W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:52 AM GMT

PDB ID	:	2IZW
Title	:	CRYSTAL STRUCTURE OF RYEGRASS MOTTLE VIRUS
Authors	:	Plevka, P.; Tars, K.; Zeltins, A.; Balke, I.; Truve, E.; Liljas, L.
Deposited on	:	2006-07-27
Resolution	:	2.90 Å(reported)

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	:	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 ⓘ

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

The reported resolution of this entry is 2.90 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		22
Ramachandran outliers		0.4%
Sidechain outliers		7.7%
RSRZ outliers		13.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
◻ Percentile relative to X-ray structures of similar resolution
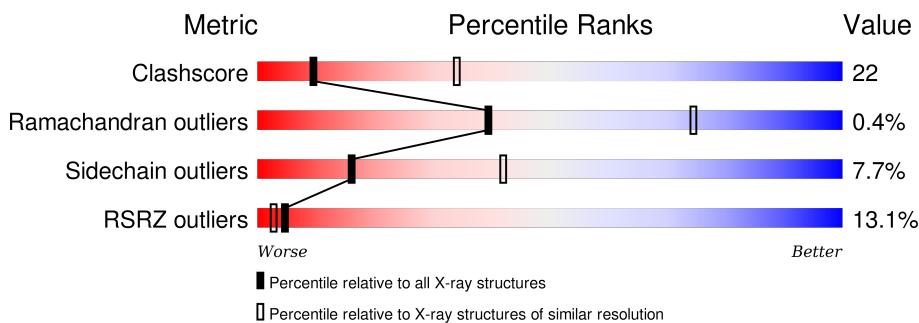
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	234	12% — 45% / 28% / • / 24%
1	B	234	8% — 42% / 31% / • / 24%
1	C	234	12% — 53% / 35% / • / 11%
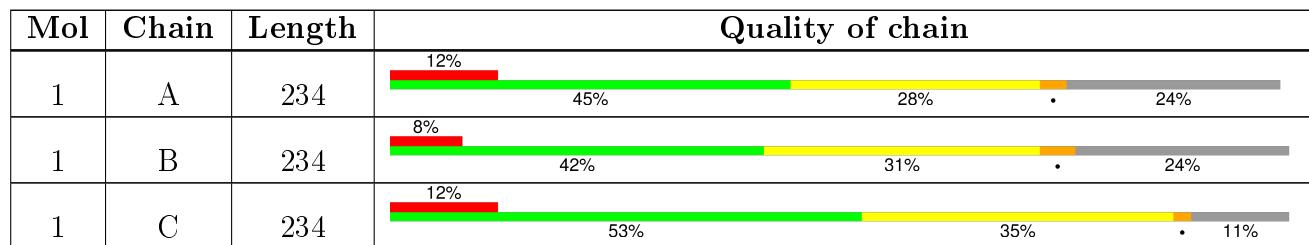
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4324 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 RYEGRASS MOTTLE VIRUS COAT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1366	861	235	266	4			
1	B	179	Total	C	N	O	S	0	0	0
			1373	865	236	268	4			
1	C	208	Total	C	N	O	S	0	0	0
			1585	996	276	308	5			

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.

