Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:29 AM GMT

PDB ID	:	2QVJ
Title	:	Crystal structure of a vesicular stomatitis virus nucleocapsid protein Ser290Trp mutant
Authors	:	Luo, M.; Green, T.J.; Zhang, X.; Tsao, J.; Qiu, S.
Deposited on	:	2007-08-08
Resolution	:	2.80 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:

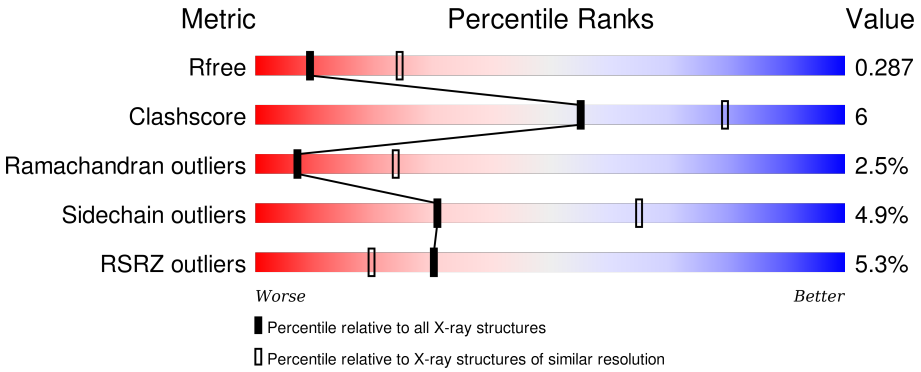
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	421	6% 79% 19%
1	B	421	5% 79% 18%
1	C	421	5% 79% 18%
1	D	421	5% 85% 14%
1	E	421	6% 85% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16675 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	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
1	B	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
1	C	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
1	D	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			
1	E	421	Total	C	N	O	S	0	0	0
			3335	2126	559	632	18			

There are 5 discrepancies between the modelled and reference sequences:

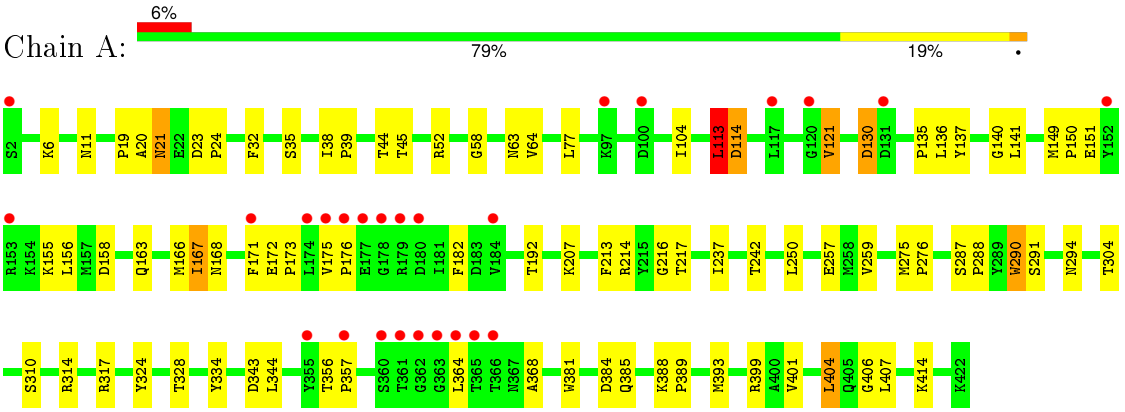
Chain	Residue	Modelled	Actual	Comment	Reference
A	290	TRP	SER	ENGINEERED	UNP P03521
B	290	TRP	SER	ENGINEERED	UNP P03521
C	290	TRP	SER	ENGINEERED	UNP P03521
D	290	TRP	SER	ENGINEERED	UNP P03521
E	290	TRP	SER	ENGINEERED	UNP P03521

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

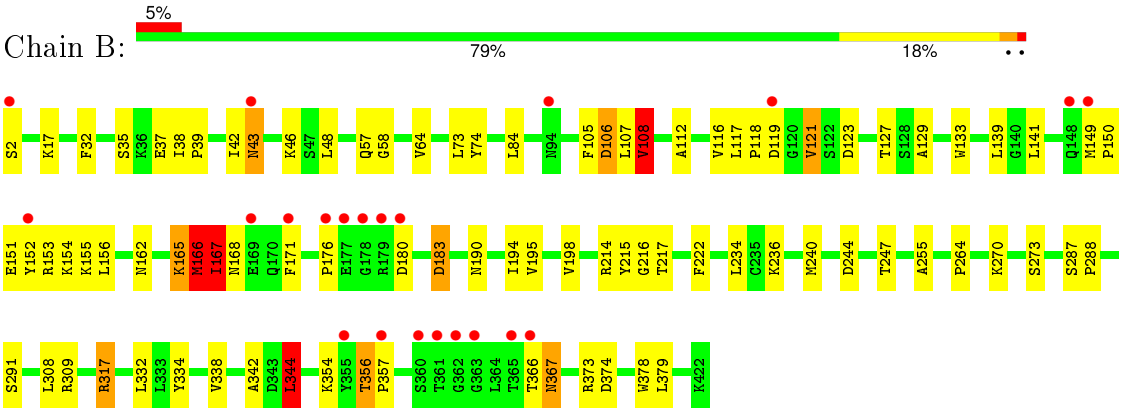
- Molecule 1: Nucleocapsid protein

Chain A:



