Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:54 AM GMT

PDB ID	:	3CJI
Title	:	Structure of Seneca Valley Virus-001
Authors	:	Venkataraman, S.; Reddy, V.S.
Deposited on	:	2008-03-13
Resolution	:	2.30 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 (i)) were used in the production of this report:

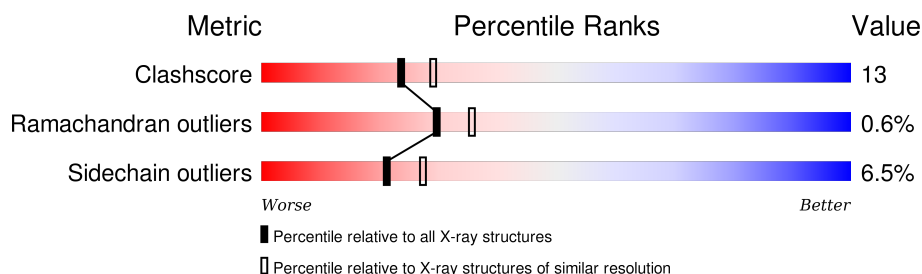|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Clashscore		13
Ramachandran outliers		0.6%
Sidechain outliers		6.5%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	263	75%　　　　　　　　　21%　　· ·
2	B	239	76%　　　　　　　　　20%　　·
3	C	284	73%　　　　　　　　　20%　· 6%
4	D	71	35%　　　10%　·　　　51%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6521 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 Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2015	1295	345	371	4			

- Molecule 2 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	0	0
			1855	1199	294	351	11			

- Molecule 3 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	268	Total	C	N	O	S	0	0	0
			2105	1333	357	407	8			

- Molecule 4 is a protein called Polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	35	Total	C	N	O	S	0	0	0
			278	174	47	56	1			

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	83	Total	O	0	0
			83	83		

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| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	74	Total 74	O 74	0	0
6	C	99	Total 99	O 99	0	0
6	D	11	Total 11	O 11	0	0

3 Residue-property plots ⓘ

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.
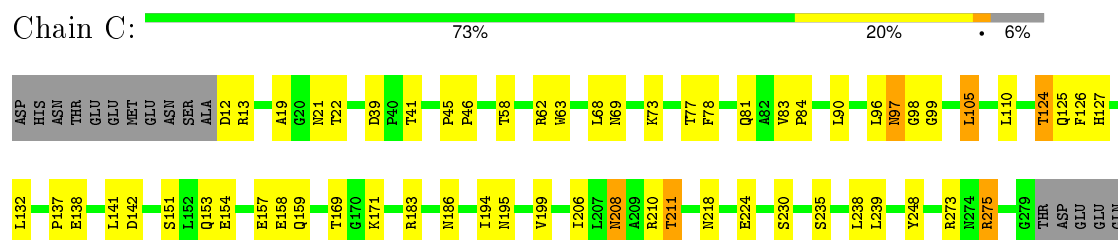
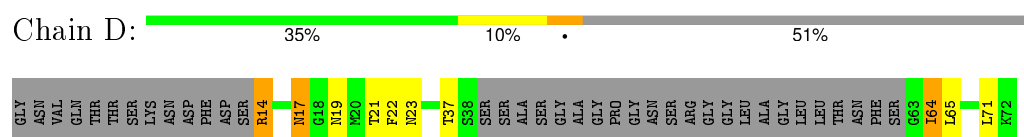Note EDS failed to run properly.

