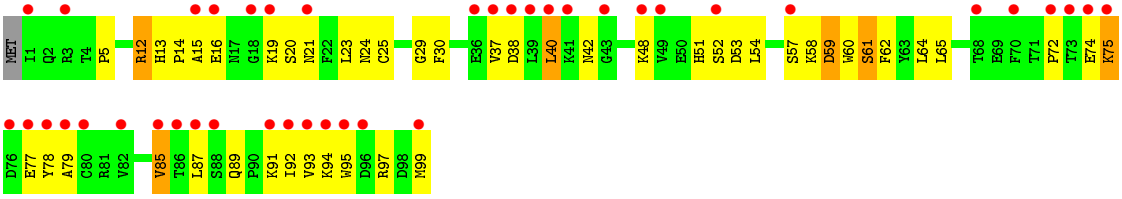
• Molecule 2: Beta-2-microglobulin



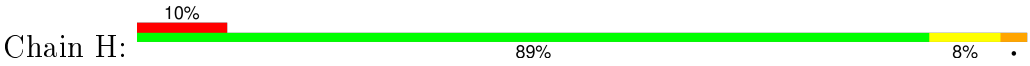
• Molecule 2: Beta-2-microglobulin

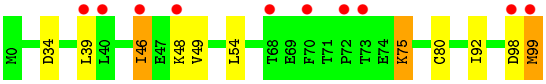


• Molecule 2: Beta-2-microglobulin

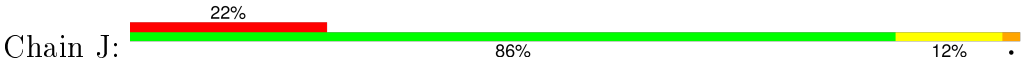


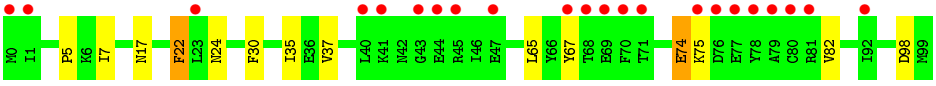
• Molecule 2: Beta-2-microglobulin



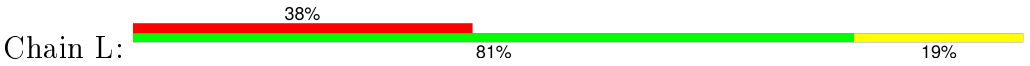


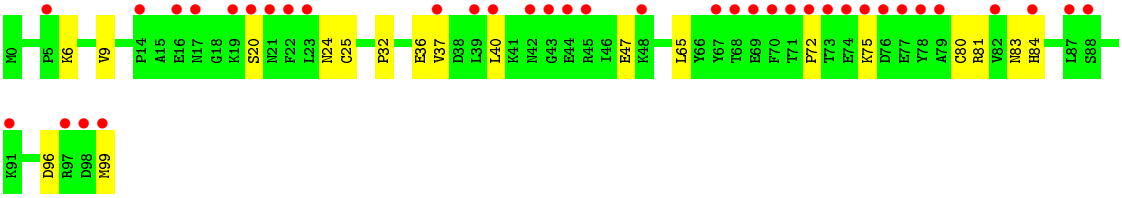
• Molecule 2: Beta-2-microglobulin



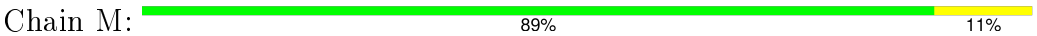


• Molecule 2: Beta-2-microglobulin





• Molecule 3: Nucleoprotein



• Molecule 3: Nucleoprotein

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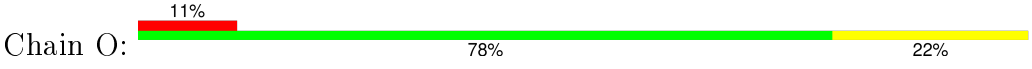


- Molecule 3: Nucleoprotein

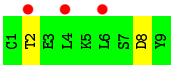
Chain P:

- Molecule 3: Nucleoprotein

Chain Q:

- Molecule 3: Nucleoprotein

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	265.54Å 81.50Å 140.07Å 90.00° 121.58° 90.00°	Depositor
Resolution (Å)	43.49 – 2.39 43.49 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.8 (43.49-2.39) 98.9 (43.49-2.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.39Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.256 , 0.291 0.261 , 0.281	Depositor DCC
R_{free} test set	4976 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	47.6	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 51.1	EDS
Estimated twinning fraction	0.095 for -h-2*l,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 99958 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	19628	wwPDB-VP
Average B, all atoms (Å^2)	62.0	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 56.23 % 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 2.8202e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.41	0/2287	0.62	0/3101
1	C	0.39	0/2287	0.62	0/3101
1	E	0.42	0/2287	0.64	0/3101
1	G	0.40	0/2287	0.61	0/3101
1	I	0.38	0/2287	0.62	0/3101
1	K	0.39	0/2287	0.62	0/3101
2	B	0.40	0/860	0.67	0/1162
2	D	0.43	0/860	0.68	0/1162
2	F	0.48	0/852	0.80	0/1152
2	H	0.41	0/860	0.61	0/1162
2	J	0.39	0/860	0.62	0/1162
2	L	0.42	0/860	0.63	0/1162
3	M	0.44	0/74	0.68	0/97
3	N	0.39	0/74	0.58	0/97
3	O	0.41	0/74	0.63	0/97
3	P	0.41	0/74	0.69	0/97
3	Q	0.43	0/74	0.69	0/97
3	R	0.39	0/74	0.60	0/97
All	All	0.41	0/19318	0.63	0/26150

