Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:09 PM GMT

PDB ID	:	1NOV
Title	:	NODAMURA VIRUS
Authors	:	Natarajan, P.; Johnson, J.E.
Deposited on	:	1997-09-16
Resolution	:	3.50 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:

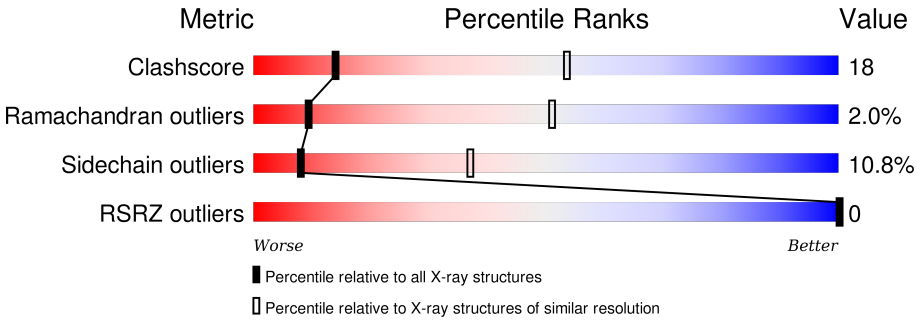
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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	355	52% 30% • • 13%
1	B	355	55% 28% • 13%
1	C	355	56% 29% 6% • 9%
2	D	44	25% 20% 55%
2	E	44	30% 9% 61%
2	F	44	18% 14% 7% 61%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7451 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 NODAMURA VIRUS COAT PROTEINS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	0	0
			2300	1468	373	445	14			
1	B	309	Total	C	N	O	S	0	0	0
			2297	1465	373	445	14			
1	C	324	Total	C	N	O	S	0	0	0
			2434	1541	412	467	14			

- Molecule 2 is a protein called NODAMURA VIRUS COAT PROTEINS.

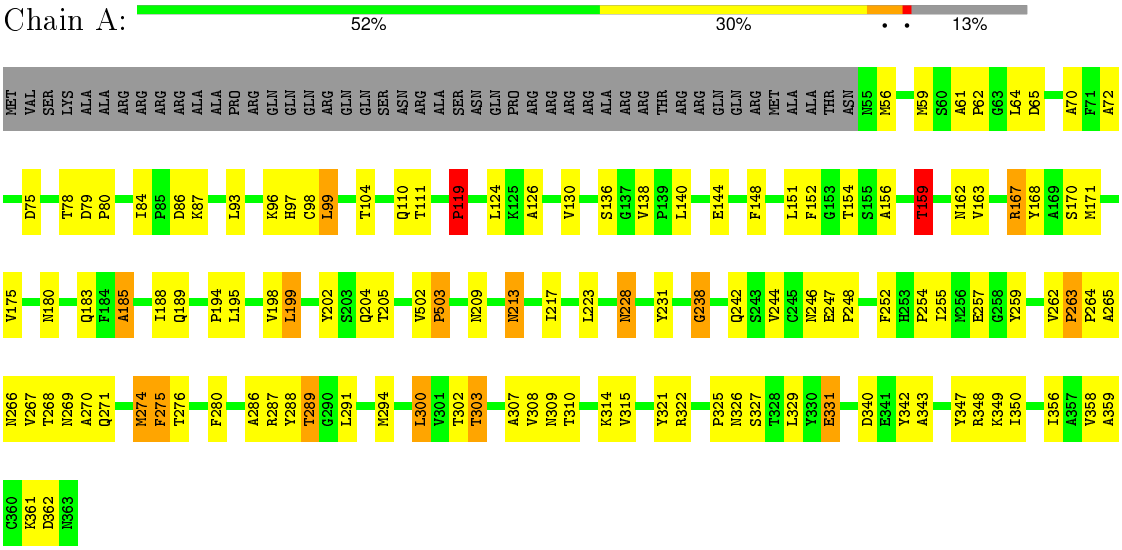
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	20	Total	C	N	O	0	0	0
			149	96	28	25			
2	E	17	Total	C	N	O	0	0	0
			134	87	25	22			
2	F	17	Total	C	N	O	0	0	0
			137	88	26	23			

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.