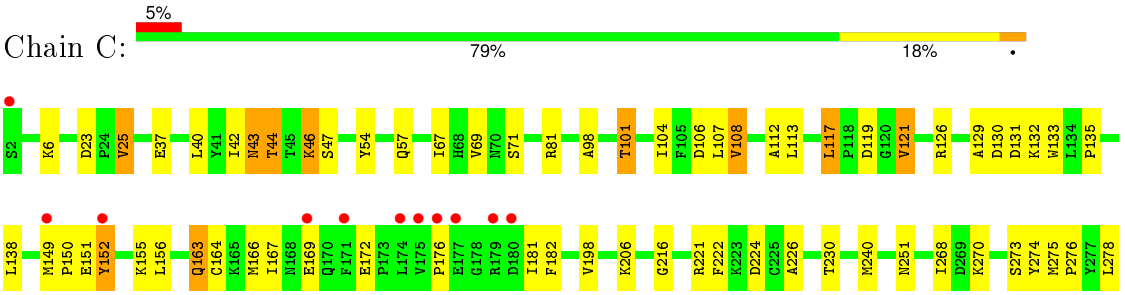
- Molecule 1: Nucleocapsid protein

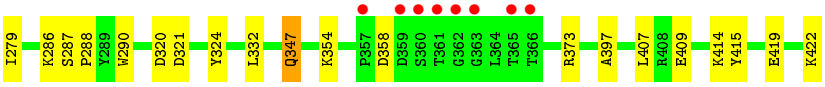
Chain B:



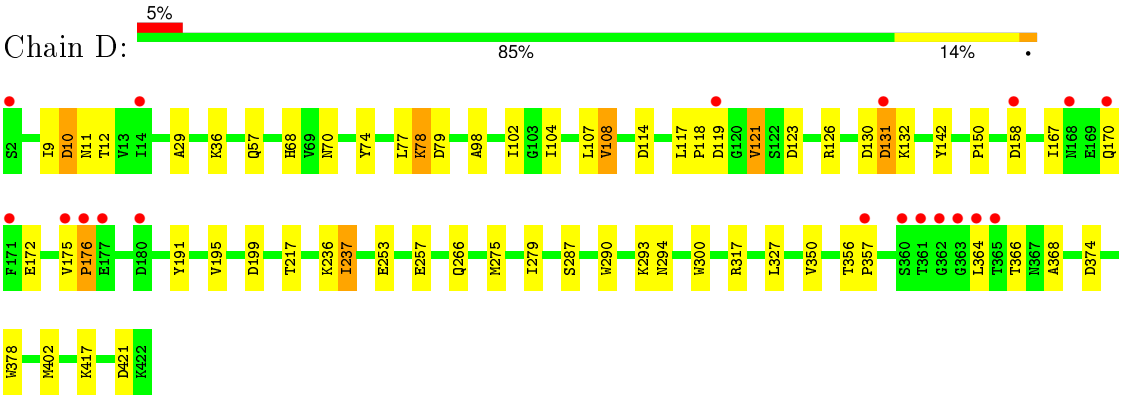
- Molecule 1: Nucleocapsid protein

Chain C:

