



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:44 AM EDT

PDB ID : 1X33  
Title : T=3 recombinant capsid of SeMV CP  
Authors : Sangita, V.; Lokesh, G.L.; Satheshkumar, P.S.; Saravanan, V.; Vijay, C.S.;  
Savithri, H.S.; Murthy, M.R.  
Deposited on : 2005-04-29  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

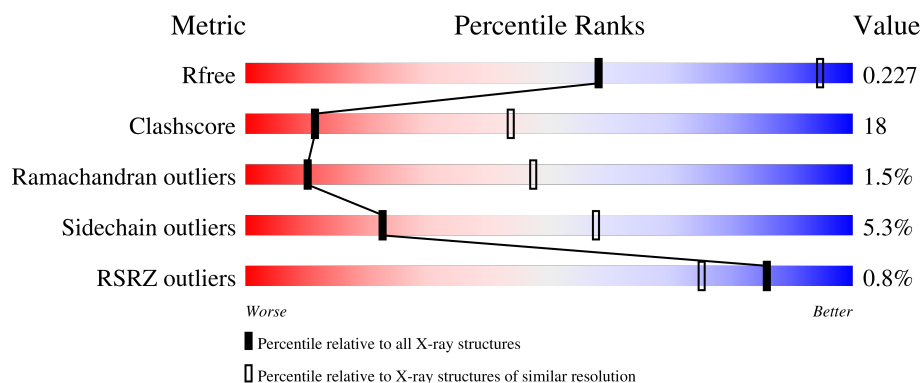
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ . 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	268	
1	B	268	
1	C	268	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4529 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.

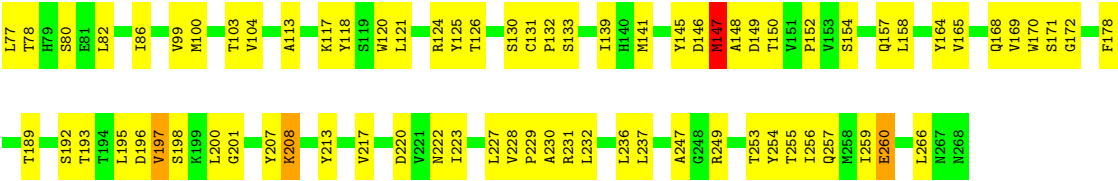
- Molecule 1 is a protein called Coat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	196	Total	C	N	O	S	0	0	0
			1447	921	236	282	8			
1	B	197	Total	C	N	O	S	0	0	0
			1447	915	237	287	8			
1	C	225	Total	C	N	O	S	0	0	0
			1632	1031	270	321	10			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		





## 4 Data and refinement statistics

Property	Value	Source
Space group	R 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	291.31Å 291.31Å 291.31Å 61.63° 61.63° 61.63°	Depositor
Resolution (Å)	15.00 – 3.60 18.31 – 3.56	Depositor EDS
% Data completeness (in resolution range)	59.1 (15.00-3.60) 58.1 (18.31-3.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.232 , 0.234 0.224 , 0.227	Depositor DCC
$R_{free}$ test set	18116 reflections (9.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	(Not available)	Xtrriage
Anisotropy	(Not available)	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.0	EDS
L-test for twinning <sup>1</sup>	$\langle  L  \rangle =$ (Not available), $\langle L^2 \rangle =$ (Not available)	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.85	EDS
Total number of atoms	4529	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *(Not available)*

<sup>1</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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	0.36	0/1479	0.66	0/2028
1	B	0.38	0/1479	0.66	0/2025
1	C	0.37	0/1666	0.65	0/2283
All	All	0.37	0/4624	0.66	0/6336