- Molecule 1: RYEGRASS MOTTLE VIRUS COAT PROTEIN
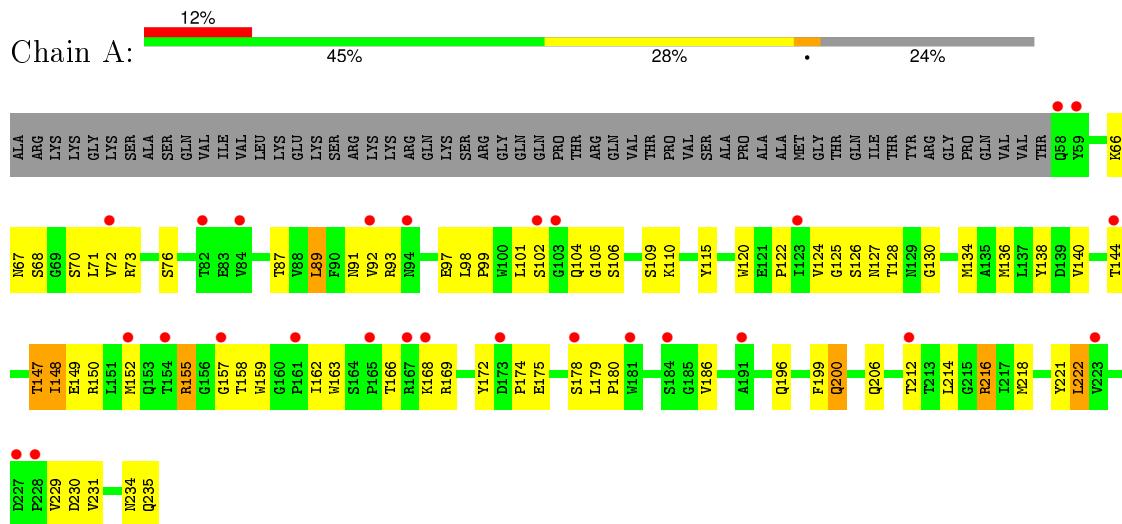
- Molecule 1: RYEGRASS MOTTLE VIRUS COAT PROTEIN
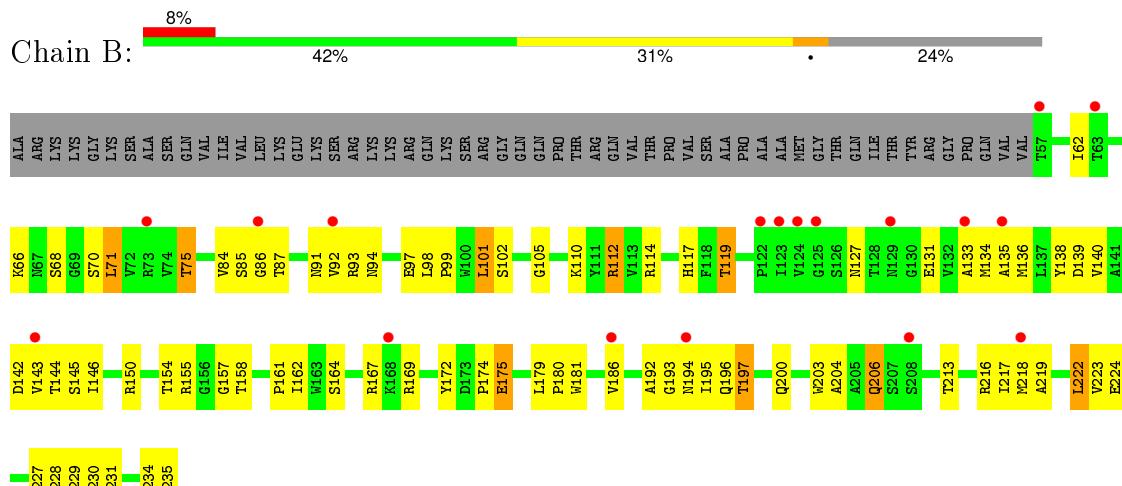
- Molecule 1: RYEGRASS MOTTLE VIRUS COAT PROTEIN
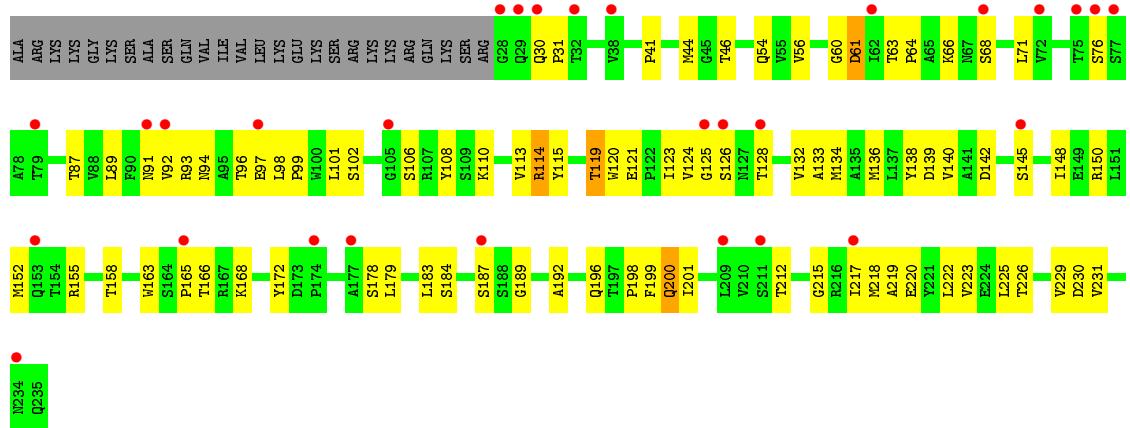
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	277.64Å 298.72Å 392.49Å 90.00° 92.74° 90.00°	Depositor
Resolution (Å)	34.90 – 2.90 34.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	40.5 (34.90-2.90) 22.2 (34.90-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.37 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.294 , (Not available) 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	17.9	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 20.7	EDS
Estimated twinning fraction	0.216 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.27, < L^2 > = 0.11$	Xtriage
Outliers	0 of 611504 reflections	Xtriage
F_o,F_c correlation	0.71	EDS
Total number of atoms	4324	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.15 % 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 6.0420e-03.*