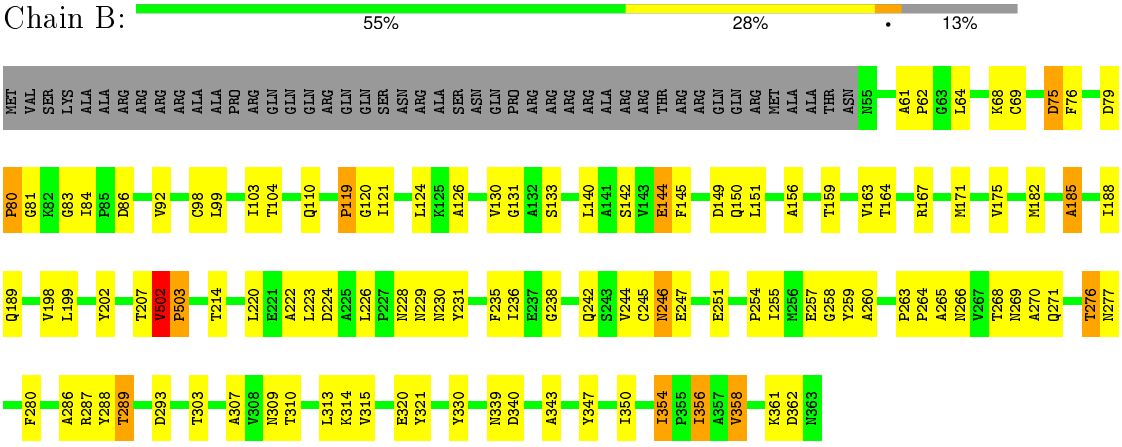
- Molecule 1: NODAMURA VIRUS COAT PROTEINS

Chain A:



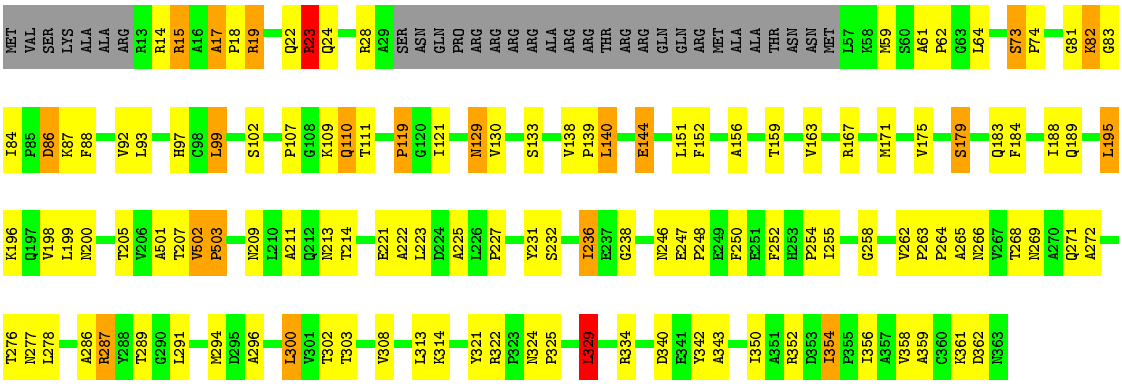
- Molecule 1: NODAMURA VIRUS COAT PROTEINS

Chain B:



- Molecule 1: NODAMURA VIRUS COAT PROTEINS

Chain C:



• Molecule 2: NODAMURA VIRUS COAT PROTEINS

Chain D:

• Molecule 2: NODAMURA VIRUS COAT PROTEINS

Chain E:

• Molecule 2: NODAMURA VIRUS COAT PROTEINS

Chain F:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	562.09Å 354.13Å 612.77Å 90.00° 110.89° 90.00°	Depositor
Resolution (Å)	8.00 – 3.50 20.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	48.1 (8.00-3.50) 51.3 (20.00-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	8.10 (at 3.29Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.296 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 78.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.38$, $< L^2 > = 0.20$	Xtriage
Outliers	0 of 1708847 reflections	Xtriage
F_o,F_c correlation	0.06	EDS
Total number of atoms	7451	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.65% 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	0.42	0/2356	0.77	2/3221 (0.1%)
1	B	0.42	0/2353	0.78	3/3217 (0.1%)
1	C	0.42	0/2490	0.79	6/3396 (0.2%)
2	D	0.47	0/151	0.71	0/203
2	E	0.48	0/136	0.78	0/182
2	F	0.50	0/139	0.88	1/186 (0.5%)
All	All	0.42	0/7625	0.78	12/10405 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	ARG	N-CA-C	6.45	128.42	111.00
1	C	329	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	263	PRO	N-CA-C	-5.63	97.45	112.10
1	C	263	PRO	N-CA-C	-5.52	97.74	112.10
1	A	503	PRO	N-CA-C	-5.49	97.83	112.10
1	C	503	PRO	N-CA-C	-5.46	97.92	112.10
1	A	263	PRO	N-CA-C	-5.36	98.18	112.10
1	B	502	VAL	C-N-CD	5.13	139.17	128.40
1	C	22	GLN	N-CA-C	-5.13	97.16	111.00
2	F	374	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	23	ARG	N-CA-C	5.09	124.75	111.00
1	B	503	PRO	N-CA-C	-5.02	99.05	112.10

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	2300	0	2250	94	0
1	B	2297	0	2241	84	0
1	C	2434	0	2387	102	0
2	D	149	0	143	8	0
2	E	134	0	134	3	0
2	F	137	0	138	10	0
All	All	7451	0	7293	269	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 18.