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	2227	0	2090	17	0
1	C	2227	0	2090	14	0
1	E	2227	0	2090	23	0
1	G	2227	0	2090	18	0
1	I	2227	0	2090	18	0
1	K	2227	0	2090	27	0
2	B	837	0	805	5	0
2	D	837	0	805	10	0
2	F	829	0	796	24	0
2	H	837	0	805	5	0
2	J	837	0	805	6	0
2	L	837	0	805	7	0
3	M	74	0	73	0	0
3	N	74	0	73	2	0
3	O	74	0	73	4	0
3	P	74	0	73	1	0
3	Q	74	0	73	0	0
3	R	74	0	73	1	0
4	A	114	0	0	0	0
4	B	44	0	0	0	0
4	C	106	0	0	0	0
4	D	40	0	0	0	0
4	E	107	0	0	0	0
4	F	28	0	0	1	0
4	G	86	0	0	0	0
4	H	33	0	0	0	0
4	I	94	0	0	1	0
4	J	28	0	0	0	0
4	K	84	0	0	1	0
4	L	27	0	0	0	0
4	M	4	0	0	0	0
4	N	3	0	0	0	0
4	O	2	0	0	0	0
4	P	3	0	0	0	0
4	Q	2	0	0	0	0
4	R	3	0	0	0	0
All	All	19628	0	17799	158	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.