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1447	0	1415	60	0
1	B	1447	0	1402	48	0
1	C	1632	0	1590	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
All	All	4529	0	4407	158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (158) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:HE2	1:B:260:GLU:OE2	1.68	0.93
1:C:99:VAL:HG12	1:C:230:ALA:O	1.83	0.78
1:C:86:ILE:HG22	1:C:247:ALA:HB3	1.68	0.75
1:A:100:MET:HE1	1:A:208:LYS:HB2	1.69	0.73
1:C:259:ILE:HG13	1:C:260:GLU:HG3	1.71	0.72
1:B:80:SER:HB2	1:B:253:THR:HG23	1.70	0.72
1:C:86:ILE:HG23	1:C:236:LEU:HD11	1.71	0.72
1:C:208:LYS:HE2	1:C:208:LYS:HA	1.71	0.71
1:A:117:LYS:HE2	1:A:260:GLU:OE1	1.91	0.70
1:A:169:VAL:HG13	1:A:247:ALA:HB1	1.73	0.69
1:A:126:THR:HG23	1:A:192:SER:HB2	1.74	0.68
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.58	0.67
1:C:200:LEU:HD23	1:C:229:PRO:HB2	1.76	0.67
1:C:147:MET:HE2	1:C:231:ARG:HD3	1.77	0.67
1:C:165:VAL:HG21	1:C:193:THR:HB	1.76	0.66
1:A:80:SER:OG	1:A:253:THR:HG23	1.95	0.66
1:A:213:TYR:CE1	1:A:217:VAL:HG21	2.32	0.65
1:B:152:PRO:HA	1:C:266:LEU:HD21	1.81	0.63
1:A:74:ILE:HG22	1:A:75:THR:N	2.14	0.62
1:C:67:VAL:HG22	1:C:77:LEU:HD23	1.82	0.62
1:B:111:VAL:HG23	1:B:112:ALA:N	2.14	0.62
1:A:76:VAL:HG22	1:A:257:GLN:HG2	1.82	0.61
1:B:126:THR:HG23	1:B:192:SER:HB2	1.82	0.61
1:A:150:THR:HB	1:B:266:LEU:CD2	2.30	0.61
1:A:158:LEU:HD23	1:A:158:LEU:O	2.00	0.61
1:C:154:SER:OG	1:C:157:GLN:HG3	2.01	0.61
1:B:145:TYR:HB3	1:C:117:LYS:HE3	1.82	0.60
1:A:118:TYR:HB2	1:A:256:ILE:HD11	1.84	0.59
1:A:150:THR:HB	1:B:266:LEU:HD22	1.85	0.59
1:C:125:TYR:CD2	1:C:232:LEU:HD22	2.38	0.59
1:A:86:ILE:HG23	1:A:236:LEU:HD11	1.84	0.58
1:B:158:LEU:HD23	1:B:158:LEU:O	2.04	0.58
1:C:126:THR:HG23	1:C:192:SER:HB2	1.86	0.57
1:C:200:LEU:HD23	1:C:229:PRO:CB	2.34	0.57
1:A:150:THR:O	1:B:266:LEU:HD22	2.04	0.57
1:A:200:LEU:HD22	1:A:229:PRO:HB2	1.87	0.56
1:B:124:ARG:HB2	1:B:194:THR:HG22	1.86	0.56
1:C:86:ILE:HG23	1:C:236:LEU:CD1	2.36	0.56
1:B:114:ASN:HD22	1:B:114:ASN:N	2.03	0.54
1:A:266:LEU:CD2	1:C:150:THR:HB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:ILE:HG13	1:B:179:ILE:HD11	1.90	0.54
1:A:100:MET:O	1:A:104:VAL:HG23	2.08	0.54
1:A:142:GLY:O	1:A:232:LEU:HD12	2.08	0.53
1:A:82:LEU:HD12	1:A:83:SER:N	2.24	0.53
1:C:208:LYS:HD3	1:C:227:LEU:HD22	1.90	0.53
1:B:217:VAL:HG13	1:B:221:VAL:HG12	1.91	0.53
1:A:89:THR:O	1:A:239:GLY:HA3	2.08	0.53
1:A:132:PRO:HD2	1:A:135:THR:OG1	2.09	0.52
1:B:128:ILE:HG13	1:B:179:ILE:CD1	2.39	0.52