- Molecule 1: Polyprotein

Chain A:
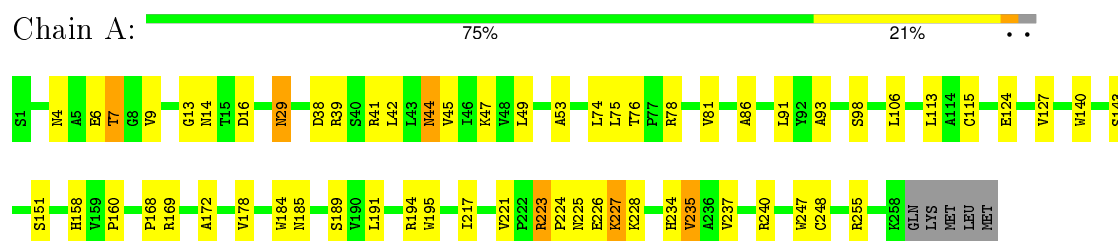
- Molecule 2: Polyprotein

Chain B:
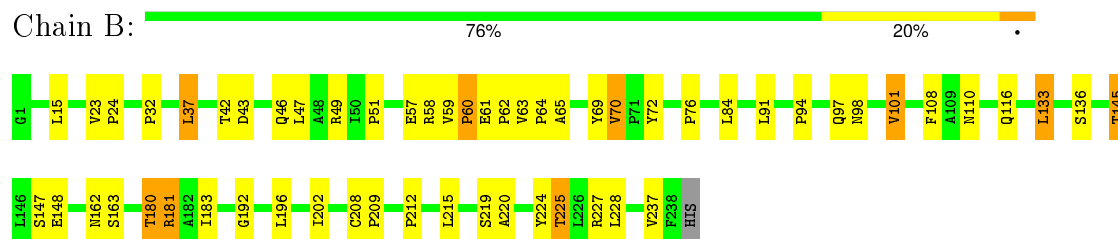
- Molecule 3: Polyprotein

Chain C:

- Molecule 4: Polyprotein

Chain D:

4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	311.51Å 311.51Å 1526.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	88.56 – 2.30	Depositor
% Data completeness (in resolution range)	80.3 (88.56-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.23	Depositor
$<I/\sigma(I)>$ [1]	1.40 (at 2.29Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.258 , 0.260	Depositor
Wilson B-factor (Å^2)	35.5	Xtriage
Anisotropy	0.073	Xtriage
Estimated twinning fraction	0.428 for -h-k,k,-l	Xtriage
L-test for twinning[2]	$<|L|>$ = 0.46, $<L^2>$ = 0.29	Xtriage
Outliers	0 of 1967686 reflections	Xtriage
Total number of atoms	6521	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	0/2078	0.60	0/2833
2	B	0.37	0/1915	0.69	0/2636
3	C	0.34	0/2164	0.66	0/2963
4	D	0.41	0/283	0.62	0/380
All	All	0.36	0/6440	0.65	0/8812

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 (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	2015	0	1951	53	0
2	B	1855	0	1815	55	0
3	C	2105	0	2030	61	0
4	D	278	0	254	15	0
5	B	1	0	0	0	0
6	A	83	0	0	0	0
6	B	74	0	0	1	0
6	C	99	0	0	0	0
6	D	11	0	0	0	0
All	All	6521	0	6050	162	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 13.