All (269) 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:C:502:VAL:HB	1:C:503:PRO:HD3	1.35	1.08
1:A:180:ASN:HB3	1:A:183:GLN:HB2	1.40	1.02
1:A:502:VAL:HB	1:A:503:PRO:HD3	1.40	0.99
1:A:156:ALA:HB3	1:A:287:ARG:HD2	1.42	0.99
1:A:171:MET:HB2	1:A:294:MET:HE3	1.49	0.94
1:C:84:ILE:HD12	1:C:167:ARG:HD3	1.52	0.89
1:B:198:VAL:HG22	1:C:254:PRO:HB2	1.57	0.87
1:A:254:PRO:HB2	1:C:198:VAL:HG22	1.59	0.85
1:A:217:ILE:H	1:A:274:MET:HE1	1.42	0.83
1:C:199:LEU:HD21	1:C:213:ASN:HB3	1.63	0.81
1:C:156:ALA:HA	1:C:159:THR:HG23	1.62	0.80
1:C:156:ALA:H	1:C:287:ARG:NH1	1.78	0.80
1:A:303:THR:HB	1:A:309:ASN:HD22	1.48	0.78
1:B:502:VAL:HB	1:B:503:PRO:CD	2.12	0.78
1:C:268:THR:OG1	1:C:271:GLN:HG3	1.84	0.78
1:A:198:VAL:HG22	1:B:254:PRO:HB2	1.67	0.75
1:B:246:ASN:HB2	1:B:293:ASP:O	1.87	0.74
1:C:188:ILE:HD12	1:C:238:GLY:HA2	1.69	0.74
1:C:358:VAL:HG21	2:F:366:PHE:HE2	1.53	0.74
1:B:350:ILE:HD13	2:E:370:VAL:HG13	1.70	0.74
1:C:502:VAL:HB	1:C:503:PRO:CD	2.15	0.73
1:C:152:PHE:O	1:C:159:THR:HA	1.87	0.73
1:C:189:GLN:HA	1:C:231:TYR:O	1.89	0.73
1:A:268:THR:HB	1:A:271:GLN:HG3	1.71	0.73
1:C:156:ALA:H	1:C:287:ARG:HH11	1.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:HD11	2:E:374:LEU:HD21	1.73	0.71
1:A:156:ALA:HB3	1:A:287:ARG:CD	2.20	0.70
1:A:325:PRO:HB3	1:C:227:PRO:HG3	1.72	0.70
1:C:214:THR:HG21	1:C:272:ALA:HA	1.71	0.70
1:C:15:ARG:O	1:C:19:ARG:HB2	1.92	0.69
1:C:156:ALA:N	1:C:287:ARG:HD3	2.08	0.69
1:A:124:LEU:HB3	1:A:140:LEU:HB3	1.74	0.69
1:B:86:ASP:HA	1:B:339:ASN:HD22	1.57	0.69
1:A:65:ASP:HB3	1:A:80:PRO:O	1.92	0.69
1:C:167:ARG:HB2	1:C:252:PHE:CD1	2.28	0.68
1:B:255:ILE:HG23	1:B:289:THR:HG22	1.76	0.67
1:C:88:PHE:HB3	1:C:167:ARG:HH22	1.60	0.66
1:A:356:ILE:H	1:A:356:ILE:HD12	1.58	0.66
1:B:133:SER:HB2	1:B:224:ASP:OD2	1.94	0.66
1:A:163:VAL:HG11	1:A:321:TYR:CD1	2.31	0.66
1:B:156:ALA:HB2	1:B:287:ARG:CG	2.25	0.66
1:A:189:GLN:HA	1:A:231:TYR:O	1.96	0.65
1:A:257:GLU:H	1:C:200:ASN:ND2	1.93	0.65
1:C:205:THR:HG22	1:C:209:ASN:OD1	1.97	0.65
1:C:23:ARG:HD3	1:C:24:GLN:H	1.62	0.65
1:C:110:GLN:HG2	1:C:130:VAL:HA	1.79	0.64
1:B:83:GLY:HA3	1:B:320:GLU:OE2	1.98	0.64
1:A:159:THR:HG23	1:A:257:GLU:HG2	1.79	0.64
1:B:156:ALA:HB2	1:B:287:ARG:HG3	1.79	0.64
1:A:358:VAL:HG11	1:A:362:ASP:HB2	1.79	0.64
1:B:207:THR:HG22	1:B:502:VAL:H	1.62	0.64
1:A:248:PRO:HD2	1:B:251:GLU:HG2	1.80	0.64
1:A:199:LEU:HD22	1:A:213:ASN:HB2	1.79	0.63
1:A:217:ILE:H	1:A:274:MET:CE	2.11	0.63
1:A:263:PRO:HG3	1:A:274:MET:SD	2.39	0.63
1:A:350:ILE:HD13	2:D:370:VAL:HG13	1.81	0.63
1:A:188:ILE:HD12	1:A:238:GLY:HA2	1.81	0.63
1:B:268:THR:HB	1:B:271:GLN:HG3	1.81	0.62
1:B:265:ALA:O	1:B:266:ASN:HB2	2.00	0.61
1:B:159:THR:HB	1:B:257:GLU:HG2	1.81	0.61
1:A:136:SER:O	1:A:276:THR:HG22	1.99	0.61
1:A:86:ASP:OD2	1:C:248:PRO:HB3	2.00	0.61
1:C:59:MET:HG2	1:C:342:TYR:HD1	1.66	0.61
1:A:180:ASN:HB3	1:A:183:GLN:CB	2.26	0.60
1:C:81:GLY:O	1:C:83:GLY:N	2.34	0.60
1:B:163:VAL:HG11	1:B:321:TYR:CD1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:ILE:O	1:B:354:ILE:HG12	2.01	0.60
1:A:349:LYS:CD	2:D:378:LEU:HD23	2.32	0.60