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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)

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	0.44	0/1399	0.68	0/1912
1	B	0.47	0/1406	0.70	0/1922
1	C	0.49	1/1623 (0.1%)	0.71	1/2221 (0.0%)
All	All	0.47	1/4428 (0.0%)	0.70	1/6055 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	220	GLU	CB-CG	5.13	1.61	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	60	GLY	N-CA-C	-5.06	100.44	113.10

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	1366	0	1333	57	0
1	B	1373	0	1340	78	0
1	C	1585	0	1556	68	0
All	All	4324	0	4229	192	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 22.

All (192) 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:154:THR:HG22	1:C:230:ASP:H	1.30	0.95
1:B:91:ASN:HD21	1:B:197:THR:HB	1.33	0.93
1:B:92:VAL:HA	1:B:101:LEU:HD12	1.53	0.90
1:C:89:LEU:HD11	1:C:140:VAL:HG23	1.55	0.88
1:B:91:ASN:ND2	1:B:197:THR:HB	1.88	0.87
1:C:125:GLY:O	1:C:128:THR:HG22	1.77	0.83
1:A:66:LYS:HB2	1:A:222:LEU:HD22	1.59	0.82
1:A:147:THR:HG23	1:A:150:ARG:HD2	1.64	0.80
1:C:114:ARG:HB2	1:C:222:LEU:HD12	1.61	0.80
1:B:91:ASN:HD21	1:B:197:THR:CB	1.98	0.76
1:C:114:ARG:HA	1:C:114:ARG:HH11	1.50	0.75
1:C:136:MET:HE2	1:C:138:TYR:CZ	2.23	0.73
1:A:136:MET:HE2	1:A:138:TYR:CZ	2.22	0.73
1:B:92:VAL:O	1:B:102:SER:HA	1.88	0.73
1:C:76:SER:HB3	1:C:212:THR:H	1.52	0.73
1:B:119:THR:HG23	1:B:218:MET:HB2	1.71	0.73
1:A:124:VAL:HB	1:A:128:THR:HG21	1.70	0.72
1:B:91:ASN:HB3	1:B:93:ARG:H	1.55	0.72
1:B:216:ARG:HB2	1:B:218:MET:HE3	1.71	0.72
1:A:125:GLY:O	1:A:128:THR:HG23	1.92	0.69
1:A:216:ARG:HB2	1:A:218:MET:HE3	1.75	0.68
1:B:145:SER:HB3	1:B:150:ARG:NH1	2.07	0.68
1:B:154:THR:HG22	1:C:230:ASP:N	2.05	0.67
1:B:92:VAL:HA	1:B:101:LEU:CD1	2.24	0.67
1:C:97:GLU:C	1:C:99:PRO:HD3	2.14	0.67
1:A:92:VAL:O	1:A:102:SER:HA	1.95	0.67
1:C:92:VAL:O	1:C:102:SER:HA	1.94	0.66
1:B:87:THR:HG21	1:B:143:VAL:HG13	1.77	0.66
1:C:96:THR:HB	1:C:97:GLU:OE1	1.94	0.66
1:B:167:ARG:HH11	1:B:167:ARG:HG3	1.62	0.64
1:B:154:THR:HB	1:C:229:VAL:HA	1.79	0.64