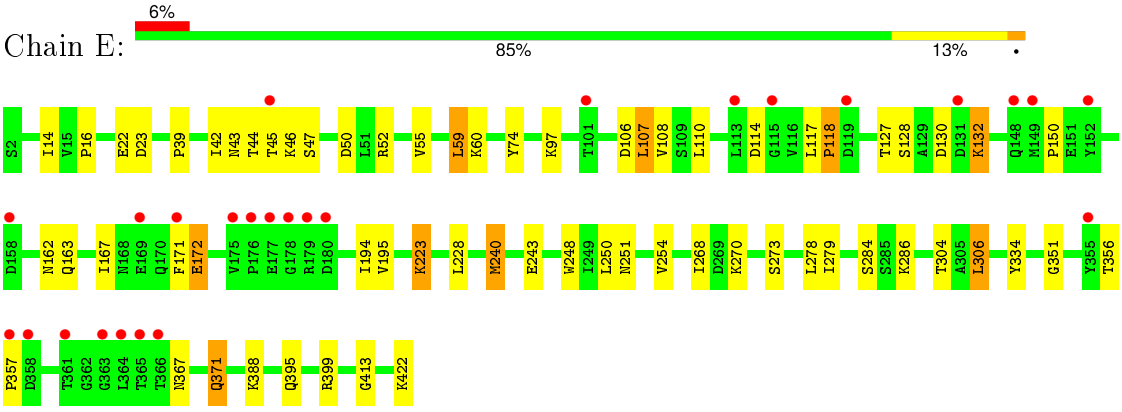




• Molecule 1: Nucleocapsid protein



• Molecule 1: Nucleocapsid protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	166.46Å 236.65Å 74.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.62 – 2.80 41.61 – 2.80	Depositor EDS
% Data completeness (in resolution range)	74.4 (41.62-2.80) 74.4 (41.61-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.24 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.243 , 0.286 0.249 , 0.287	Depositor DCC
R_{free} test set	2796 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 54826 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	16675	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, 0.375 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	0.34	0/3413	0.49	0/4622
1	B	0.34	0/3413	0.55	2/4622 (0.0%)
1	C	0.34	0/3413	0.50	0/4622
1	D	0.34	0/3413	0.48	0/4622
1	E	0.37	0/3413	0.49	0/4622
All	All	0.35	0/17065	0.50	2/23110 (0.0%)

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	2
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	MET	N-CA-C	11.57	142.25	111.00
1	B	167	ILE	N-CA-CB	-7.18	94.29	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	165	LYS	Peptide
1	B	167	ILE	Peptide
1	E	106	ASP	Peptide

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	3335	0	3292	48	0
1	B	3335	0	3292	56	0
1	C	3335	0	3292	49	0
1	D	3335	0	3292	36	0
1	E	3335	0	3292	32	0
All	All	16675	0	16460	209	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 6.