1:B:175:VAL:O	1:B:238:GLY:HA3	2.03	0.59
1:B:268:THR:HG22	1:B:270:ALA:H	1.66	0.59
1:C:163:VAL:HG11	1:C:321:TYR:CD1	2.38	0.59
1:C:175:VAL:O	1:C:238:GLY:HA3	2.03	0.58
1:A:152:PHE:O	1:A:159:THR:HA	2.02	0.58
1:A:349:LYS:HD2	2:D:378:LEU:HD23	1.84	0.58
1:B:244:VAL:HG13	1:B:347:TYR:CZ	2.38	0.58
1:C:262:VAL:HG21	1:C:278:LEU:HD12	1.84	0.58
1:A:110:GLN:HB3	1:A:300:LEU:HD21	1.86	0.58
2:D:368:GLU:HG2	2:D:371:ARG:HH21	1.69	0.58
1:A:502:VAL:HB	1:A:503:PRO:CD	2.25	0.58
1:C:167:ARG:HB2	1:C:252:PHE:HD1	1.66	0.58
1:A:265:ALA:O	1:A:266:ASN:HB2	2.03	0.58
1:A:194:PRO:O	1:B:164:THR:HG21	2.03	0.58
1:A:259:TYR:O	1:A:287:ARG:HB3	2.04	0.57
1:C:354:ILE:HD11	2:F:366:PHE:HE1	1.68	0.57
1:B:156:ALA:HB3	1:B:287:ARG:NH1	2.20	0.57
1:B:220:LEU:O	1:B:223:LEU:HB2	2.05	0.56
1:A:213:ASN:HD22	1:C:213:ASN:ND2	2.02	0.56
1:C:156:ALA:HA	1:C:159:THR:CG2	2.36	0.56
1:A:140:LEU:HD11	1:A:223:LEU:HD11	1.88	0.56
1:B:124:LEU:HB3	1:B:140:LEU:HB3	1.88	0.56
1:C:350:ILE:HD13	2:F:370:VAL:HG13	1.88	0.55
1:B:84:ILE:HD12	1:B:84:ILE:H	1.71	0.55
1:A:303:THR:CB	1:A:309:ASN:HD22	2.17	0.55
1:C:247:GLU:HG3	1:C:248:PRO:HD2	1.88	0.55
1:B:149:ASP:HB2	1:B:150:GLN:NE2	2.21	0.55
1:A:244:VAL:HG13	1:A:347:TYR:CZ	2.42	0.55
1:B:244:VAL:HG12	1:B:245:CYS:N	2.21	0.55
1:C:73:SER:N	1:C:74:PRO:HD2	2.22	0.55
1:A:340:ASP:OD2	1:A:343:ALA:HB2	2.08	0.54
1:C:358:VAL:HG11	1:C:362:ASP:HB2	1.90	0.54
1:B:214:THR:HG23	1:B:264:PRO:HD2	1.90	0.54
1:C:156:ALA:HB2	1:C:287:ARG:HG2	1.89	0.53
1:C:144:GLU:HG2	1:C:286:ALA:HB2	1.90	0.53
1:C:156:ALA:H	1:C:287:ARG:HD3	1.72	0.53
1:A:202:TYR:HE1	1:A:204:GLN:HG3	1.71	0.53
1:B:358:VAL:HG11	1:B:362:ASP:HB2	1.91	0.53
1:A:268:THR:HG22	1:A:270:ALA:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:VAL:O	1:A:238:GLY:HA3	2.09	0.53
1:A:167:ARG:HD2	1:A:252:PHE:CE1	2.45	0.52
1:A:138:VAL:O	1:A:276:THR:HB	2.10	0.52
1:A:72:ALA:HB1	1:A:75:ASP:OD2	2.09	0.52
1:B:189:GLN:OE1	1:B:226:LEU:HD11	2.10	0.52
1:A:267:VAL:HG23	1:C:211:ALA:CB	2.40	0.52
1:C:19:ARG:HH12	1:C:24:GLN:HA	1.74	0.51
1:A:61:ALA:N	1:A:62:PRO:HD2	2.25	0.51
1:A:167:ARG:HD2	1:A:252:PHE:CZ	2.45	0.51
1:C:156:ALA:HB2	1:C:287:ARG:CG	2.41	0.51
1:A:70:ALA:HA	1:A:170:SER:HB3	1.93	0.51
1:C:156:ALA:CB	1:C:287:ARG:HH11	2.23	0.51
1:A:326:ASN:HD22	1:C:221:GLU:HB3	1.75	0.51
1:C:88:PHE:HZ	1:C:322:ARG:NH1	2.08	0.51
1:A:99:LEU:O	1:A:314:LYS:HA	2.11	0.51
1:A:183:GLN:HG2	1:A:308:VAL:HB	1.92	0.50
1:C:340:ASP:OD2	1:C:343:ALA:HB2	2.11	0.50
1:B:202:TYR:HE2	1:B:214:THR:HG1	1.59	0.50
2:F:378:LEU:O	2:F:378:LEU:HD22	2.12	0.50
1:A:275:PHE:CD1	1:A:276:THR:HG23	2.47	0.50
1:B:188:ILE:HD12	1:B:238:GLY:HA2	1.93	0.50
1:C:99:LEU:O	1:C:314:LYS:HA	2.12	0.50
1:B:214:THR:HG23	1:B:264:PRO:CD	2.42	0.49
1:A:59:MET:CG	1:A:342:TYR:HD2	2.25	0.49
1:B:156:ALA:HB2	1:B:287:ARG:CD	2.42	0.49
1:A:228:ASN:H	1:A:228:ASN:ND2	2.11	0.49
1:B:99:LEU:O	1:B:314:LYS:HA	2.11	0.49
1:A:148:PHE:CE2	1:A:286:ALA:HB1	2.48	0.49
1:C:82:LYS:NZ	1:C:334:ARG:HD2	2.27	0.49
1:B:121:ILE:HG12	1:B:142:SER:HB2	1.95	0.48
2:D:369:ARG:HB2	2:D:369:ARG:HH11	1.78	0.48