1:B:150:THR:O	1:C:266:LEU:HG	2.10	0.52
1:C:141:MET:O	1:C:164:TYR:HA	2.09	0.52
1:B:89:THR:O	1:B:239:GLY:HA3	2.10	0.52
1:A:237:LEU:HD23	1:A:237:LEU:N	2.26	0.51
1:C:100:MET:O	1:C:104:VAL:HG23	2.12	0.50
1:C:131:CYS:HB2	1:C:132:PRO:CD	2.41	0.50
1:C:147:MET:HE2	1:C:231:ARG:CD	2.40	0.50
1:A:226:PRO:HG2	1:A:227:LEU:HD13	1.94	0.50
1:A:79:HIS:CD2	1:A:80:SER:H	2.31	0.49
1:C:237:LEU:HD23	1:C:237:LEU:N	2.27	0.49
1:C:237:LEU:HD23	1:C:237:LEU:H	1.77	0.49
1:C:74:ILE:HG22	1:C:259:ILE:CG2	2.43	0.49
1:B:259:ILE:C	1:B:260:GLU:HG2	2.32	0.49
1:A:266:LEU:HD22	1:C:150:THR:HB	1.95	0.48
1:B:101:PRO:HD3	1:B:118:TYR:CE2	2.48	0.48
1:A:140:HIS:ND1	1:A:166:SER:HB2	2.29	0.48
1:B:223:ILE:O	1:B:227:LEU:HD13	2.13	0.48
1:C:165:VAL:CG2	1:C:193:THR:HB	2.41	0.48
1:A:100:MET:CE	1:A:208:LYS:HB2	2.40	0.48
1:A:137:GLY:C	1:A:169:VAL:HG23	2.34	0.48
1:A:160:ASN:N	1:A:160:ASN:HD22	2.10	0.48
1:B:146:ASP:O	1:B:148:ALA:N	2.46	0.48
1:B:100:MET:HB3	1:B:228:VAL:HG12	1.95	0.48
1:B:249:ARG:HG2	1:B:249:ARG:NH1	2.28	0.48
1:C:130:SER:HB3	1:C:249:ARG:NH1	2.29	0.48
1:C:146:ASP:O	1:C:148:ALA:N	2.47	0.48
1:C:124:ARG:HD3	1:C:178:PHE:CD1	2.49	0.47
1:B:197:VAL:HA	1:B:200:LEU:HD13	1.96	0.47
1:C:256:ILE:HG12	1:C:257:GLN:N	2.29	0.47
1:B:111:VAL:CG2	1:B:112:ALA:N	2.78	0.47
1:B:237:LEU:O	1:B:238:ASP:O	2.33	0.47
1:C:56:GLN:NE2	1:C:171:SER:HA	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:CYS:SG	1:A:178:PHE:N	2.88	0.47
1:C:220:ASP:OD2	1:C:222:ASN:HB2	2.15	0.47
1:C:145:TYR:CD1	1:C:145:TYR:N	2.84	0.46
1:A:237:LEU:HD23	1:A:237:LEU:H	1.79	0.46
1:A:86:ILE:HG23	1:A:236:LEU:CD1	2.46	0.46
1:A:141:MET:HB3	1:A:232:LEU:HD11	1.98	0.46
1:A:145:TYR:CD1	1:A:230:ALA:HB2	2.50	0.46
1:A:77:LEU:HD23	1:A:77:LEU:O	2.16	0.46
1:C:223:ILE:HG22	1:C:223:ILE:O	2.16	0.46
1:A:154:SER:OG	1:A:157:GLN:HG3	2.16	0.46
1:A:82:LEU:HD12	1:A:83:SER:H	1.81	0.45
1:C:197:VAL:O	1:C:200:LEU:HD13	2.15	0.45
1:A:159:SER:HA	1:A:164:TYR:CD1	2.51	0.45
1:A:74:ILE:CG2	1:A:75:THR:N	2.79	0.45
1:B:213:TYR:CE2	1:B:217:VAL:HG21	2.52	0.45
1:A:266:LEU:HD23	1:C:150:THR:HB	1.99	0.45
1:B:89:THR:O	1:B:238:ASP:O	2.34	0.45
1:B:227:LEU:HD12	1:B:227:LEU:N	2.31	0.45
1:C:139:ILE:HA	1:C:236:LEU:HD23	1.99	0.45
1:C:171:SER:OG	1:C:172:GLY:N	2.49	0.45
1:B:77:LEU:O	1:B:77:LEU:HD23	2.17	0.44
1:A:100:MET:HB3	1:A:228:VAL:HG12	2.00	0.44
1:A:169:VAL:CG1	1:A:247:ALA:HB1	2.45	0.44
1:A:180:ASN:O	1:A:180:ASN:CG	2.55	0.44
1:A:108:LEU:HA	1:A:111:VAL:CG1	2.48	0.44
1:A:150:THR:HB	1:B:266:LEU:HD23	1.99	0.44