All (162) 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)
3:C:141:LEU:HD21	3:C:194:ILE:HD11	1.42	1.00
3:C:69:ASN:H	3:C:81:GLN:HE22	1.04	0.97
2:B:209:PRO:HG3	3:C:248:TYR:HA	1.49	0.94
1:A:255:ARG:H	2:B:98:ASN:HD21	1.09	0.92
3:C:124:THR:CG2	3:C:126:PHE:H	1.84	0.90
4:D:64:ILE:HD13	4:D:64:ILE:H	1.38	0.89
2:B:42:THR:H	2:B:46:GLN:HE22	1.18	0.88
1:A:13:GLY:H	2:B:116:GLN:HE22	1.22	0.86
3:C:22:THR:HG21	3:C:63:TRP:HB2	1.60	0.83
1:A:6:GLU:OE2	3:C:211:THR:HG21	1.78	0.82
2:B:145:THR:HG22	2:B:148:GLU:H	1.43	0.82
3:C:124:THR:HG22	3:C:126:PHE:H	1.44	0.81
2:B:43:ASP:H	2:B:46:GLN:HE21	1.27	0.79
3:C:141:LEU:CD2	3:C:194:ILE:HD11	2.12	0.79
2:B:181:ARG:HB2	2:B:181:ARG:HH11	1.49	0.77
1:A:29:ASN:HD22	1:A:29:ASN:H	1.30	0.76
2:B:42:THR:H	2:B:46:GLN:NE2	1.84	0.76
3:C:275:ARG:HG3	3:C:275:ARG:HH11	1.51	0.76
1:A:76:THR:HG22	1:A:78:ARG:H	1.53	0.74
1:A:44:ASN:HD22	1:A:45:VAL:H	1.34	0.73
2:B:202:ILE:HD13	2:B:212:PRO:HG3	1.70	0.73
1:A:13:GLY:H	2:B:116:GLN:NE2	1.88	0.71
1:A:14:ASN:ND2	1:A:16:ASP:H	1.90	0.70
3:C:169:THR:CG2	3:C:171:LYS:HB2	2.21	0.70
3:C:97:ASN:C	3:C:97:ASN:HD22	1.96	0.69
3:C:69:ASN:N	3:C:81:GLN:HE22	1.85	0.69
2:B:110:ASN:HD22	2:B:227:ARG:HE	1.41	0.68
3:C:84:PRO:HG3	3:C:142:ASP:HB3	1.74	0.68
2:B:181:ARG:HB2	2:B:181:ARG:NH1	2.08	0.67
1:A:7:THR:HG22	1:A:9:VAL:H	1.59	0.67
4:D:17:ASN:ND2	4:D:19:ASN:H	1.93	0.66
3:C:124:THR:HG23	3:C:126:PHE:H	1.59	0.66
1:A:172:ALA:HB2	1:A:178:VAL:HG23	1.78	0.65
1:A:93:ALA:H	3:C:186:ASN:ND2	1.94	0.65
2:B:110:ASN:ND2	2:B:227:ARG:HH21	1.95	0.65
2:B:59:VAL:O	2:B:61:GLU:N	2.30	0.65
1:A:221:VAL:HG12	1:A:223:ARG:HB2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:THR:HG22	3:C:171:LYS:HB2	1.78	0.65
4:D:14:ARG:HB2	4:D:14:ARG:HH11	1.63	0.64
2:B:70:VAL:CG1	2:B:72:TYR:H	2.11	0.63
1:A:143:SER:H	1:A:185:ASN:ND2	1.96	0.63
1:A:38:ASP:OD2	1:A:240:ARG:HD3	1.99	0.62
3:C:105:LEU:CD2	3:C:230:SER:HB3	2.29	0.62
2:B:145:THR:HG22	2:B:148:GLU:N	2.15	0.61
1:A:29:ASN:HD22	1:A:29:ASN:N	1.97	0.61
1:A:224:PRO:HG2	1:A:227:LYS:HD2	1.83	0.61
2:B:145:THR:HG23	2:B:147:SER:H	1.66	0.60
1:A:14:ASN:HD22	1:A:16:ASP:H	1.47	0.60
2:B:61:GLU:N	2:B:62:PRO:HD3	2.16	0.60
1:A:93:ALA:H	3:C:186:ASN:HD22	1.50	0.60
3:C:208:ASN:HB3	3:C:211:THR:HG23	1.83	0.60
1:A:44:ASN:ND2	1:A:45:VAL:H	1.99	0.60
3:C:69:ASN:H	3:C:81:GLN:NE2	1.86	0.60
2:B:209:PRO:HG3	3:C:248:TYR:CA	2.27	0.60
4:D:14:ARG:HB2	4:D:14:ARG:NH1	2.16	0.60
4:D:17:ASN:HD21	4:D:19:ASN:HB3	1.68	0.59