All (158) 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:80:CYS:SG	2.09	0.91
1:G:204:TRP:HZ2	2:H:99:MET:HB3	1.43	0.83
1:K:12:VAL:HG12	1:K:94:THR:HG22	1.59	0.83
1:E:261:VAL:HG22	1:E:270:LEU:HB2	1.69	0.75
2:F:25:CYS:SG	4:F:103:HOH:O	2.45	0.74
1:K:226:GLN:HE21	3:O:8:ASP:HB2	1.53	0.74
1:E:207:GLY:HA2	1:E:240:THR:HG21	1.69	0.73
1:K:207:GLY:HA2	1:K:240:THR:HG21	1.71	0.71
1:E:101:CYS:HG	1:E:164:CYS:HG	1.40	0.68
1:K:226:GLN:OE1	4:K:312:HOH:O	2.12	0.67
1:I:44:LYS:HG3	1:I:64:THR:OG1	1.94	0.67
1:E:207:GLY:HA2	1:E:240:THR:CG2	2.24	0.66
1:K:207:GLY:HA2	1:K:240:THR:CG2	2.25	0.66
1:I:5:MET:HB2	1:I:168:LEU:HD13	1.78	0.66
1:K:226:GLN:NE2	3:O:8:ASP:HB2	2.10	0.65
1:G:189:MET:HE2	1:G:274:TRP:HB2	1.78	0.65
2:B:97:ARG:HG2	2:B:98:ASP:N	2.11	0.65
2:L:96:ASP:HB3	2:L:99:MET:HG2	1.79	0.65
1:G:10:THR:HG21	2:H:54:LEU:HD23	1.79	0.65
1:C:204:TRP:HZ2	2:D:99:MET:HB2	1.62	0.65
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.77	0.65
1:K:261:VAL:HG13	1:K:270:LEU:HB2	1.78	0.64
1:C:5:MET:HB2	1:C:168:LEU:HD13	1.81	0.63
1:A:203:CYS:HG	1:A:259:CYS:HG	1.43	0.63
2:F:24:ASN:HB3	2:F:65:LEU:HD11	1.80	0.63
1:E:5:MET:HB2	1:E:168:LEU:HD13	1.80	0.62
2:L:24:ASN:HB3	2:L:65:LEU:HD11	1.82	0.61
1:K:5:MET:HB2	1:K:168:LEU:HD13	1.82	0.61
2:F:79:ALA:HB2	2:F:94:LYS:HA	1.82	0.61
1:C:70:HIS:CE1	3:N:6:LEU:HD13	2.35	0.61
1:A:268:LYS:HD3	1:I:268:LYS:HD3	1.81	0.61
1:I:33:PHE:HD2	1:I:52:ILE:HG13	1.65	0.60
1:E:163:ARG:HG3	3:O:1:CYS:SG	2.41	0.60
2:F:5:PRO:HB3	2:F:30:PHE:HB3	1.83	0.60
1:G:5:MET:HB2	1:G:168:LEU:HD13	1.82	0.60
1:G:203:CYS:HG	1:G:259:CYS:HG	1.47	0.60
2:D:20:SER:HB3	1:I:106:ASP:HA	1.83	0.60
1:E:150:VAL:HG22	1:K:229:GLU:HB2	1.84	0.60
2:J:7:ILE:HG12	2:J:82:VAL:HG21	1.82	0.59
1:A:188:HIS:HB2	1:C:16:GLY:HA3	1.82	0.59
2:F:23:LEU:HG	2:F:78:TYR:CE2	2.37	0.59
1:C:203:CYS:SG	1:C:259:CYS:SG	3.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:203:CYS:HG	1:I:259:CYS:HG	1.51	0.58
1:E:150:VAL:CG2	1:K:229:GLU:HB2	2.34	0.58
1:E:10:THR:HG21	2:F:54:LEU:HD23	1.86	0.57
1:A:203:CYS:SG	1:A:259:CYS:SG	3.00	0.57
1:E:146:LYS:HG2	1:K:248:VAL:HG11	1.87	0.56
1:A:230:LEU:HD12	1:A:245:ALA:HB2	1.87	0.56
1:I:101:CYS:HG	1:I:164:CYS:HG	1.51	0.56
1:A:256:ARG:HH11	1:I:256:ARG:HD2	1.72	0.55
2:L:40:LEU:HD11	2:L:81:ARG:HB2	1.89	0.55
1:I:203:CYS:SG	1:I:259:CYS:SG	3.05	0.55
2:D:97:ARG:C	2:D:99:MET:H	2.11	0.54
2:B:73:THR:HB	2:B:75:LYS:HE3	1.90	0.54
2:F:12:ARG:HG2	2:F:13:HIS:CE1	2.43	0.54
2:L:20:SER:HA	2:L:72:PRO:HD2	1.90	0.53
1:E:226:GLN:HG3	3:P:8:ASP:HB2	1.90	0.53