All (209) 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:B:167:ILE:HG22	1:B:168:ASN:CB	1.37	1.54
1:B:167:ILE:HG22	1:B:168:ASN:CG	1.55	1.27
1:B:167:ILE:CG2	1:B:168:ASN:HB2	1.70	1.21
1:B:167:ILE:CG2	1:B:168:ASN:CG	2.30	0.99
1:B:167:ILE:HG22	1:B:168:ASN:HB2	0.96	0.94
1:D:57:GLN:HG2	1:D:123:ASP:HB2	1.49	0.93
1:B:37:GLU:HB2	1:B:108:VAL:HG21	1.50	0.91
1:B:167:ILE:CG2	1:B:168:ASN:CB	2.33	0.88
1:E:107:LEU:HD23	1:E:107:LEU:N	1.94	0.82
1:B:356:THR:H	1:B:357:PRO:HD2	1.50	0.77
1:B:167:ILE:CG2	1:B:168:ASN:ND2	2.50	0.74
1:B:356:THR:H	1:B:357:PRO:CD	2.01	0.73
1:D:57:GLN:HB3	1:D:121:VAL:HG12	1.71	0.72
1:B:57:GLN:HG2	1:B:123:ASP:HB2	1.72	0.71
1:C:25:VAL:HG21	1:C:288:PRO:HA	1.72	0.71
1:B:129:ALA:HB1	1:B:133:TRP:HE1	1.56	0.71
1:D:199:ASP:HB2	1:D:217:THR:HG22	1.73	0.71
1:E:107:LEU:H	1:E:107:LEU:HD23	1.54	0.70
1:D:175:VAL:HB	1:D:176:PRO:HD3	1.72	0.70
1:E:107:LEU:H	1:E:107:LEU:CD2	2.00	0.70
1:A:214:ARG:HA	1:A:217:THR:HG22	1.75	0.69
1:B:167:ILE:HG22	1:B:168:ASN:ND2	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:ILE:HG12	1:A:168:ASN:H	1.58	0.69
1:B:167:ILE:CB	1:B:168:ASN:HB2	2.24	0.68
1:E:55:VAL:O	1:E:59:LEU:HB2	1.94	0.68
1:A:389:PRO:HA	1:A:393:MET:HE3	1.77	0.67
1:C:57:GLN:HB3	1:C:121:VAL:HB	1.76	0.67
1:C:415:TYR:O	1:C:419:GLU:HB2	1.94	0.67
1:E:108:VAL:O	1:E:108:VAL:HG12	1.95	0.65
1:B:166:MET:SD	1:B:166:MET:N	2.69	0.65
1:D:356:THR:N	1:D:357:PRO:CD	2.59	0.65
1:A:21:ASN:HD22	1:A:21:ASN:H	1.44	0.65
1:A:356:THR:H	1:A:357:PRO:HD3	1.62	0.65
1:C:42:ILE:HD11	1:C:71:SER:HA	1.79	0.64
1:C:126:ARG:HH22	1:C:129:ALA:HB3	1.61	0.64
1:B:166:MET:C	1:B:167:ILE:HG12	2.19	0.63
1:B:166:MET:O	1:B:167:ILE:HG12	2.00	0.62
1:B:162:ASN:HA	1:B:165:LYS:HE3	1.81	0.62
1:A:175:VAL:HB	1:A:176:PRO:HD3	1.82	0.62
1:A:401:VAL:O	1:A:404:LEU:HB2	2.00	0.61
1:A:257:GLU:HB3	1:A:294:ASN:HD22	1.64	0.61
1:C:37:GLU:HB2	1:C:108:VAL:HG21	1.81	0.61
1:B:356:THR:N	1:B:357:PRO:HD2	2.15	0.61
1:C:224:ASP:OD1	1:C:279:ILE:HG13	2.00	0.61
1:D:57:GLN:CG	1:D:123:ASP:HB2	2.28	0.61
1:E:228:LEU:HD11	1:E:268:ILE:HD11	1.83	0.61
1:B:166:MET:C	1:B:167:ILE:CG1	2.68	0.60
1:B:57:GLN:HB3	1:B:121:VAL:HG12	1.84	0.60
1:A:58:GLY:HA3	1:A:64:VAL:HB	1.84	0.59
1:D:356:THR:H	1:D:357:PRO:HD3	1.68	0.59
1:B:2:SER:HA	1:D:350:VAL:HG21	1.84	0.59
1:C:43:ASN:HB3	1:C:112:ALA:H	1.68	0.58
1:C:278:LEU:HD12	1:C:279:ILE:HG12	1.84	0.58
1:A:52:ARG:HD3	1:A:130:ASP:HB3	1.86	0.58
1:A:364:LEU:H	1:A:368:ALA:HB2	1.68	0.58
1:E:306:LEU:HD11	1:E:413:GLY:HA2	1.86	0.58
1:B:244:ASP:O	1:B:247:THR:HG22	2.03	0.58
1:A:314:ARG:HD2	1:A:404:LEU:HD21	1.87	0.57
1:B:356:THR:N	1:B:357:PRO:CD	2.68	0.56
1:C:226:ALA:O	1:C:230:THR:HG23	2.04	0.56
1:A:214:ARG:HA	1:A:217:THR:CG2	2.37	0.55
1:B:117:LEU:H	1:B:118:PRO:HD3	1.71	0.55
1:A:290:TRP:HE3	1:A:291:SER:H	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:LEU:HB3	1:C:354:LYS:HE2	1.89	0.54
1:B:17:LYS:HB2	1:C:268:ILE:HD11	1.89	0.54
1:D:117:LEU:N	1:D:118:PRO:CD	2.70	0.54
1:C:117:LEU:HD12	1:C:117:LEU:H	1.72	0.54
1:C:409:GLU:HA	1:C:414:LYS:HD2	1.89	0.54
1:A:135:PRO:HB2	1:A:213:PHE:CE1	2.43	0.53
1:B:270:LYS:HD3	1:B:273:SER:HB2	1.90	0.53
1:B:117:LEU:N	1:B:118:PRO:CD	2.72	0.53
1:C:270:LYS:HD3	1:C:273:SER:HB2	1.90	0.52
1:C:126:ARG:NH2	1:C:129:ALA:HB3	2.24	0.52
1:A:140:GLY:HA2	1:A:216:GLY:HA3	1.90	0.52
1:B:105:PHE:C	1:B:107:LEU:H	2.14	0.51
1:C:132:LYS:HG2	1:C:166:MET:HB3	1.91	0.51
1:C:275:MET:HG3	1:C:276:PRO:HD3	1.92	0.51
1:E:23:ASP:OD1	1:E:286:LYS:HE2	2.11	0.51
1:C:130:ASP:O	1:C:135:PRO:HD2	2.10	0.51
1:C:44:THR:HG23	1:C:46:LYS:HE2	1.93	0.50
1:A:290:TRP:HE3	1:A:291:SER:N	2.08	0.50
1:A:344:LEU:HB3	1:E:250:LEU:HB3	1.93	0.50
1:A:137:TYR:OH	1:A:173:PRO:HD3	2.12	0.50
1:D:130:ASP:O	1:D:132:LYS:N	2.44	0.50
1:D:195:VAL:HG13	1:D:217:THR:HG23	1.94	0.50
1:A:135:PRO:HB2	1:A:213:PHE:HE1	1.75	0.50
1:B:255:ALA:HB2	1:C:347:GLN:HG2	1.92	0.49
1:D:70:ASN:HD21	1:D:191:TYR:HB2	1.78	0.49
1:C:320:ASP:HA	1:C:324:TYR:OH	2.13	0.49
1:D:300:TRP:HB2	1:D:327:LEU:HD22	1.94	0.49
1:B:374:ASP:O	1:B:378:TRP:HD1	1.95	0.49
1:C:81:ARG:HB3	1:C:101:THR:HG22	1.94	0.49
1:E:52:ARG:HD3	1:E:130:ASP:HB3	1.94	0.49
1:A:6:LYS:HD3	1:A:11:ASN:HA	1.94	0.49
1:A:63:ASN:HD21	1:A:121:VAL:HG21	1.78	0.48
1:C:67:ILE:HD12	1:C:117:LEU:HD11	1.96	0.47
1:A:324:TYR:O	1:A:328:THR:HG23	2.13	0.47
1:B:117:LEU:N	1:B:118:PRO:HD3	2.30	0.47
1:E:44:THR:HB	1:E:46:LYS:HE3	1.95	0.47
1:E:44:THR:O	1:E:46:LYS:HG2	2.15	0.47
1:E:251:ASN:HB2	1:E:254:VAL:HG23	1.97	0.47
1:B:354:LYS:HE3	1:B:356:THR:HB	1.96	0.47
1:D:356:THR:H	1:D:357:PRO:CD	2.23	0.47
1:B:43:ASN:HA	1:B:112:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:371:GLN:H	1:E:371:GLN:CD	2.18	0.47
1:D:107:LEU:O	1:D:108:VAL:HG23	2.14	0.46
1:B:317:ARG:NE	1:B:317:ARG:H	2.13	0.46
1:E:270:LYS:HD2	1:E:273:SER:HB3	1.98	0.46