1:A:130:GLY:C	1:A:162:ILE:HG13	2.18	0.63
1:B:66:LYS:HB2	1:B:222:LEU:CD2	2.28	0.63
1:B:93:ARG:NH1	1:B:186:VAL:HG13	2.14	0.62
1:A:234:ASN:O	1:A:235:GLN:HG3	2.00	0.62
1:A:155:ARG:HG3	1:B:227:ASP:HA	1.82	0.61
1:C:114:ARG:CB	1:C:222:LEU:HD12	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ARG:O	1:B:154:THR:HG23	2.01	0.61
1:C:92:VAL:HG23	1:C:93:ARG:HG3	1.81	0.61
1:A:158:THR:HG23	1:A:168:LYS:HG3	1.82	0.60
1:A:186:VAL:HG22	1:A:235:GLN:O	2.02	0.60
1:B:114:ARG:CB	1:B:222:LEU:HD12	2.32	0.60
1:C:145:SER:HB3	1:C:150:ARG:NH1	2.16	0.59
1:C:123:ILE:HG22	1:C:123:ILE:O	2.01	0.59
1:B:234:ASN:O	1:B:235:GLN:HG3	2.02	0.59
1:A:91:ASN:HD22	1:A:93:ARG:H	1.50	0.59
1:A:115:TYR:CE2	1:A:222:LEU:HB2	2.37	0.59
1:C:199:PHE:HE1	1:C:201:ILE:HD11	1.68	0.59
1:B:192:ALA:O	1:B:196:GLN:HG3	2.03	0.58
1:B:71:LEU:O	1:B:97:GLU:HB3	2.04	0.58
1:B:94:ASN:ND2	1:B:97:GLU:H	2.02	0.58
1:B:172:TYR:O	1:B:174:PRO:HD3	2.04	0.58
1:C:123:ILE:HG13	1:C:215:GLY:HA2	1.85	0.57
1:C:41:PRO:HG3	1:C:44:MET:HG3	1.85	0.57
1:B:179:LEU:HB2	1:B:180:PRO:HD2	1.86	0.56
1:B:112:ARG:HG2	1:B:181:TRP:CZ3	2.40	0.56
1:A:136:MET:HE2	1:A:138:TYR:CE2	2.41	0.56
1:C:187:SER:H	1:C:196:GLN:HE22	1.53	0.56
1:A:162:ILE:HD11	1:A:206:GLN:O	2.06	0.56
1:C:192:ALA:O	1:C:196:GLN:HG3	2.06	0.55
1:C:158:THR:HG21	1:C:168:LYS:O	2.06	0.55
1:B:91:ASN:HD21	1:B:197:THR:CG2	2.18	0.55
1:B:167:ARG:NH1	1:B:167:ARG:HG3	2.22	0.55
1:A:91:ASN:ND2	1:A:93:ARG:H	2.05	0.54
1:C:97:GLU:O	1:C:99:PRO:HD3	2.07	0.54
1:B:134:MET:HE3	1:B:217:ILE:HG23	1.88	0.54
1:A:134:MET:O	1:A:157:GLY:HA2	2.07	0.54
1:C:54:GLN:HB2	1:C:66:LYS:HB3	1.88	0.54
1:C:68:SER:HA	1:C:219:ALA:O	2.07	0.54
1:B:193:GLY:O	1:B:197:THR:HG23	2.07	0.54
1:B:114:ARG:HB2	1:B:222:LEU:HD12	1.88	0.54
1:C:106:SER:HB2	1:C:231:VAL:HG23	1.90	0.54
1:A:97:GLU:C	1:A:99:PRO:HD3	2.29	0.53
1:C:134:MET:HE1	1:C:217:ILE:HD13	1.89	0.53
1:C:30:GLN:HB3	1:C:31:PRO:HD2	1.90	0.53
1:A:155:ARG:HG2	1:B:228:PRO:HD2	1.91	0.53
1:B:94:ASN:ND2	1:B:97:GLU:HB2	2.24	0.53
1:B:216:ARG:HB2	1:B:218:MET:CE	2.37	0.52