1:I:154:GLU:OE1	1:I:157:ARG:NH2	2.40	0.52
2:L:25:CYS:HG	2:L:80:CYS:HG	1.57	0.52
1:A:111:ARG:HD3	1:A:128:GLU:HG3	1.91	0.52
1:K:203:CYS:SG	1:K:259:CYS:SG	3.04	0.52
2:L:32:PRO:O	2:L:84:HIS:HE1	1.92	0.52
2:F:30:PHE:O	2:F:61:SER:O	2.26	0.52
1:C:236:ALA:O	2:D:12:ARG:HG3	2.10	0.52
2:F:42:ASN:HA	2:F:77:GLU:HB3	1.92	0.51
1:K:109:PHE:HD1	1:K:165:VAL:HG11	1.76	0.51
1:K:63:GLU:OE2	3:R:2:THR:HG22	2.09	0.51
1:C:63:GLU:OE2	3:N:2:THR:HG22	2.10	0.51
1:A:189:MET:HE2	1:A:274:TRP:HB2	1.94	0.50
1:K:35:ARG:HG2	1:K:48:ARG:HB2	1.93	0.50
2:H:80:CYS:O	2:H:92:ILE:HA	2.11	0.50
2:J:37:VAL:HG22	2:J:82:VAL:HG12	1.94	0.50
2:F:91:LYS:HE2	1:G:131:ARG:HG2	1.94	0.49
1:E:216:THR:HG23	1:E:260:HIS:HB2	1.94	0.49
1:E:213:ILE:HD11	1:E:243:LYS:HD2	1.95	0.49
2:H:39:LEU:O	2:H:46:ILE:HG12	2.12	0.49
1:C:101:CYS:SG	1:C:164:CYS:SG	3.04	0.49
1:A:130:LEU:O	1:A:157:ARG:NH1	2.46	0.49
1:G:189:MET:HE2	1:G:201:LEU:HD22	1.94	0.48
1:E:28:VAL:HG11	1:E:179:LEU:HD13	1.96	0.48
2:H:39:LEU:HD13	2:H:49:VAL:HG11	1.95	0.48
2:F:78:TYR:O	2:F:95:TRP:HB2	2.13	0.48
2:D:97:ARG:O	2:D:99:MET:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:VAL:HG22	2:B:82:VAL:HG12	1.95	0.48
2:F:13:HIS:HB2	2:F:21:ASN:HB3	1.96	0.48
2:D:7:ILE:HD13	2:D:91:LYS:HG2	1.96	0.48
1:K:103:VAL:HG13	1:K:107:GLY:HA2	1.96	0.47
1:K:93:HIS:ND1	1:K:118:TYR:OH	2.47	0.47
1:A:268:LYS:HD2	1:A:269:PRO:HD2	1.96	0.47
1:C:119:ASP:HB3	2:D:0:MET:HG3	1.97	0.47
1:G:101:CYS:SG	1:G:164:CYS:SG	3.11	0.46
1:I:130:LEU:O	1:I:157:ARG:NH1	2.48	0.46
1:C:156:ARG:HD3	1:C:156:ARG:HA	1.80	0.46
2:B:97:ARG:HG2	2:B:98:ASP:H	1.77	0.46
1:A:189:MET:HE3	1:A:217:TRP:HH2	1.80	0.46
1:G:95:ILE:HD12	1:G:117:ALA:O	2.15	0.46
2:F:57:SER:HB2	2:F:58:LYS:HG3	1.97	0.46
1:G:101:CYS:HG	1:G:164:CYS:HG	1.57	0.46
1:C:200:THR:HG22	1:C:248:VAL:HG22	1.98	0.46
2:L:36:GLU:HB3	2:L:83:ASN:HB3	1.98	0.46
1:K:62:GLN:HE21	1:K:66:ASN:HD21	1.64	0.46
2:J:22:PHE:HD2	2:J:67:TYR:HB2	1.81	0.45
1:E:101:CYS:SG	1:E:164:CYS:SG	3.07	0.45
2:D:37:VAL:HA	2:D:81:ARG:O	2.17	0.45
1:I:33:PHE:CD2	1:I:52:ILE:HG13	2.48	0.45
2:F:75:LYS:HB2	2:F:97:ARG:HH22	1.82	0.45
1:I:268:LYS:HD2	1:I:269:PRO:HD2	1.99	0.45
1:E:213:ILE:HG23	1:E:263:HIS:HD2	1.81	0.45
1:A:13:SER:HA	1:A:20:PRO:HB3	1.98	0.45
2:F:40:LEU:HD11	2:F:79:ALA:HB3	1.98	0.44
1:G:224:GLN:O	1:G:228:THR:HG21	2.18	0.44
2:F:19:LYS:HB3	2:F:20:SER:HB2	1.99	0.44
1:A:156:ARG:HD3	1:A:156:ARG:HA	1.89	0.44
1:E:66:ASN:O	1:E:70:HIS:ND1	2.51	0.44
2:F:51:HIS:O	2:F:64:LEU:CD2	2.65	0.44
1:K:227:ASP:OD1	3:O:8:ASP:HB3	2.17	0.44
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.53	0.44