1:A:32:PHE:HA	1:A:35:SER:O	2.16	0.46
1:C:149:MET:O	1:C:151:GLU:N	2.40	0.46
1:D:417:LYS:O	1:D:421:ASP:HB3	2.14	0.46
1:A:237:ILE:CD1	1:A:310:SER:HB2	2.45	0.46
1:D:130:ASP:C	1:D:132:LYS:H	2.20	0.45
1:A:356:THR:N	1:A:357:PRO:HD3	2.30	0.45
1:E:42:ILE:HD11	1:E:194:ILE:HD11	1.97	0.45
1:C:321:ASP:HB3	1:D:236:LYS:HD3	1.98	0.45
1:A:141:LEU:HD13	1:A:182:PHE:CE2	2.52	0.45
1:D:29:ALA:H	1:D:266:GLN:HE22	1.65	0.45
1:A:259:VAL:HG12	1:E:14:ILE:HD12	1.99	0.45
1:C:287:SER:HB3	1:C:290:TRP:HB2	1.97	0.45
1:C:181:ILE:HG13	1:C:182:PHE:N	2.32	0.45
1:A:356:THR:N	1:A:357:PRO:CD	2.80	0.44
1:C:133:TRP:HB2	1:C:163:GLN:HE21	1.82	0.44
1:A:19:PRO:HB3	1:B:222:PHE:CZ	2.52	0.44
1:E:304:THR:HG21	1:E:334:TYR:CD2	2.52	0.44
1:D:257:GLU:HG2	1:D:294:ASN:HD22	1.83	0.44
1:A:113:LEU:HD13	1:A:113:LEU:H	1.82	0.44
1:C:152:TYR:HA	1:C:155:LYS:HB2	2.00	0.44
1:B:287:SER:HA	1:B:288:PRO:HD3	1.87	0.44
1:D:287:SER:HB3	1:D:290:TRP:HB2	1.99	0.44
1:C:130:ASP:C	1:C:132:LYS:H	2.21	0.44
1:E:39:PRO:HB3	1:E:110:LEU:HD13	1.99	0.44
1:C:23:ASP:HB2	1:C:286:LYS:HE3	2.00	0.44
1:B:42:ILE:HG12	1:B:74:TYR:HB2	1.99	0.44
1:B:342:ALA:HB1	1:B:344:LEU:HD23	2.00	0.44
1:B:214:ARG:O	1:B:216:GLY:N	2.51	0.44
1:C:69:VAL:HG13	1:C:138:LEU:HD13	1.99	0.44
1:D:10:ASP:HB3	1:D:12:THR:OG1	2.17	0.43
1:A:399:ARG:HB3	1:E:422:LYS:HE3	1.99	0.43
1:E:356:THR:N	1:E:357:PRO:CD	2.81	0.43
1:A:77:LEU:HB3	1:A:104:ILE:HD12	2.00	0.43
1:B:195:VAL:HG13	1:B:217:THR:HG22	2.00	0.43
1:E:130:ASP:C	1:E:132:LYS:H	2.22	0.43
1:C:332:LEU:HD13	1:C:397:ALA:HB2	2.00	0.43
1:B:32:PHE:HA	1:B:35:SER:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:ILE:HD11	1:C:198:VAL:HG22	2.01	0.43
1:C:130:ASP:C	1:C:132:LYS:N	2.71	0.43
1:E:240:MET:H	1:E:240:MET:HG2	1.70	0.43
1:D:126:ARG:HH22	1:D:170:GLN:HE22	1.66	0.43
1:C:407:LEU:HD13	1:C:414:LYS:HA	2.00	0.43
1:D:279:ILE:HD11	1:D:287:SER:HB2	2.00	0.43
1:B:149:MET:O	1:B:151:GLU:N	2.40	0.43
1:E:278:LEU:HD13	1:E:284:SER:HB3	2.01	0.43
1:D:374:ASP:O	1:D:378:TRP:HD1	2.01	0.43
1:B:38:ILE:HA	1:B:39:PRO:HD3	1.88	0.42
1:C:324:TYR:HD2	1:D:237:ILE:HD11	1.84	0.42
1:C:54:TYR:CE1	1:C:119:ASP:HA	2.54	0.42
1:B:57:GLN:CG	1:B:123:ASP:HB2	2.47	0.42
1:C:149:MET:C	1:C:151:GLU:H	2.22	0.42
1:D:199:ASP:HB2	1:D:217:THR:CG2	2.47	0.42
1:D:293:LYS:HA	1:D:293:LYS:HD2	1.81	0.42
1:C:240:MET:CE	1:C:373:ARG:HD3	2.50	0.42
1:C:37:GLU:CB	1:C:108:VAL:HG21	2.49	0.42
1:C:67:ILE:CD1	1:C:117:LEU:HD11	2.50	0.42
1:B:366:THR:HG22	1:B:367:ASN:HD22	1.84	0.42
1:B:180:ASP:HA	1:B:183:ASP:HB2	2.00	0.42
1:E:60:LYS:HA	1:E:172:GLU:HB3	2.01	0.42
1:A:21:ASN:HD22	1:A:21:ASN:N	2.15	0.42
1:C:270:LYS:HB3	1:C:273:SER:HB2	2.02	0.42
1:D:364:LEU:H	1:D:368:ALA:HB2	1.85	0.42
1:A:287:SER:HA	1:A:288:PRO:HD3	1.87	0.42
1:D:77:LEU:C	1:D:79:ASP:H	2.22	0.42
1:B:38:ILE:HD11	1:B:107:LEU:HB3	2.02	0.41
1:E:240:MET:HE1	1:E:248:TRP:CD1	2.55	0.41
1:B:194:ILE:O	1:B:198:VAL:HG23	2.20	0.41
1:D:142:TYR:HB2	1:D:191:TYR:OH	2.20	0.41
1:C:164:CYS:SG	1:C:169:GLU:HG2	2.61	0.41
1:A:304:THR:HG21	1:A:334:TYR:CD2	2.55	0.41
1:A:167:ILE:CG1	1:A:168:ASN:H	2.29	0.41
1:D:68:HIS:CE1	1:D:118:PRO:HB2	2.55	0.41
1:D:68:HIS:HE1	1:D:118:PRO:HB2	1.86	0.41
1:C:107:LEU:HD21	1:C:274:TYR:HE2	1.86	0.41
1:E:127:THR:OG1	1:E:128:SER:N	2.53	0.41
1:B:129:ALA:HB1	1:B:133:TRP:NE1	2.29	0.41
1:A:149:MET:O	1:A:151:GLU:N	2.47	0.41
1:A:356:THR:H	1:A:357:PRO:CD	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:THR:HB	1:E:16:PRO:HB2	2.02	0.41
1:C:221:ARG:HG2	1:C:222:PHE:CD2	2.55	0.41
1:C:133:TRP:O	1:C:163:GLN:NE2	2.54	0.41
1:B:334:TYR:O	1:B:338:VAL:HG23	2.20	0.41
1:D:74:TYR:CE2	1:D:78:LYS:HD2	2.56	0.41
1:E:42:ILE:HD13	1:E:74:TYR:HB2	2.03	0.41
1:A:113:LEU:HB2	1:A:114:ASP:H	1.70	0.41
1:A:23:ASP:HA	1:A:24:PRO:HD3	1.82	0.41
1:E:395:GLN:O	1:E:399:ARG:HG2	2.21	0.41
1:A:155:LYS:O	1:A:158:ASP:HB3	2.21	0.41
1:A:38:ILE:HA	1:A:39:PRO:HD3	1.90	0.41
1:A:381:TRP:O	1:A:385:GLN:HG2	2.21	0.41
1:E:223:LYS:HG3	1:E:279:ILE:HD13	2.02	0.41
1:C:422:LYS:HB2	1:D:402:MET:SD	2.61	0.41
1:E:117:LEU:O	1:E:118:PRO:C	2.59	0.40
1:A:275:MET:HB3	1:A:276:PRO:HD3	2.03	0.40
1:A:149:MET:C	1:A:151:GLU:H	2.24	0.40
1:A:404:LEU:HD22	1:A:407:LEU:HD21	2.04	0.40
1:B:106:ASP:C	1:B:107:LEU:HD12	2.42	0.40
1:D:104:ILE:H	1:D:104:ILE:HG13	1.73	0.40
1:B:58:GLY:HA3	1:B:64:VAL:HB	2.02	0.40
1:B:240:MET:HE1	1:B:373:ARG:HD3	2.03	0.40
1:B:190:ASN:O	1:B:194:ILE:HG13	2.21	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	419/421 (100%)	383 (91%)	26 (6%)	10 (2%)	7 25
1	B	419/421 (100%)	373 (89%)	35 (8%)	11 (3%)	7 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	419/421 (100%)	376 (90%)	32 (8%)	11 (3%)	7 22
1	D	419/421 (100%)	372 (89%)	36 (9%)	11 (3%)	7 22
1	E	419/421 (100%)	379 (90%)	30 (7%)	10 (2%)	7 25
All	All	2095/2105 (100%)	1883 (90%)	159 (8%)	53 (2%)	7 24