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Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:HB2	1:B:222:LEU:HD23	1.91	0.52
1:B:71:LEU:HB2	1:B:217:ILE:O	2.09	0.52
1:A:148:ILE:O	1:A:152:MET:HG3	2.09	0.52
1:C:61:ASP:HB3	1:C:226:THR:OG1	2.10	0.52
1:B:195:ILE:HG22	1:B:195:ILE:O	2.08	0.52
1:A:106:SER:HB2	1:A:231:VAL:HG13	1.92	0.52
1:C:56:VAL:O	1:C:64:PRO:HD2	2.09	0.51
1:B:229:VAL:HG11	1:B:234:ASN:HB2	1.92	0.51
1:C:136:MET:HE3	1:C:199:PHE:HB2	1.92	0.51
1:A:179:LEU:HB2	1:A:180:PRO:HD2	1.91	0.51
1:C:115:TYR:CE2	1:C:222:LEU:HB2	2.46	0.51
1:B:86:GLY:HA3	1:B:203:TRP:CE2	2.45	0.51
1:C:148:ILE:O	1:C:152:MET:HG3	2.10	0.51
1:A:89:LEU:HD11	1:A:140:VAL:HG13	1.92	0.50
1:A:93:ARG:HH12	1:A:235:GLN:HA	1.75	0.50
1:C:91:ASN:HB2	1:C:94:ASN:HB2	1.93	0.50
1:A:76:SER:HB3	1:A:212:THR:H	1.76	0.50
1:B:229:VAL:HG12	1:B:230:ASP:N	2.27	0.50
1:C:66:LYS:HB2	1:C:222:LEU:HD23	1.93	0.49
1:A:162:ILE:HD13	1:A:214:LEU:HD23	1.94	0.49
1:A:216:ARG:HB2	1:A:218:MET:CE	2.42	0.49
1:C:120:TRP:HB3	1:C:166:THR:HB	1.93	0.49
1:C:108:TYR:CG	1:C:225:LEU:HB3	2.47	0.49
1:A:130:GLY:HA2	1:A:206:GLN:NE2	2.27	0.48
1:A:109:SER:OG	1:A:229:VAL:HG21	2.13	0.48
1:C:119:THR:HG23	1:C:218:MET:HB2	1.94	0.48
1:C:178:SER:O	1:C:179:LEU:HD12	2.12	0.48
1:C:198:PRO:O	1:C:199:PHE:HB3	2.13	0.48
1:A:92:VAL:HG23	1:A:93:ARG:HG3	1.94	0.48
1:C:92:VAL:HA	1:C:101:LEU:HG	1.94	0.48
1:C:91:ASN:HB3	1:C:93:ARG:H	1.79	0.48
1:B:62:ILE:HG23	1:B:224:GLU:HB3	1.95	0.48
1:C:66:LYS:HB2	1:C:222:LEU:CD2	2.44	0.48
1:A:72:VAL:CG1	1:A:73:ARG:N	2.76	0.48
1:C:97:GLU:N	1:C:97:GLU:OE1	2.46	0.48
1:B:134:MET:O	1:B:157:GLY:HA2	2.14	0.48
1:B:62:ILE:CG2	1:B:224:GLU:HB3	2.44	0.48
1:B:154:THR:CB	1:C:229:VAL:HA	2.42	0.48
1:A:71:LEU:HD21	1:A:98:LEU:HD21	1.95	0.48
1:B:97:GLU:C	1:B:99:PRO:HD3	2.35	0.47
1:C:120:TRP:H	1:C:166:THR:CG2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:SER:HB2	1:A:214:LEU:HD11	1.97	0.46
1:B:112:ARG:NH1	1:B:224:GLU:OE2	2.45	0.46
1:B:92:VAL:HB	1:B:105:GLY:HA3	1.97	0.46
1:A:67:ASN:CG	1:A:68:SER:H	2.17	0.46
1:C:136:MET:HE2	1:C:138:TYR:OH	2.15	0.46
1:C:89:LEU:HD13	1:C:200:GLN:CG	2.46	0.46
1:B:66:LYS:HB2	1:B:222:LEU:HD22	1.98	0.46
1:A:136:MET:HE2	1:A:138:TYR:OH	2.15	0.46
1:A:230:ASP:OD2	1:C:150:ARG:HD3	2.16	0.46
1:C:41:PRO:CG	1:C:44:MET:HG3	2.45	0.46
1:B:133:ALA:HA	1:B:158:THR:O	2.16	0.46
1:B:98:LEU:N	1:B:99:PRO:HD3	2.30	0.45
1:B:229:VAL:CG1	1:B:234:ASN:HB2	2.45	0.45
1:C:110:LYS:HG2	1:C:183:LEU:CD2	2.47	0.45
1:B:139:ASP:HB3	1:B:142:ASP:OD1	2.16	0.45
1:B:216:ARG:HD3	1:B:218:MET:HE1	1.97	0.45
1:A:109:SER:OG	1:A:229:VAL:CG2	2.64	0.45
1:A:214:LEU:N	1:A:214:LEU:CD1	2.80	0.45