1:I:101:CYS:SG	1:I:164:CYS:SG	3.10	0.44
1:E:186:LYS:HD2	1:E:206:LEU:HD12	1.98	0.44
2:F:13:HIS:HB3	2:F:14:PRO:HD2	1.99	0.44
1:K:147:TRP:HA	1:K:150:VAL:HG12	2.00	0.44
2:J:24:ASN:HB3	2:J:65:LEU:HD11	2.00	0.44
1:A:189:MET:CE	1:A:274:TRP:HB2	2.47	0.43
1:G:16:GLY:C	1:G:18:GLY:H	2.20	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:93:HIS:ND1	1:G:118:TYR:OH	2.47	0.43
1:K:193:PRO:HA	1:K:199:ALA:HA	2.00	0.43
1:I:147:TRP:HA	1:I:150:VAL:HG12	2.00	0.43
1:G:203:CYS:SG	1:G:259:CYS:SG	3.04	0.43
2:F:74:GLU:HA	2:F:75:LYS:HG2	2.00	0.43
2:F:57:SER:HA	2:F:58:LYS:HA	1.80	0.43
1:C:61:ASP:HB3	1:C:65:ARG:HH21	1.84	0.43
1:K:109:PHE:HD1	1:K:165:VAL:CG1	2.31	0.43
1:K:71:SER:O	1:K:75:ARG:HG2	2.18	0.43
1:E:147:TRP:HA	1:E:150:VAL:HG12	2.00	0.42
1:K:203:CYS:HG	1:K:259:CYS:HG	1.45	0.42
2:F:59:ASP:CG	2:F:60:TRP:H	2.22	0.42
2:F:51:HIS:C	2:F:53:ASP:H	2.23	0.42
1:K:58:GLU:H	1:K:58:GLU:HG3	1.59	0.42
1:E:248:VAL:HG21	1:G:146:LYS:HG2	2.02	0.42
1:E:139:ALA:O	1:E:142:ILE:HG12	2.20	0.42
2:F:29:GLY:HA2	2:F:61:SER:HB3	2.01	0.41
1:G:227:ASP:HB3	1:G:248:VAL:HG13	2.02	0.41
2:J:5:PRO:HB3	2:J:30:PHE:HB3	2.01	0.41
1:K:139:ALA:O	1:K:142:ILE:HG23	2.20	0.41
1:I:214:THR:HB	1:I:262:GLN:HB2	2.02	0.41
1:E:259:CYS:O	1:E:271:THR:HA	2.21	0.41
2:D:5:PRO:HB3	2:D:30:PHE:HB3	2.03	0.41
1:K:214:THR:HB	1:K:262:GLN:HB2	2.03	0.41
1:I:264:GLU:HG2	4:I:369:HOH:O	2.20	0.41
1:C:20:PRO:HD2	1:C:75:ARG:HG2	2.03	0.41
1:A:214:THR:HB	1:A:262:GLN:HB2	2.02	0.41
1:C:214:THR:HB	1:C:262:GLN:HB2	2.02	0.41
1:I:193:PRO:HA	1:I:199:ALA:HA	2.03	0.41
1:G:129:ASP:HB3	1:G:131:ARG:HD2	2.03	0.40
2:J:17:ASN:HD21	2:J:74:GLU:N	2.20	0.40
1:G:93:HIS:CG	1:G:118:TYR:HH	2.38	0.40
1:A:62:GLN:HE21	1:A:66:ASN:HD21	1.69	0.40
2:D:35:ILE:HD11	2:D:64:LEU:CD1	2.51	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	272/274 (99%)	267 (98%)	4 (2%)	1 (0%)	39	56
1	C	272/274 (99%)	267 (98%)	4 (2%)	1 (0%)	39	56
1	E	272/274 (99%)	265 (97%)	7 (3%)	0	100	100
1	G	272/274 (99%)	266 (98%)	5 (2%)	1 (0%)	39	56
1	I	272/274 (99%)	268 (98%)	3 (1%)	1 (0%)	39	56
1	K	272/274 (99%)	267 (98%)	5 (2%)	0	100	100
2	B	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	19	28
2	D	98/100 (98%)	94 (96%)	2 (2%)	2 (2%)	9	11
2	F	97/100 (97%)	74 (76%)	13 (13%)	10 (10%)	1	0
2	H	98/100 (98%)	91 (93%)	5 (5%)	2 (2%)	9	11
2	J	98/100 (98%)	91 (93%)	6 (6%)	1 (1%)	19	28
2	L	98/100 (98%)	90 (92%)	7 (7%)	1 (1%)	19	28
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	2261/2298 (98%)	2172 (96%)	68 (3%)	21 (1%)	21	30