1:C:167:ARG:HB2	1:C:252:PHE:CE1	2.47	0.48
1:C:61:ALA:N	1:C:62:PRO:HD2	2.28	0.48
1:B:198:VAL:HG12	1:B:199:LEU:N	2.29	0.48
1:B:260:ALA:HA	1:B:287:ARG:HD3	1.95	0.48
1:A:358:VAL:CG1	1:A:362:ASP:HB2	2.42	0.48
1:B:189:GLN:HA	1:B:231:TYR:O	2.14	0.48
1:B:276:THR:CG2	1:B:277:ASN:N	2.77	0.48
1:C:199:LEU:CD2	1:C:213:ASN:HB3	2.38	0.48
1:C:19:ARG:HH11	1:C:24:GLN:HG2	1.78	0.47
1:A:59:MET:HE2	1:A:64:LEU:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:VAL:HB	1:B:503:PRO:HD3	1.91	0.47
1:B:246:ASN:O	1:B:247:GLU:HG3	2.13	0.47
1:A:110:GLN:HG3	1:A:130:VAL:HA	1.96	0.47
1:B:229:ASN:O	1:B:356:ILE:HD12	2.14	0.47
1:C:358:VAL:CG1	1:C:362:ASP:HB2	2.44	0.47
1:B:61:ALA:N	1:B:62:PRO:HD2	2.29	0.47
1:B:182:MET:HG2	1:B:182:MET:O	2.14	0.47
1:C:354:ILE:HD11	2:F:366:PHE:CE1	2.48	0.47
1:A:257:GLU:H	1:C:200:ASN:HD22	1.60	0.47
1:C:262:VAL:O	1:C:264:PRO:HD3	2.15	0.47
1:C:358:VAL:HG21	2:F:366:PHE:CE2	2.40	0.47
1:C:265:ALA:O	1:C:266:ASN:HB2	2.15	0.47
2:F:366:PHE:O	2:F:370:VAL:HG23	2.15	0.47
1:A:98:CYS:HA	1:A:315:VAL:O	2.14	0.47
1:A:213:ASN:ND2	1:C:213:ASN:ND2	2.63	0.47
1:A:502:VAL:CB	1:A:503:PRO:HD3	2.29	0.46
1:C:97:HIS:HE1	1:C:321:TYR:OH	1.99	0.46
1:B:303:THR:HB	1:B:309:ASN:HD22	1.80	0.46
1:B:110:GLN:NE2	1:B:131:GLY:H	2.13	0.46
1:C:59:MET:CG	1:C:342:TYR:HD1	2.26	0.46
1:A:97:HIS:HE1	1:A:321:TYR:OH	1.99	0.46
1:A:348:ARG:HG2	1:A:348:ARG:HH11	1.81	0.46
1:C:84:ILE:HG22	1:C:86:ASP:HB3	1.98	0.46
1:A:247:GLU:O	1:A:348:ARG:NH2	2.49	0.46
1:C:198:VAL:HG12	1:C:199:LEU:N	2.30	0.46
1:B:502:VAL:HB	1:B:503:PRO:HD2	1.93	0.46
1:B:110:GLN:CG	1:B:130:VAL:HA	2.45	0.46
1:C:156:ALA:N	1:C:287:ARG:HH11	2.11	0.46
1:B:163:VAL:HG12	1:B:255:ILE:HD12	1.98	0.46
1:B:75:ASP:N	1:B:75:ASP:OD1	2.49	0.46
1:A:168:TYR:HB3	1:A:294:MET:CE	2.47	0.45
1:C:189:GLN:HG2	1:C:232:SER:OG	2.16	0.45
1:A:188:ILE:CD1	1:A:238:GLY:HA2	2.46	0.45
1:C:152:PHE:HE1	1:C:255:ILE:HD13	1.81	0.45
1:C:358:VAL:CG2	2:F:366:PHE:HE2	2.25	0.45
1:B:188:ILE:HG13	1:B:235:PHE:HA	1.99	0.45
1:A:244:VAL:HG13	1:A:347:TYR:CE2	2.51	0.45
1:B:120:GLY:O	1:B:145:PHE:HB2	2.16	0.45
1:B:68:LYS:HD2	1:B:80:PRO:HG2	1.98	0.45
1:C:156:ALA:HB3	1:C:287:ARG:HH11	1.82	0.45
1:C:358:VAL:HG12	1:C:359:ALA:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:ARG:HD3	1:C:15:ARG:HA	1.38	0.45
1:A:198:VAL:HG12	1:A:199:LEU:N	2.32	0.45
1:C:358:VAL:HG12	1:C:359:ALA:N	2.32	0.45
1:C:110:GLN:HB2	1:C:300:LEU:HD21	1.99	0.45
1:B:144:GLU:HG2	1:B:286:ALA:HB2	1.98	0.45
1:A:119:PRO:HB2	1:A:289:THR:OG1	2.16	0.45
1:A:325:PRO:HD2	1:C:222:ALA:HB2	1.99	0.45
1:B:159:THR:HG22	1:B:255:ILE:CG2	2.47	0.44
1:B:358:VAL:CG1	1:B:362:ASP:HB2	2.47	0.44
1:A:280:PHE:CE2	1:A:288:TYR:HB2	2.53	0.44
1:B:156:ALA:HB3	1:B:287:ARG:HH11	1.81	0.44
1:A:59:MET:HE2	1:A:64:LEU:CA	2.47	0.44
1:B:222:ALA:HB2	1:C:324:ASN:OD1	2.18	0.44
1:C:236:ILE:HD13	1:C:236:ILE:HA	1.84	0.44
1:A:148:PHE:CE1	1:A:152:PHE:HB2	2.53	0.44
1:A:228:ASN:HD21	1:B:330:TYR:HD2	1.65	0.44
1:C:171:MET:HB2	1:C:294:MET:HE2	2.00	0.44
1:B:103:ILE:HD11	1:B:313:LEU:HD22	1.99	0.44