1:A:91:SER:O	1:A:93:VAL:HG23	2.18	0.44
1:C:228:VAL:HG23	1:C:229:PRO:HD2	2.00	0.44
1:B:128:ILE:CG1	1:B:179:ILE:HD11	2.48	0.43
1:B:237:LEU:CD2	1:B:237:LEU:H	2.31	0.43
1:C:207:TYR:C	1:C:207:TYR:CD1	2.92	0.43
1:A:140:HIS:CE1	1:A:166:SER:HB2	2.53	0.43
1:A:77:LEU:CD2	1:A:256:ILE:HG23	2.48	0.43
1:C:59:MET:HE2	1:C:60:VAL:N	2.34	0.43
1:B:77:LEU:HD23	1:B:77:LEU:C	2.38	0.43
1:A:108:LEU:HA	1:A:111:VAL:HG12	2.01	0.43
1:B:221:VAL:HG23	1:B:222:ASN:N	2.34	0.43
1:C:197:VAL:HA	1:C:200:LEU:CD1	2.49	0.43
1:C:121:LEU:HD12	1:C:257:GLN:HG3	2.00	0.43
1:C:213:TYR:CE2	1:C:217:VAL:HG21	2.54	0.43
1:B:146:ASP:OD2	1:C:208:LYS:HE3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:VAL:HG21	1:C:120:TRP:CZ2	2.54	0.43
1:C:130:SER:HB3	1:C:249:ARG:HH12	1.83	0.43
1:C:200:LEU:HD12	1:C:200:LEU:N	2.33	0.43
1:A:121:LEU:HD12	1:A:121:LEU:HA	1.82	0.43
1:B:121:LEU:HA	1:B:121:LEU:HD23	1.74	0.43
1:C:118:TYR:HB2	1:C:256:ILE:HD11	2.00	0.43
1:B:118:TYR:HB2	1:B:256:ILE:HD11	2.01	0.42
1:B:152:PRO:CA	1:C:266:LEU:HD21	2.48	0.42
1:A:116:SER:HB2	1:A:260:GLU:HB2	2.01	0.42
1:A:131:CYS:HB2	1:A:132:PRO:CD	2.49	0.42
1:A:112:ALA:HA	1:A:258:MET:CE	2.49	0.42
1:B:137:GLY:HA2	1:B:238:ASP:CB	2.50	0.42
1:C:99:VAL:HG22	1:C:99:VAL:O	2.19	0.42
1:C:196:ASP:O	1:C:198:SER:N	2.53	0.42
1:A:223:ILE:O	1:A:223:ILE:HG22	2.19	0.42
1:A:243:THR:HG23	1:A:243:THR:O	2.19	0.42
1:A:217:VAL:HG12	1:A:217:VAL:O	2.19	0.42
1:B:159:SER:HA	1:B:164:TYR:CD1	2.55	0.42
1:B:256:ILE:HG12	1:B:257:GLN:N	2.34	0.42
1:C:133:SER:HA	1:C:170:TRP:CD2	2.55	0.42
1:C:200:LEU:O	1:C:201:GLY:C	2.57	0.41
1:A:131:CYS:SG	1:A:169:VAL:HG12	2.61	0.41
1:B:103:THR:O	1:B:104:VAL:C	2.57	0.41
1:A:80:SER:HA	1:A:252:CYS:O	2.21	0.41
1:B:114:ASN:N	1:B:114:ASN:ND2	2.69	0.41
1:B:154:SER:OG	1:B:157:GLN:HG3	2.20	0.41
1:C:146:ASP:HB3	1:C:149:ASP:OD2	2.20	0.41
1:A:99:VAL:HG23	1:A:231:ARG:HA	2.02	0.41
1:C:80:SER:OG	1:C:253:THR:HG23	2.21	0.41
1:C:78:THR:HG23	1:C:255:THR:OG1	2.21	0.40
1:A:180:ASN:O	1:A:181:GLY:C	2.59	0.40
1:B:217:VAL:O	1:B:217:VAL:HG12	2.22	0.40
1:B:226:PRO:HG2	1:B:227:LEU:HD12	2.02	0.40
1:C:113:ALA:HA	1:C:207:TYR:CE2	2.56	0.40
1:C:77:LEU:CD1	1:C:254:TYR:HE1	2.34	0.40
1:C:146:ASP:C	1:C:148:ALA:N	2.75	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	194/268 (72%)	171 (88%)	19 (10%)	4 (2%)	7	40
1	B	195/268 (73%)	173 (89%)	20 (10%)	2 (1%)	15	55
1	C	223/268 (83%)	202 (91%)	18 (8%)	3 (1%)	12	50
All	All	612/804 (76%)	546 (89%)	57 (9%)	9 (2%)	10	47