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	ARG
2	D	98	ASP
2	F	15	ALA
2	F	52	SER

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Mol	Chain	Res	Type
2	F	62	PHE
2	F	85	VAL
2	F	89	GLN
1	G	17	ARG
2	F	16	GLU
2	F	48	LYS
2	F	61	SER
2	L	75	LYS
2	B	98	ASP
2	F	72	PRO
2	H	48	LYS
2	D	75	LYS
2	H	75	LYS
2	F	59	ASP
1	I	16	GLY
2	J	75	LYS
1	A	16	GLY

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	231/231 (100%)	215 (93%)	16 (7%)	19 30
1	C	231/231 (100%)	213 (92%)	18 (8%)	16 24
1	E	231/231 (100%)	207 (90%)	24 (10%)	9 12
1	G	231/231 (100%)	214 (93%)	17 (7%)	17 26
1	I	231/231 (100%)	216 (94%)	15 (6%)	21 33
1	K	231/231 (100%)	206 (89%)	25 (11%)	8 11
2	B	95/95 (100%)	89 (94%)	6 (6%)	22 35
2	D	95/95 (100%)	88 (93%)	7 (7%)	17 26
2	F	94/95 (99%)	84 (89%)	10 (11%)	8 12
2	H	95/95 (100%)	90 (95%)	5 (5%)	28 44
2	J	95/95 (100%)	91 (96%)	4 (4%)	36 56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	L	95/95 (100%)	91 (96%)	4 (4%)	36 56
3	M	9/9 (100%)	8 (89%)	1 (11%)	8 10
3	N	9/9 (100%)	8 (89%)	1 (11%)	8 10
3	O	9/9 (100%)	9 (100%)	0	100 100
3	P	9/9 (100%)	9 (100%)	0	100 100
3	Q	9/9 (100%)	8 (89%)	1 (11%)	8 10
3	R	9/9 (100%)	8 (89%)	1 (11%)	8 10
All	All	2009/2010 (100%)	1854 (92%)	155 (8%)	16 24

All (155) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	48	ARG
1	A	61	ASP
1	A	63	GLU
1	A	89	GLU
1	A	110	LEU
1	A	111	ARG
1	A	116	ASP
1	A	156	ARG
1	A	176	LYS
1	A	180	GLN
1	A	183	ASP
1	A	194	ILE
1	A	196	ASP
1	A	222	GLU
1	A	228	THR
2	B	9	VAL
2	B	36	GLU
2	B	45	ARG
2	B	70	PHE
2	B	75	LYS
2	B	97	ARG
1	C	12	VAL
1	C	14	ARG
1	C	35	ARG
1	C	61	ASP
1	C	63	GLU
1	C	110	LEU