1:B:207:THR:HG23	1:C:501:ALA:O	2.17	0.43
1:A:126:ALA:HB2	1:A:140:LEU:HD23	2.00	0.43
1:C:179:SER:OG	1:C:308:VAL:O	2.36	0.43
1:C:184:PHE:CG	1:C:236:ILE:HG12	2.53	0.43
1:B:84:ILE:HD12	1:B:84:ILE:N	2.33	0.43
1:A:326:ASN:HA	1:C:225:ALA:HB2	2.00	0.43
2:F:371:ARG:O	2:F:375:LYS:N	2.49	0.43
1:B:340:ASP:OD2	1:B:343:ALA:HB2	2.19	0.43
1:B:156:ALA:HB1	1:B:258:GLY:H	1.84	0.43
1:C:156:ALA:HB1	1:C:258:GLY:H	1.84	0.43
1:B:110:GLN:HG3	1:B:130:VAL:HA	2.01	0.43
1:B:185:ALA:HB3	1:B:307:ALA:HB2	2.01	0.43
1:B:69:CYS:HA	1:B:79:ASP:OD1	2.18	0.43
2:E:367:TRP:CZ3	2:E:370:VAL:HG11	2.54	0.43
1:B:202:TYR:HE2	1:B:214:THR:OG1	2.01	0.43
1:C:140:LEU:HD11	1:C:223:LEU:HD11	2.01	0.43
1:A:59:MET:HG3	1:A:342:TYR:HD2	1.84	0.43
1:A:262:VAL:O	1:A:264:PRO:HD3	2.18	0.43
1:A:185:ALA:HB3	1:A:307:ALA:HB2	2.00	0.42
1:C:15:ARG:CZ	1:C:18:PRO:HG2	2.50	0.42
1:A:162:ASN:HA	1:A:327:SER:HB2	2.00	0.42
1:B:354:ILE:HA	1:B:354:ILE:HD13	1.77	0.42
1:C:152:PHE:HB3	1:C:159:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:LYS:HB3	1:B:76:PHE:CE2	2.55	0.42
1:B:222:ALA:HB2	1:C:325:PRO:HD2	2.02	0.42
1:B:226:LEU:HD13	1:B:230:ASN:ND2	2.35	0.42
1:C:156:ALA:CB	1:C:258:GLY:H	2.33	0.42
1:C:156:ALA:N	1:C:287:ARG:NH1	2.57	0.42
2:D:371:ARG:O	2:D:374:LEU:HD23	2.19	0.42
1:C:84:ILE:HD13	1:C:250:PHE:CD2	2.54	0.42
1:C:107:PRO:HA	1:C:303:THR:HG22	2.01	0.42
1:B:198:VAL:CG2	1:C:254:PRO:HB2	2.41	0.41
1:A:322:ARG:NH1	1:C:246:ASN:HB2	2.34	0.41
1:C:93:LEU:HD11	1:C:329:LEU:HB2	2.01	0.41
1:A:86:ASP:OD2	1:A:167:ARG:NH2	2.53	0.41
1:C:269:ASN:OD1	1:C:277:ASN:HB3	2.20	0.41
1:C:138:VAL:HA	1:C:139:PRO:HD3	1.87	0.41
1:C:198:VAL:HG12	1:C:199:LEU:H	1.85	0.41
1:B:244:VAL:CG1	1:B:245:CYS:N	2.83	0.41
2:F:367:TRP:CE3	2:F:367:TRP:HA	2.55	0.41
1:A:79:ASP:HB3	1:A:96:LYS:HD3	2.02	0.41
1:B:126:ALA:HB2	1:B:140:LEU:HD23	2.00	0.41
1:A:205:THR:HA	1:A:209:ASN:HA	2.02	0.41
1:B:98:CYS:HA	1:B:315:VAL:O	2.19	0.41
1:B:244:VAL:HG13	1:B:347:TYR:CE2	2.54	0.41
1:B:104:THR:HG23	1:B:310:THR:HG22	2.03	0.41
1:A:359:ALA:C	1:A:361:LYS:H	2.24	0.41
1:C:121:ILE:HD12	1:C:121:ILE:N	2.36	0.41
2:D:378:LEU:HD13	2:D:378:LEU:O	2.21	0.41
1:C:109:LYS:HE2	1:C:129:ASN:ND2	2.36	0.41
1:A:274:MET:HE3	1:A:274:MET:HB3	1.80	0.41
1:C:17:ALA:CB	1:C:18:PRO:CD	2.99	0.41
1:B:259:TYR:HB3	1:B:288:TYR:HB3	2.03	0.41
1:A:93:LEU:HD11	1:A:329:LEU:HB3	2.03	0.41
1:B:185:ALA:HB3	1:B:307:ALA:CB	2.51	0.41
1:C:195:LEU:HD11	1:C:296:ALA:HB2	2.03	0.40
1:B:142:SER:HB3	1:B:280:PHE:CD1	2.57	0.40
1:A:163:VAL:HG12	1:A:255:ILE:HD12	2.03	0.40
1:A:329:LEU:O	1:A:331:GLU:N	2.54	0.40
1:C:214:THR:CG2	1:C:272:ALA:HA	2.45	0.40
2:D:366:PHE:O	2:D:370:VAL:HG23	2.22	0.40
1:A:84:ILE:HG22	1:A:86:ASP:HB2	2.04	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	307/355 (86%)	280 (91%)	20 (6%)	7 (2%)	8 48
1	B	307/355 (86%)	282 (92%)	19 (6%)	6 (2%)	9 51
1	C	320/355 (90%)	291 (91%)	24 (8%)	5 (2%)	12 55
2	D	18/44 (41%)	14 (78%)	2 (11%)	2 (11%)	0 7
2	E	15/44 (34%)	15 (100%)	0	0	100 100
2	F	15/44 (34%)	14 (93%)	1 (7%)	0	100 100
All	All	982/1197 (82%)	896 (91%)	66 (7%)	20 (2%)	9 51