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	ALA
1	B	238	ASP
1	A	181	GLY
1	B	147	MET
1	C	147	MET
1	C	197	VAL
1	A	147	MET
1	A	152	PRO
1	C	152	PRO

### 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	156/220 (71%)	151 (97%)	5 (3%)	39	70
1	B	156/220 (71%)	149 (96%)	7 (4%)	27	62
1	C	174/220 (79%)	160 (92%)	14 (8%)	12	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	486/660 (74%)	460 (95%)	26 (5%)	22	58

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	166	SER
1	A	177	CYS
1	A	198	SER
1	A	233	VAL
1	B	77	LEU
1	B	162	ARG
1	B	180	ASN
1	B	198	SER
1	B	237	LEU
1	B	249	ARG
1	B	260	GLU
1	C	50	SER
1	C	54	SER
1	C	59	MET
1	C	61	ARG
1	C	82	LEU
1	C	103	THR
1	C	147	MET
1	C	158	LEU
1	C	168	GLN
1	C	169	VAL
1	C	189	THR
1	C	195	LEU
1	C	208	LYS
1	C	260	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	HIS
1	A	160	ASN
1	B	114	ASN
1	B	160	ASN
1	B	180	ASN
1	C	56	GLN

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Mol	Chain	Res	Type
1	C	168	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are 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](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	196/268 (73%)	-0.80	0 100 100	9, 19, 56, 98	0
1	B	197/268 (73%)	-0.72	3 (1%) 73 60	9, 22, 92, 98	0
1	C	225/268 (83%)	-0.82	2 (0%) 84 73	9, 21, 64, 92	0
All	All	618/804 (76%)	-0.78	5 (0%) 86 75	9, 21, 75, 98	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	SER	3.9
1	C	45	THR	3.0
1	B	242	SER	3.0
1	B	241	SER	2.7
1	C	44	PRO	2.4

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	271	1/1	0.97	0.10	23,23,23,23	0
2	CA	C	270	1/1	0.97	0.16	23,23,23,23	0
2	CA	B	269	1/1	0.98	0.08	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.