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Mol	Chain	Res	Type
1	C	116	ASP
1	C	121	LYS
1	C	138	MET
1	C	156	ARG
1	C	183	ASP
1	C	188	HIS
1	C	190	THR
1	C	194	ILE
1	C	196	ASP
1	C	222	GLU
1	C	228	THR
1	C	230	LEU
2	D	9	VAL
2	D	34	ASP
2	D	37	VAL
2	D	42	ASN
2	D	46	ILE
2	D	70	PHE
2	D	97	ARG
1	E	19	GLU
1	E	35	ARG
1	E	52	ILE
1	E	54	GLN
1	E	63	GLU
1	E	68	LYS
1	E	90	ASP
1	E	110	LEU
1	E	111	ARG
1	E	113	TYR
1	E	116	ASP
1	E	121	LYS
1	E	142	ILE
1	E	156	ARG
1	E	177	GLU
1	E	181	ARG
1	E	183	ASP
1	E	186	LYS
1	E	194	ILE
1	E	213	ILE
1	E	219	ARG
1	E	222	GLU
1	E	224	GLN

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Mol	Chain	Res	Type
1	E	240	THR
2	F	12	ARG
2	F	37	VAL
2	F	38	ASP
2	F	40	LEU
2	F	75	LYS
2	F	85	VAL
2	F	87	LEU
2	F	92	ILE
2	F	93	VAL
2	F	99	MET
1	G	12	VAL
1	G	17	ARG
1	G	35	ARG
1	G	63	GLU
1	G	68	LYS
1	G	98	MET
1	G	103	VAL
1	G	116	ASP
1	G	129	ASP
1	G	134	THR
1	G	138	MET
1	G	156	ARG
1	G	183	ASP
1	G	194	ILE
1	G	222	GLU
1	G	248	VAL
1	G	268	LYS
2	H	34	ASP
2	H	46	ILE
2	H	75	LYS
2	H	98	ASP
2	H	99	MET
1	I	17	ARG
1	I	21	ARG
1	I	35	ARG
1	I	44	LYS
1	I	52	ILE
1	I	63	GLU
1	I	90	ASP
1	I	98	MET
1	I	110	LEU

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Mol	Chain	Res	Type
1	I	116	ASP
1	I	156	ARG
1	I	183	ASP
1	I	194	ILE
1	I	222	GLU
1	I	228	THR
2	J	22	PHE
2	J	35	ILE
2	J	74	GLU
2	J	98	ASP
1	K	11	SER
1	K	28	VAL
1	K	35	ARG
1	K	58	GLU
1	K	61	ASP
1	K	63	GLU
1	K	68	LYS
1	K	90	ASP
1	K	103	VAL
1	K	110	LEU
1	K	116	ASP
1	K	138	MET
1	K	142	ILE
1	K	156	ARG
1	K	163	ARG
1	K	178	THR
1	K	180	GLN
1	K	183	ASP
1	K	188	HIS
1	K	194	ILE
1	K	216	THR
1	K	222	GLU
1	K	231	VAL
1	K	240	THR
1	K	261	VAL
2	L	6	LYS
2	L	9	VAL
2	L	37	VAL
2	L	47	GLU
3	M	8	ASP
3	N	8	ASP
3	Q	8	ASP

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Mol	Chain	Res	Type
3	R	8	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	115	GLN
1	C	62	GLN
1	C	127	ASN
2	F	13	HIS
2	F	31	HIS
2	F	51	HIS
1	G	54	GLN
1	G	96	GLN
1	G	155	GLN
1	G	174	ASN
2	J	17	ASN
1	K	62	GLN
1	K	226	GLN
2	L	84	HIS

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

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	274/274 (100%)	0.21	3 (1%) 82 82	18, 44, 72, 110	0
1	C	274/274 (100%)	0.73	20 (7%) 18 18	34, 58, 93, 109	0
1	E	274/274 (100%)	1.01	39 (14%) 4 3	36, 60, 90, 114	0
1	G	274/274 (100%)	0.80	33 (12%) 6 5	32, 63, 101, 127	0
1	I	274/274 (100%)	0.47	13 (4%) 35 36	26, 56, 101, 127	0
1	K	274/274 (100%)	1.12	40 (14%) 3 3	36, 69, 123, 145	0
2	B	100/100 (100%)	0.36	1 (1%) 84 83	24, 43, 77, 97	0
2	D	100/100 (100%)	0.73	9 (9%) 12 11	32, 51, 78, 85	0
2	F	99/100 (99%)	2.10	41 (41%) 0 0	41, 81, 120, 128	0
2	H	100/100 (100%)	0.84	10 (10%) 9 9	32, 60, 84, 96	0
2	J	100/100 (100%)	1.30	22 (22%) 1 1	34, 71, 107, 116	0
2	L	100/100 (100%)	1.93	38 (38%) 0 0	38, 83, 131, 147	0
3	M	9/9 (100%)	-0.19	0 100 100	28, 35, 43, 48	0
3	N	9/9 (100%)	0.99	1 (11%) 7 7	50, 55, 74, 75	0
3	O	9/9 (100%)	0.98	1 (11%) 7 7	60, 63, 65, 76	0
3	P	9/9 (100%)	1.26	2 (22%) 1 1	54, 62, 66, 78	0
3	Q	9/9 (100%)	-0.08	0 100 100	36, 38, 47, 50	0
3	R	9/9 (100%)	1.79	3 (33%) 0 1	74, 83, 86, 102	0
All	All	2297/2298 (99%)	0.85	276 (12%) 6 5	18, 59, 105, 147	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	21	ASN	9.0
2	F	39	LEU	8.1
2	L	78	TYR	8.1