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	356	THR
1	C	113	LEU
1	D	98	ALA
1	E	45	THR
1	A	44	THR
1	A	113	LEU
1	A	343	ASP
1	B	43	ASN
1	B	108	VAL
1	B	176	PRO
1	C	44	THR
1	C	176	PRO
1	D	131	ASP
1	D	167	ILE
1	E	47	SER
1	A	20	ALA
1	A	406	GLY
1	B	344	LEU
1	C	131	ASP
1	D	119	ASP
1	E	22	GLU
1	E	114	ASP
1	E	367	ASN
1	A	150	PRO
1	A	167	ILE
1	B	367	ASN
1	C	98	ALA
1	C	216	GLY
1	D	78	LYS
1	D	176	PRO
1	E	150	PRO
1	A	114	ASP
1	A	121	VAL

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Mol	Chain	Res	Type
1	B	46	LYS
1	B	121	VAL
1	C	108	VAL
1	C	150	PRO
1	C	167	ILE
1	D	9	ILE
1	D	114	ASP
1	D	121	VAL
1	E	167	ILE
1	B	150	PRO
1	B	215	TYR
1	C	47	SER
1	C	172	GLU
1	D	150	PRO
1	E	118	PRO
1	E	351	GLY
1	A	172	GLU
1	B	264	PRO
1	E	172	GLU
1	D	172	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	362/362 (100%)	344 (95%)	18 (5%)	30	64
1	B	362/362 (100%)	336 (93%)	26 (7%)	18	45
1	C	362/362 (100%)	346 (96%)	16 (4%)	35	69
1	D	362/362 (100%)	350 (97%)	12 (3%)	45	79
1	E	362/362 (100%)	346 (96%)	16 (4%)	35	69
All	All	1810/1810 (100%)	1722 (95%)	88 (5%)	31	65