1:A:98:LEU:N	1:A:99:PRO:HD3	2.31	0.45
1:B:135:ALA:HB1	1:B:154:THR:OG1	2.16	0.45
1:A:104:GLN:HA	1:A:104:GLN:OE1	2.17	0.45
1:A:136:MET:HE3	1:A:199:PHE:HB2	1.99	0.45
1:C:87:THR:HA	1:C:201:ILE:O	2.16	0.44
1:A:126:SER:HA	1:A:163:TRP:CG	2.53	0.44
1:B:234:ASN:O	1:B:235:GLN:CG	2.65	0.44
1:A:120:TRP:CD1	1:A:122:PRO:HG3	2.53	0.44
1:B:154:THR:CG2	1:C:230:ASP:H	2.16	0.44
1:C:120:TRP:H	1:C:166:THR:HG22	1.83	0.44
1:C:46:THR:HB	1:C:121:GLU:OE1	2.18	0.44
1:C:136:MET:HE2	1:C:138:TYR:CE2	2.52	0.44
1:B:94:ASN:HD21	1:B:97:GLU:CB	2.31	0.44
1:A:101:LEU:HD13	1:A:221:TYR:CE2	2.53	0.44
1:B:179:LEU:HD13	1:B:181:TRP:O	2.18	0.44
1:B:143:VAL:HG12	1:B:143:VAL:O	2.18	0.43
1:A:130:GLY:HA2	1:A:206:GLN:HE22	1.82	0.43
1:B:131:GLU:HG2	1:B:206:GLN:HG3	2.01	0.43
1:B:114:ARG:HB3	1:B:222:LEU:HD12	1.99	0.43
1:A:89:LEU:HD13	1:A:200:GLN:HG2	2.01	0.43
1:B:175:GLU:H	1:B:175:GLU:CD	2.22	0.43
1:B:92:VAL:HB	1:B:105:GLY:CA	2.49	0.43
1:B:94:ASN:HD21	1:B:97:GLU:HB2	1.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:SER:HA	1:B:218:MET:CE	2.49	0.42
1:B:75:THR:HA	1:B:213:THR:HA	2.00	0.42
1:A:70:SER:HB2	1:A:218:MET:HE1	2.01	0.42
1:C:89:LEU:HD13	1:C:200:GLN:HG3	2.01	0.42
1:C:126:SER:HA	1:C:163:TRP:CG	2.53	0.42
1:C:98:LEU:N	1:C:99:PRO:HD3	2.33	0.42
1:C:124:VAL:CG1	1:C:128:THR:HG21	2.50	0.42
1:A:92:VAL:HB	1:A:105:GLY:HA3	2.00	0.42
1:C:132:VAL:CG2	1:C:133:ALA:N	2.82	0.42
1:A:196:GLN:HB2	1:A:196:GLN:HE21	1.64	0.42
1:A:172:TYR:O	1:A:174:PRO:HD3	2.20	0.42
1:C:44:MET:CE	1:C:165:PRO:HD2	2.49	0.41
1:C:113:VAL:HB	1:C:172:TYR:CE2	2.55	0.41
1:B:161:PRO:HG2	1:B:164:SER:HB3	2.02	0.41
1:C:132:VAL:HG22	1:C:133:ALA:N	2.34	0.41
1:B:94:ASN:HD21	1:B:97:GLU:H	1.68	0.41
1:B:68:SER:HA	1:B:219:ALA:O	2.20	0.41
1:A:178:SER:OG	1:B:110:LYS:HE2	2.20	0.41
1:B:140:VAL:HG23	1:B:194:ASN:OD1	2.21	0.41
1:A:158:THR:HG22	1:A:159:TRP:N	2.36	0.41
1:B:136:MET:HE2	1:B:138:TYR:CZ	2.55	0.41
1:A:155:ARG:CG	1:B:227:ASP:HA	2.51	0.41
1:A:120:TRP:HB3	1:A:166:THR:HG23	2.03	0.41
1:C:115:TYR:CE2	1:C:222:LEU:CB	3.03	0.41
1:A:71:LEU:CD2	1:A:98:LEU:HD21	2.51	0.41
1:B:117:HIS:HB3	1:B:169:ARG:HD2	2.03	0.41
1:A:110:LYS:HE3	1:C:138:TYR:CD2	2.56	0.40
1:B:85:SER:HB3	1:B:146:ILE:HB	2.03	0.40
1:B:134:MET:CE	1:B:217:ILE:HG23	2.50	0.40
1:C:93:ARG:HD2	1:C:184:SER:OG	2.20	0.40
1:B:84:VAL:O	1:B:204:ALA:HA	2.21	0.40
1:C:139:ASP:HB3	1:C:142:ASP:OD2	2.22	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	176/234 (75%)	158 (90%)	17 (10%)	1 (1%)	30	67
1	B	177/234 (76%)	166 (94%)	11 (6%)	0	100	100
1	C	206/234 (88%)	195 (95%)	10 (5%)	1 (0%)	34	71
All	All	559/702 (80%)	519 (93%)	38 (7%)	2 (0%)	39	74