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Mol	Chain	Res	Type	RSRZ
1	K	47	PRO	7.5
2	F	79	ALA	7.4
1	K	18	GLY	6.9
1	K	49	ALA	6.4
1	I	18	GLY	6.1
1	K	172	LEU	6.1
1	K	52	ILE	6.0
2	J	79	ALA	5.6
2	F	37	VAL	5.6
2	F	41	LYS	5.5
2	L	76	ASP	5.5
2	L	74	GLU	5.4
2	F	76	ASP	5.4
1	E	59	TYR	5.4
1	C	41	ALA	5.4
1	I	56	GLY	5.3
1	K	51	TRP	5.3
1	K	44	LYS	5.2
2	F	40	LEU	5.2
2	F	91	LYS	5.2
1	K	237	GLY	5.1
2	F	16	GLU	5.1
1	K	62	GLN	4.9
1	E	47	PRO	4.9
2	F	87	LEU	4.9
2	L	22	PHE	4.8
1	K	59	TYR	4.8
2	L	37	VAL	4.8
2	F	93	VAL	4.8
2	F	68	THR	4.7
2	F	78	TYR	4.6
2	F	82	VAL	4.6
2	L	79	ALA	4.6
1	K	65	ARG	4.5
2	L	82	VAL	4.5
1	E	194	ILE	4.4
2	J	0	MET	4.3
1	E	16	GLY	4.3
2	F	21	ASN	4.3
2	J	78	TYR	4.3
1	G	34	VAL	4.3
2	J	81	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
2	L	45	ARG	4.2
2	L	68	THR	4.2
2	H	72	PRO	4.2
2	L	39	LEU	4.1
1	K	40	ALA	4.1
1	G	172	LEU	4.1
1	E	176	LYS	4.1
2	H	40	LEU	4.0
3	R	6	LEU	4.0
2	L	75	LYS	3.9
2	F	15	ALA	3.9
2	D	75	LYS	3.9
1	C	60	TRP	3.8
1	K	36	PHE	3.8
3	N	1	CYS	3.8
1	G	16	GLY	3.7
2	L	19	LYS	3.7
2	F	77	GLU	3.7
1	C	54	GLN	3.6
1	E	91	GLY	3.6
1	G	171	TYR	3.6
2	F	38	ASP	3.6
1	I	57	PRO	3.6
1	K	84	TYR	3.6
2	F	86	THR	3.6
1	G	158	VAL	3.6
1	K	38	SER	3.6
1	K	41	ALA	3.6
2	J	40	LEU	3.6
2	L	77	GLU	3.5
2	L	69	GLU	3.5
1	A	41	ALA	3.5
1	I	107	GLY	3.5
2	L	99	MET	3.4
1	G	15	PRO	3.4
2	H	70	PHE	3.4
2	J	67	TYR	3.4
1	E	239	GLY	3.4
2	L	23	LEU	3.4
1	G	175	GLY	3.4
2	J	71	THR	3.4
2	F	74	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
2	J	68	THR	3.3
1	K	70	HIS	3.3
2	F	80	CYS	3.3
1	K	14	ARG	3.3
1	G	126	LEU	3.2
1	E	38	SER	3.2
1	K	43	GLN	3.2
2	F	57	SER	3.2
2	L	97	ARG	3.2
2	L	17	ASN	3.2
1	E	113	TYR	3.1
1	C	16	GLY	3.1
1	G	95	ILE	3.1
2	F	19	LYS	3.1
1	G	110	LEU	3.1
2	L	48	LYS	3.1
1	G	142	ILE	3.1
1	E	69	ALA	3.1
2	D	99	MET	3.1
1	C	196	ASP	3.1
2	F	95	TRP	3.1
2	F	92	ILE	3.1
1	G	41	ALA	3.0
2	J	76	ASP	3.0
2	F	18	GLY	3.0
1	E	267	PRO	3.0
1	I	59	TYR	2.9
1	A	177	GLU	2.9
1	C	56	GLY	2.9
1	G	140	ALA	2.9
1	C	47	PRO	2.9
2	F	73	THR	2.9
2	F	36	GLU	2.9
1	G	51	TRP	2.9
2	H	68	THR	2.8
1	G	104	GLY	2.8
2	F	49	VAL	2.8
2	L	91	LYS	2.8
1	G	179	LEU	2.8
1	K	249	VAL	2.8
1	K	55	GLU	2.8
1	K	61	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	54	GLN	2.7
1	G	17	ARG	2.7
2	H	98	ASP	2.7
2	L	40	LEU	2.7
2	J	45	ARG	2.7
1	A	1	GLY	2.7
1	I	175	GLY	2.7
2	F	48	LYS	2.7
2	J	75	LYS	2.7
2	D	74	GLU	2.7
3	R	4	LEU	2.7
2	F	52	SER	2.7
1	C	178	THR	2.7
1	K	56	GLY	2.7
1	C	61	ASP	2.7
1	G	61	ASP	2.6
2	F	72	PRO	2.6
1	C	106	ASP	2.6
1	C	70	HIS	2.6
1	G	107	GLY	2.6
1	G	60	TRP	2.6
1	G	1	GLY	2.6
1	E	76	ALA	2.6
2	J	80	CYS	2.6
2	J	23	LEU	2.6
1	C	52	ILE	2.6
1	C	57	PRO	2.6
1	E	70	HIS	2.6
1	G	91	GLY	2.6
1	G	109	PHE	2.5
2	F	70	PHE	2.5
1	K	158	VAL	2.5
1	G	177	GLU	2.5
1	C	252	GLY	2.5
2	L	43	GLY	2.5
3	P	1	CYS	2.5
2	F	85	VAL	2.5
2	J	44	GLU	2.5
1	C	75	ARG	2.5
1	I	40	ALA	2.5
1	K	60	TRP	2.5
1	K	173	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	71	THR	2.5
1	E	168	LEU	2.5
1	E	170	ARG	2.5
2	F	75	LYS	2.5
2	J	47	GLU	2.5
1	E	33	PHE	2.5
2	F	43	GLY	2.4
1	G	174	ASN	2.4
1	E	50	PRO	2.4
1	E	189	MET	2.4
1	E	231	VAL	2.4
2	J	69	GLU	2.4
1	E	166	ASP	2.4
2	L	84	HIS	2.4
2	L	16	GLU	2.4
1	K	248	VAL	2.4
1	C	139	ALA	2.4
1	K	28	VAL	2.4
1	K	176	LYS	2.4
2	F	1	ILE	2.4
1	I	51	TRP	2.4
2	F	88	SER	2.4
2	D	73	THR	2.4
2	B	7	ILE	2.4
1	I	181	ARG	2.4
1	K	50	PRO	2.4
2	H	73	THR	2.4
1	E	112	GLY	2.3
1	K	162	GLY	2.3
2	L	87	LEU	2.3
1	G	52	ILE	2.3
1	G	84	TYR	2.3
1	E	48	ARG	2.3
1	E	54	GLN	2.3
1	K	48	ARG	2.3
1	I	41	ALA	2.3
2	F	99	MET	2.3
1	K	17	ARG	2.3
1	K	54	GLN	2.3
2	J	70	PHE	2.3
2	J	43	GLY	2.3
2	D	81	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
2	J	92	ILE	2.3
2	L	73	THR	2.3
2	J	77	GLU	2.3
2	L	88	SER	2.3
1	E	81	LEU	2.3
1	E	110	LEU	2.3
1	K	196	ASP	2.3
2	D	0	MET	2.3
1	E	20	PRO	2.3
2	D	1	ILE	2.3
1	E	64	THR	2.2
2	D	86	THR	2.2
3	P	2	THR	2.2
2	F	94	LYS	2.2
2	L	20	SER	2.2
1	E	157	ARG	2.2
1	G	194	ILE	2.2
2	J	1	ILE	2.2
1	I	268	LYS	2.2
1	E	265	GLY	2.2
2	D	98	ASP	2.2
2	F	96	ASP	2.2
1	E	82	ARG	2.2
2	J	41	LYS	2.2
2	H	46	ILE	2.2
1	C	248	VAL	2.2
1	G	65	ARG	2.2
2	H	48	LYS	2.2
1	G	59	TYR	2.2
2	L	70	PHE	2.2
1	C	179	LEU	2.2
1	E	42	SER	2.2
2	L	42	ASN	2.1
1	E	268	LYS	2.1
2	L	72	PRO	2.1
1	C	85	TYR	2.1
3	R	2	THR	2.1
1	E	177	GLU	2.1
1	K	57	PRO	2.1
1	E	141	GLN	2.1
2	H	39	LEU	2.1
3	O	9	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	63	GLU	2.1
2	L	98	ASP	2.1
1	G	248	VAL	2.1
1	E	80	THR	2.1
2	L	44	GLU	2.1
2	F	3	ARG	2.1
2	L	5	PRO	2.1
2	L	14	PRO	2.1
1	E	174	ASN	2.0
1	K	201	LEU	2.0
1	E	51	TRP	2.0
1	I	60	TRP	2.0
1	K	252	GLY	2.0
1	K	85	TYR	2.0
2	L	67	TYR	2.0
1	E	15	PRO	2.0
1	C	108	ARG	2.0
1	E	173	GLU	2.0
1	I	55	GLU	2.0
1	K	205	ALA	2.0
2	H	99	MET	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.