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	45	THR
1	A	113	LEU
1	A	130	ASP
1	A	136	LEU
1	A	156	LEU
1	A	163	GLN
1	A	166	MET
1	A	171	PHE
1	A	192	THR
1	A	207	LYS
1	A	250	LEU
1	A	290	TRP
1	A	317	ARG
1	A	384	ASP
1	A	388	LYS
1	A	404	LEU
1	A	414	LYS
1	B	48	LEU
1	B	73	LEU
1	B	84	LEU
1	B	106	ASP
1	B	108	VAL
1	B	116	VAL
1	B	119	ASP
1	B	127	THR
1	B	139	LEU
1	B	141	LEU
1	B	152	TYR
1	B	153	ARG
1	B	154	LYS
1	B	155	LYS
1	B	156	LEU
1	B	166	MET
1	B	171	PHE
1	B	183	ASP
1	B	234	LEU
1	B	236	LYS
1	B	291	SER
1	B	308	LEU
1	B	309	ARG
1	B	317	ARG
1	B	332	LEU

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Mol	Chain	Res	Type
1	B	344	LEU
1	C	6	LYS
1	C	25	VAL
1	C	40	LEU
1	C	43	ASN
1	C	46	LYS
1	C	101	THR
1	C	106	ASP
1	C	117	LEU
1	C	121	VAL
1	C	152	TYR
1	C	156	LEU
1	C	163	GLN
1	C	206	LYS
1	C	251	ASN
1	C	347	GLN
1	C	358	ASP
1	D	10	ASP
1	D	11	ASN
1	D	36	LYS
1	D	102	ILE
1	D	108	VAL
1	D	131	ASP
1	D	158	ASP
1	D	237	ILE
1	D	253	GLU
1	D	275	MET
1	D	317	ARG
1	D	366	THR
1	E	43	ASN
1	E	50	ASP
1	E	59	LEU
1	E	97	LYS
1	E	107	LEU
1	E	132	LYS
1	E	162	ASN
1	E	163	GLN
1	E	171	PHE
1	E	195	VAL
1	E	223	LYS
1	E	240	MET
1	E	243	GLU