1:A:140:TRP:HE3	1:A:168:PRO:HD2	1.68	0.59
3:C:12:ASP:CG	3:C:13:ARG:H	2.06	0.59
3:C:137:PRO:HA	3:C:235:SER:O	2.03	0.58
2:B:57:GLU:HG2	2:B:69:TYR:CZ	2.38	0.58
1:A:115:CYS:SG	2:B:47:LEU:HD22	2.43	0.58
2:B:145:THR:CG2	2:B:147:SER:HB3	2.33	0.58
2:B:108:PHE:O	2:B:180:THR:HG21	2.04	0.58
3:C:39:ASP:OD1	3:C:41:THR:HB	2.03	0.58
2:B:101:VAL:HG22	2:B:219:SER:HA	1.86	0.58
3:C:97:ASN:ND2	3:C:99:GLY:H	2.03	0.57
2:B:49:ARG:HH12	4:D:65:LEU:HD12	1.69	0.56
3:C:97:ASN:HD22	3:C:99:GLY:H	1.54	0.56
2:B:51:PRO:HA	2:B:219:SER:HB3	1.87	0.55
2:B:209:PRO:CG	3:C:248:TYR:HA	2.30	0.55
2:B:133:LEU:HD23	2:B:133:LEU:N	2.22	0.55
3:C:22:THR:HG21	3:C:63:TRP:CB	2.35	0.54
3:C:124:THR:HG22	3:C:126:PHE:N	2.19	0.54
2:B:202:ILE:HD13	2:B:212:PRO:CG	2.36	0.54
3:C:105:LEU:HD22	3:C:230:SER:HB3	1.89	0.53
4:D:64:ILE:CD1	4:D:64:ILE:H	2.18	0.53
1:A:158:HIS:HD2	1:A:226:GLU:OE1	1.92	0.53
2:B:43:ASP:H	2:B:46:GLN:NE2	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG12	1:A:86:ALA:HB2	1.91	0.52
1:A:39:ARG:C	1:A:240:ARG:HG3	2.30	0.52
4:D:64:ILE:HG12	4:D:64:ILE:O	2.10	0.51
2:B:70:VAL:HG12	2:B:72:TYR:H	1.75	0.51
1:A:44:ASN:HD22	1:A:45:VAL:N	2.05	0.51
3:C:22:THR:HG22	3:C:63:TRP:HD1	1.76	0.50
3:C:83:VAL:HB	3:C:238:LEU:HB3	1.92	0.50
1:A:49:LEU:CD2	1:A:53:ALA:HB2	2.41	0.50
1:A:124:GLU:HB3	1:A:240:ARG:HB3	1.94	0.50
1:A:140:TRP:CE3	1:A:168:PRO:HD2	2.47	0.49
3:C:22:THR:CG2	3:C:63:TRP:HB2	2.38	0.49
2:B:70:VAL:HG13	2:B:72:TYR:H	1.76	0.49
3:C:73:LYS:HE3	3:C:248:TYR:CE1	2.48	0.49
3:C:19:ALA:O	3:C:22:THR:HB	2.13	0.49
3:C:97:ASN:HD22	3:C:98:GLY:N	2.11	0.49
3:C:153:GLN:O	3:C:157:GLU:HG3	2.14	0.48
3:C:124:THR:HB	3:C:127:HIS:ND1	2.29	0.48
3:C:73:LYS:HE3	3:C:248:TYR:CZ	2.48	0.48
1:A:98:SER:O	3:C:183:ARG:HG2	2.14	0.48
2:B:58:ARG:NH1	2:B:63:VAL:HB	2.29	0.47
2:B:101:VAL:CG2	2:B:219:SER:HA	2.43	0.47
2:B:76:PRO:HD2	2:B:84:LEU:HD11	1.96	0.47
3:C:275:ARG:CG	3:C:275:ARG:HH11	2.23	0.47
1:A:143:SER:H	1:A:185:ASN:HD21	1.62	0.47
1:A:184:TRP:CH2	1:A:191:LEU:HB2	2.49	0.47
1:A:49:LEU:HD22	1:A:53:ALA:HB2	1.97	0.47
3:C:169:THR:HG21	3:C:171:LYS:HB2	1.95	0.46
3:C:132:LEU:HD11	3:C:199:VAL:HG12	1.98	0.46
3:C:275:ARG:HG3	3:C:275:ARG:NH1	2.26	0.46
1:A:7:THR:HG23	4:D:71:LEU:HD22	1.98	0.46
1:A:217:ILE:HD11	1:A:237:VAL:HG21	1.98	0.46
4:D:37:THR:HG22	4:D:37:THR:O	2.15	0.46
4:D:17:ASN:HD22	4:D:17:ASN:C	2.19	0.46
2:B:145:THR:HG21	2:B:147:SER:HB3	1.97	0.46
1:A:7:THR:HG22	1:A:9:VAL:N	2.27	0.45
1:A:151:SER:HB3	1:A:160:PRO:HA	1.97	0.45