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	189	GLY
1	A	148	ILE

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	147/194 (76%)	135 (92%)	12 (8%)	14	39
1	B	148/194 (76%)	132 (89%)	16 (11%)	8	24
1	C	171/194 (88%)	163 (95%)	8 (5%)	32	68
All	All	466/582 (80%)	430 (92%)	36 (8%)	16	42

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	89	LEU
1	A	127	ASN
1	A	144	THR
1	A	147	THR
1	A	149	GLU
1	A	155	ARG

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Mol	Chain	Res	Type
1	A	169	ARG
1	A	175	GLU
1	A	200	GLN
1	A	216	ARG
1	A	222	LEU
1	B	71	LEU
1	B	75	THR
1	B	101	LEU
1	B	112	ARG
1	B	119	THR
1	B	127	ASN
1	B	144	THR
1	B	155	ARG
1	B	162	ILE
1	B	175	GLU
1	B	197	THR
1	B	200	GLN
1	B	206	GLN
1	B	222	LEU
1	B	223	VAL
1	B	231	VAL
1	C	61	ASP
1	C	63	THR
1	C	71	LEU
1	C	114	ARG
1	C	119	THR
1	C	155	ARG
1	C	200	GLN
1	C	223	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	235	GLN
1	B	91	ASN
1	B	94	ASN
1	B	196	GLN
1	B	206	GLN
1	C	67	ASN
1	C	91	ASN
1	C	117	HIS

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Mol	Chain	Res	Type
1	C	153	GLN
1	C	196	GLN
1	C	200	GLN

5.3.3   RNA (i)

There are no RNA molecules in this entry.

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

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

5.5   Carbohydrates (i)

There are no carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

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)

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, 95th 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	178/234 (76%)	1.12	27 (15%)	3	1	28, 45, 68, 113	0
1	B	179/234 (76%)	1.01	18 (10%)	9	5	28, 43, 67, 95	0
1	C	208/234 (88%)	1.14	29 (13%)	4	2	21, 43, 71, 108	0
All	All	565/702 (80%)	1.09	74 (13%)	5	3	21, 44, 68, 113	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	28	GLY	6.5
1	A	167	ARG	5.5
1	C	211	SER	5.4
1	A	94	ASN	4.9
1	B	86	GLY	4.3
1	C	77	SER	4.1
1	C	97	GLU	4.1
1	B	143	VAL	3.9
1	A	103	GLY	3.9
1	C	91	ASN	3.9
1	C	128	THR	3.9
1	A	168	LYS	3.6
1	B	135	ALA	3.6
1	C	153	GLN	3.4
1	C	209	LEU	3.4
1	A	223	VAL	3.3
1	C	145	SER	3.3
1	C	79	THR	3.2
1	A	173	ASP	3.1
1	B	125	GLY	3.0
1	B	218	MET	3.0
1	C	126	SER	2.9
1	B	124	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	29	GLN	2.8
1	C	72	VAL	2.7
1	A	154	THR	2.7
1	C	32	THR	2.7
1	B	194	ASN	2.7
1	C	234	ASN	2.6
1	A	212	THR	2.6
1	A	178	SER	2.6
1	C	177	ALA	2.6
1	C	75	THR	2.5
1	A	227	ASP	2.5
1	C	68	SER	2.5
1	C	62	ILE	2.5
1	B	123	ILE	2.5
1	A	161	PRO	2.5
1	A	157	GLY	2.4
1	A	228	PRO	2.4
1	C	30	GLN	2.4
1	A	59	TYR	2.3
1	C	92	VAL	2.3
1	B	92	VAL	2.3
1	B	133	ALA	2.3
1	C	105	GLY	2.3
1	C	76	SER	2.3
1	A	181	TRP	2.3
1	B	168	LYS	2.3
1	A	72	VAL	2.3
1	A	84	VAL	2.3
1	C	217	ILE	2.3
1	B	129	ASN	2.2
1	B	186	VAL	2.2
1	B	57	THR	2.2
1	B	63	THR	2.2
1	C	187	SER	2.2
1	A	184	SER	2.2
1	A	82	THR	2.2
1	A	191	ALA	2.2
1	C	165	PRO	2.1
1	A	92	VAL	2.1
1	C	38	VAL	2.1
1	A	144	THR	2.1
1	A	165	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	125	GLY	2.1
1	A	123	ILE	2.1
1	A	152	MET	2.0
1	B	122	PRO	2.0
1	A	58	GLN	2.0
1	A	102	SER	2.0
1	C	174	PRO	2.0
1	B	73	ARG	2.0
1	B	208	SER	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.