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Mol	Chain	Res	Type
1	E	306	LEU
1	E	371	GLN
1	E	388	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	57	GLN
1	A	294	ASN
1	A	346	GLN
1	A	395	GLN
1	B	251	ASN
1	B	346	GLN
1	B	367	ASN
1	B	385	GLN
1	C	21	ASN
1	C	57	GLN
1	C	163	GLN
1	C	187	ASN
1	C	294	ASN
1	C	302	GLN
1	C	346	GLN
1	C	367	ASN
1	D	70	ASN
1	D	163	GLN
1	D	170	GLN
1	D	266	GLN
1	D	294	ASN
1	E	43	ASN
1	E	57	GLN
1	E	70	ASN
1	E	162	ASN
1	E	395	GLN

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	421/421 (100%)	0.01	26 (6%)	24	15	11, 29, 69, 93	0
1	B	421/421 (100%)	0.03	22 (5%)	31	20	12, 27, 71, 87	0
1	C	421/421 (100%)	-0.06	19 (4%)	37	26	11, 27, 67, 88	0
1	D	421/421 (100%)	0.01	19 (4%)	37	26	13, 29, 66, 84	0
1	E	421/421 (100%)	0.01	26 (6%)	24	15	13, 34, 69, 90	0
All	All	2105/2105 (100%)	0.00	112 (5%)	30	20	11, 29, 69, 93	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	357	PRO	9.2
1	C	2	SER	9.1
1	D	2	SER	8.5
1	D	357	PRO	8.4
1	E	176	PRO	7.8
1	B	176	PRO	7.5
1	A	176	PRO	7.1
1	A	361	THR	6.8
1	A	363	GLY	6.6
1	C	362	GLY	6.5
1	C	177	GLU	6.0
1	C	176	PRO	5.9
1	C	357	PRO	5.9
1	C	363	GLY	5.9
1	E	177	GLU	5.8
1	B	362	GLY	5.7
1	B	361	THR	5.5
1	B	2	SER	5.3
1	A	2	SER	5.3
1	E	363	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	D	362	GLY	5.1
1	B	363	GLY	5.0
1	D	363	GLY	4.9
1	D	361	THR	4.7
1	A	365	THR	4.7
1	E	366	THR	4.6
1	B	366	THR	4.6
1	A	177	GLU	4.6
1	D	360	SER	4.6
1	C	365	THR	4.4
1	E	180	ASP	4.3
1	C	366	THR	4.1
1	C	360	SER	4.0
1	B	365	THR	3.9
1	B	179	ARG	3.8
1	B	177	GLU	3.7
1	B	178	GLY	3.7
1	A	357	PRO	3.7
1	B	360	SER	3.7
1	A	179	ARG	3.6
1	B	180	ASP	3.6
1	E	358	ASP	3.5
1	B	171	PHE	3.5
1	A	175	VAL	3.5
1	C	359	ASP	3.5
1	D	365	THR	3.5
1	A	180	ASP	3.4
1	E	364	LEU	3.4
1	B	148	GLN	3.2
1	C	152	TYR	3.2
1	A	355	TYR	3.1
1	D	177	GLU	3.1
1	A	171	PHE	3.0
1	C	180	ASP	3.0
1	E	357	PRO	2.9
1	C	174	LEU	2.9
1	E	365	THR	2.9
1	D	131	ASP	2.9
1	C	361	THR	2.9
1	E	131	ASP	2.8
1	B	119	ASP	2.8
1	D	158	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	180	ASP	2.7
1	B	355	TYR	2.7
1	B	43	ASN	2.7
1	E	178	GLY	2.7
1	A	117	LEU	2.6
1	A	100	ASP	2.6
1	E	148	GLN	2.6
1	E	361	THR	2.6
1	A	184	VAL	2.6
1	C	175	VAL	2.6
1	E	45	THR	2.5
1	E	152	TYR	2.5
1	A	366	THR	2.5
1	C	149	MET	2.5
1	C	171	PHE	2.5
1	A	174	LEU	2.5
1	D	364	LEU	2.5
1	D	119	ASP	2.4
1	E	171	PHE	2.3
1	C	169	GLU	2.3
1	A	178	GLY	2.3
1	A	362	GLY	2.3
1	E	115	GLY	2.3
1	A	131	ASP	2.3
1	D	175	VAL	2.3
1	A	364	LEU	2.3
1	E	355	TYR	2.3
1	D	170	GLN	2.3
1	D	14	ILE	2.2
1	A	153	ARG	2.2
1	D	176	PRO	2.2
1	E	179	ARG	2.2
1	E	149	MET	2.2
1	E	113	LEU	2.2
1	E	119	ASP	2.1
1	B	169	GLU	2.1
1	B	152	TYR	2.1
1	E	158	ASP	2.1
1	B	149	MET	2.1
1	C	179	ARG	2.1
1	A	97	LYS	2.1
1	A	360	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	175	VAL	2.1
1	E	101	THR	2.1
1	E	169	GLU	2.1
1	A	120	GLY	2.0
1	A	152	TYR	2.0
1	B	94	ASN	2.0
1	D	168	ASN	2.0
1	D	171	PHE	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.