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	THR
2	D	380	PHE
1	C	17	ALA
1	C	82	LYS
1	A	56	MET
1	A	87	LYS
1	A	119	PRO
1	A	331	GLU
2	D	377	GLY
1	B	119	PRO
1	C	87	LYS
1	A	238	GLY
1	B	185	ALA
1	B	502	VAL
1	C	119	PRO
1	A	185	ALA
1	B	361	LYS
1	C	502	VAL
1	B	236	ILE
1	B	81	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	246/287 (86%)	221 (90%)	25 (10%)	9 40
1	B	245/287 (85%)	227 (93%)	18 (7%)	17 57
1	C	259/287 (90%)	223 (86%)	36 (14%)	4 25
2	D	13/34 (38%)	13 (100%)	0	100 100
2	E	13/34 (38%)	12 (92%)	1 (8%)	16 54
2	F	14/34 (41%)	9 (64%)	5 (36%)	0 1
All	All	790/963 (82%)	705 (89%)	85 (11%)	8 37

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	THR
1	A	99	LEU
1	A	104	THR
1	A	111	THR
1	A	119	PRO
1	A	144	GLU
1	A	151	LEU
1	A	154	THR
1	A	159	THR
1	A	167	ARG
1	A	195	LEU
1	A	199	LEU
1	A	213	ASN
1	A	228	ASN
1	A	242	GLN
1	A	246	ASN
1	A	269	ASN
1	A	274	MET
1	A	275	PHE
1	A	289	THR
1	A	291	LEU
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	302	THR
1	A	303	THR
1	A	310	THR
1	B	64	LEU
1	B	75	ASP
1	B	80	PRO
1	B	92	VAL
1	B	119	PRO
1	B	144	GLU
1	B	151	LEU
1	B	167	ARG
1	B	171	MET
1	B	228	ASN
1	B	242	GLN
1	B	246	ASN
1	B	269	ASN
1	B	276	THR
1	B	289	THR
1	B	354	ILE
1	B	356	ILE
1	B	358	VAL
2	E	378	LEU
1	C	14	ARG
1	C	19	ARG
1	C	23	ARG
1	C	28	ARG
1	C	64	LEU
1	C	73	SER
1	C	86	ASP
1	C	92	VAL
1	C	99	LEU
1	C	102	SER
1	C	110	GLN
1	C	111	THR
1	C	119	PRO
1	C	129	ASN
1	C	133	SER
1	C	140	LEU
1	C	144	GLU
1	C	151	LEU
1	C	179	SER
1	C	183	GLN