1:A:4:ASN:HD21	2:B:162:ASN:HA	1.81	0.45
2:B:181:ARG:HG2	2:B:183:ILE:HG13	1.99	0.44
2:B:98:ASN:HD22	3:C:195:ASN:HD21	1.65	0.44
3:C:22:THR:HG21	3:C:63:TRP:H	1.82	0.44
1:A:75:LEU:HD11	1:A:217:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:THR:HG23	3:C:125:GLN:N	2.32	0.44
4:D:17:ASN:ND2	4:D:19:ASN:N	2.64	0.44
1:A:29:ASN:ND2	1:A:29:ASN:N	2.65	0.44
3:C:97:ASN:C	3:C:97:ASN:ND2	2.68	0.44
2:B:220:ALA:HB1	2:B:224:TYR:HB3	2.00	0.44
3:C:158:GLU:O	3:C:159:GLN:HB2	2.17	0.44
2:B:58:ARG:HH12	2:B:63:VAL:HB	1.83	0.44
3:C:77:THR:O	3:C:78:PHE:HB2	2.18	0.44
1:A:195:TRP:HA	3:C:138:GLU:HB3	2.01	0.43
3:C:151:SER:OG	3:C:154:GLU:HG3	2.19	0.43
1:A:6:GLU:HA	3:C:206:ILE:HB	2.00	0.42
2:B:225:THR:HB	6:B:562:HOH:O	2.19	0.42
2:B:63:VAL:C	2:B:65:ALA:H	2.23	0.42
3:C:21:ASN:OD1	3:C:62:ARG:NH2	2.51	0.42
1:A:189:SER:HA	2:B:32:PRO:HG2	2.02	0.42
1:A:7:THR:CG2	4:D:71:LEU:HD22	2.49	0.42
1:A:225:ASN:O	1:A:228:LYS:HB2	2.20	0.42
3:C:84:PRO:HG3	3:C:142:ASP:CB	2.44	0.42
2:B:47:LEU:N	2:B:47:LEU:HD12	2.35	0.42
2:B:58:ARG:O	2:B:59:VAL:C	2.58	0.42
2:B:91:LEU:HD21	2:B:224:TYR:OH	2.19	0.42
4:D:22:PHE:CD2	4:D:23:ASN:N	2.87	0.42
4:D:64:ILE:N	4:D:64:ILE:HD13	2.19	0.42
1:A:247:TRP:CG	2:B:37:LEU:HD13	2.55	0.42
2:B:63:VAL:O	2:B:65:ALA:N	2.53	0.41
2:B:63:VAL:HG13	2:B:65:ALA:H	1.85	0.41
1:A:47:LYS:HG2	1:A:234:HIS:CE1	2.55	0.41
1:A:13:GLY:N	2:B:116:GLN:HE22	2.04	0.41
3:C:183:ARG:HH11	3:C:183:ARG:HG3	1.84	0.41
1:A:184:TRP:HH2	1:A:191:LEU:HB2	1.85	0.41
3:C:169:THR:HG22	3:C:171:LYS:N	2.35	0.41
1:A:227:LYS:N	1:A:227:LYS:HE2	2.35	0.41
2:B:23:VAL:HA	2:B:24:PRO:HD3	1.87	0.41
3:C:169:THR:HG22	3:C:171:LYS:H	1.86	0.41
1:A:217:ILE:HD11	1:A:237:VAL:CG2	2.50	0.41
1:A:127:VAL:HG13	1:A:235:VAL:HG13	2.03	0.41
2:B:136:SER:O	2:B:192:GLY:HA3	2.21	0.41
2:B:94:PRO:O	2:B:97:GLN:HB2	2.21	0.41
3:C:12:ASP:CG	3:C:13:ARG:N	2.72	0.40
1:A:4:ASN:ND2	2:B:163:SER:H	2.18	0.40
3:C:45:PRO:HA	3:C:46:PRO:HD3	1.96	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:273:ARG:HG3	3:C:273:ARG:HH11	1.86	0.40
1:A:113:LEU:HD23	1:A:113:LEU:HA	1.95	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	256/263 (97%)	246 (96%)	9 (4%)	1 (0%)	39	48
2	B	236/239 (99%)	222 (94%)	11 (5%)	3 (1%)	15	15
3	C	266/284 (94%)	256 (96%)	10 (4%)	0	100	100
4	D	31/71 (44%)	30 (97%)	0	1 (3%)	5	3
All	All	789/857 (92%)	754 (96%)	30 (4%)	5 (1%)	30	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	PRO
4	D	21	THR
1	A	248	CYS
2	B	64	PRO
2	B	228	LEU

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	216/221 (98%)	203 (94%)	13 (6%)	24	31
2	B	213/214 (100%)	199 (93%)	14 (7%)	21	27
3	C	235/250 (94%)	220 (94%)	15 (6%)	22	28
4	D	30/56 (54%)	27 (90%)	3 (10%)	9	11
All	All	694/741 (94%)	649 (94%)	45 (6%)	21	27

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	29	ASN
1	A	41	ARG
1	A	42	LEU
1	A	44	ASN
1	A	74	LEU
1	A	91	LEU
1	A	106	LEU
1	A	169	ARG
1	A	194	ARG
1	A	223	ARG
1	A	227	LYS
1	A	235	VAL
2	B	15	LEU
2	B	37	LEU
2	B	60	PRO
2	B	70	VAL
2	B	101	VAL
2	B	133	LEU
2	B	145	THR
2	B	180	THR
2	B	181	ARG
2	B	196	LEU
2	B	208	CYS
2	B	215	LEU
2	B	225	THR
2	B	237	VAL
3	C	58	THR
3	C	68	LEU
3	C	90	LEU
3	C	96	LEU

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Mol	Chain	Res	Type
3	C	97	ASN
3	C	105	LEU
3	C	110	LEU
3	C	124	THR
3	C	208	ASN
3	C	210	ARG
3	C	211	THR
3	C	218	ASN
3	C	224	GLU
3	C	239	LEU
3	C	275	ARG
4	D	14	ARG
4	D	17	ASN
4	D	64	ILE

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	4	ASN
1	A	14	ASN
1	A	29	ASN
1	A	44	ASN
1	A	103	ASN
1	A	158	HIS
1	A	185	ASN
1	A	234	HIS
1	A	243	ASN
2	B	46	GLN
2	B	97	GLN
2	B	98	ASN
2	B	110	ASN
2	B	116	GLN
2	B	142	GLN
2	B	162	ASN
3	C	81	GLN
3	C	97	ASN
3	C	186	ASN
3	C	208	ASN
3	C	218	ASN
3	C	228	GLN
3	C	234	ASN
4	D	17	ASN

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Mol	Chain	Res	Type
4	D	19	ASN
4	D	27	ASN
4	D	31	ASN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

5.4   Non-standard residues in protein, DNA, RNA chains (i)

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7   Other polymers (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS failed to run properly - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands (i)

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers (i)

EDS failed to run properly - this section will therefore be empty.