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Mol	Chain	Res	Type
1	C	195	LEU
1	C	196	LYS
1	C	207	THR
1	C	236	ILE
1	C	276	THR
1	C	287	ARG
1	C	289	THR
1	C	291	LEU
1	C	300	LEU
1	C	302	THR
1	C	313	LEU
1	C	329	LEU
1	C	352	ARG
1	C	354	ILE
1	C	356	ILE
1	C	361	LYS
2	F	366	PHE
2	F	369	ARG
2	F	374	LEU
2	F	378	LEU
2	F	379	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	197	GLN
1	A	228	ASN
1	A	229	ASN
1	A	253	HIS
1	A	309	ASN
1	A	326	ASN
1	B	97	HIS
1	B	110	GLN
1	B	213	ASN
1	B	309	ASN
1	B	326	ASN
1	B	339	ASN
1	C	97	HIS
1	C	110	GLN
1	C	129	ASN
1	C	200	ASN

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Mol	Chain	Res	Type
1	C	213	ASN
1	C	229	ASN
1	C	230	ASN
1	C	253	HIS
1	C	363	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	309/355 (87%)	-0.85	0	100	100	20, 20, 20, 20	0
1	B	309/355 (87%)	-0.86	0	100	100	20, 20, 20, 20	0
1	C	324/355 (91%)	-0.86	0	100	100	20, 20, 20, 20	0
2	D	20/44 (45%)	-0.65	0	100	100	20, 20, 20, 20	0
2	E	17/44 (38%)	-0.74	0	100	100	20, 20, 20, 20	0
2	F	17/44 (38%)	-0.73	0	100	100	20, 20, 20, 20	0
All	All	996/1197 (83%)	-0.85	0	100	100	20, 20, 20, 20	0

There are no RSRZ outliers to report.

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

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.