Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 07:12 PM EDT

PDB ID	:	1OPO
Title	:	THE STRUCTURE OF CARNATION MOTTLE VIRUS
Authors	:	Morgunova, E.; Dauter, Z.; Fry, E.; Stuart, D.; Stel'mashchuk, V.; Mikhailov, A.M.; Wilson, K.S.; Vainshtein, B.K.
Deposited on	:	2003-03-06
Resolution	:	3.20 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

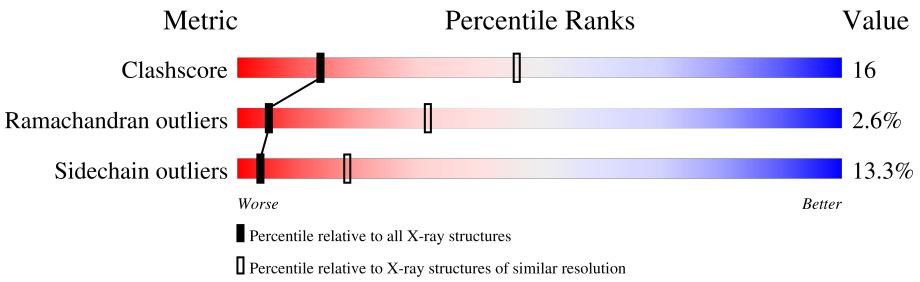
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.20 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	48% 23% 6% 23%
1	B	348	49% 22% 6% 23%
1	C	348	49% 24% • 23%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	500	-	-	X	-
2	SO4	B	501	-	X	-	-

2 Entry composition (i)

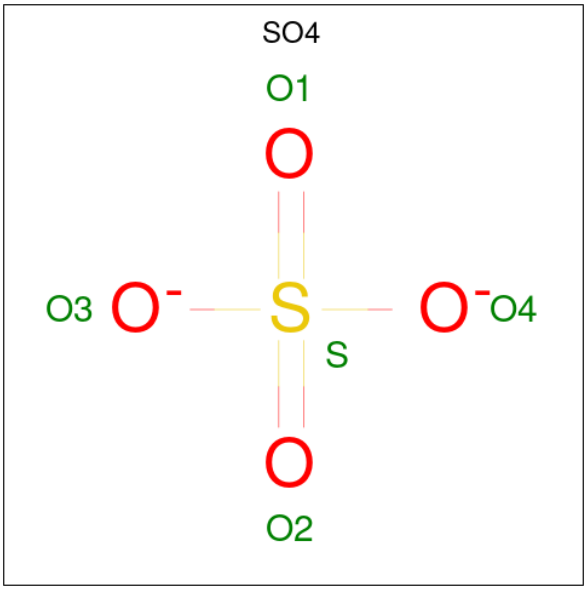
There are 3 unique types of molecules in this entry. The entry contains 6130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	267	2035	1294	336	398	7	0	0	0
1	B	267	2035	1294	336	398	7	0	0	0
1	C	268	2044	1300	338	399	7	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	B	1	5	4	1	0	0
2	C	1	5	4	1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

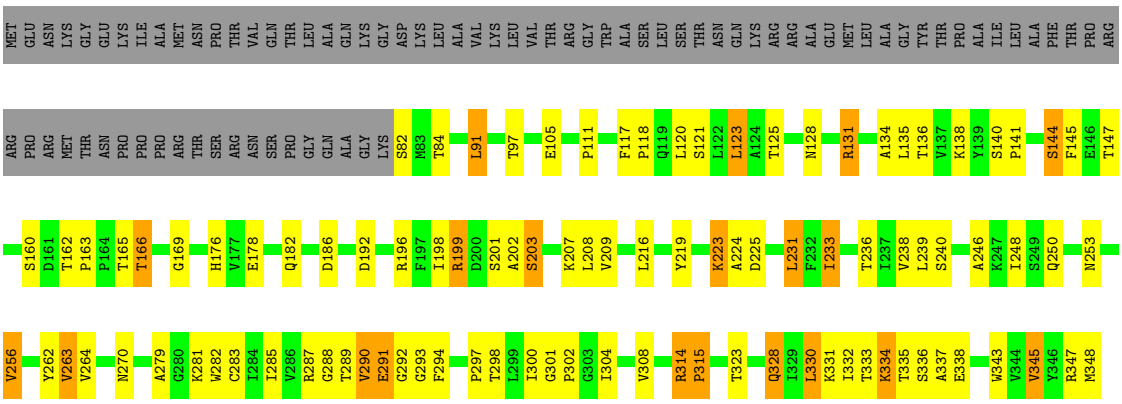
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 was not executed.

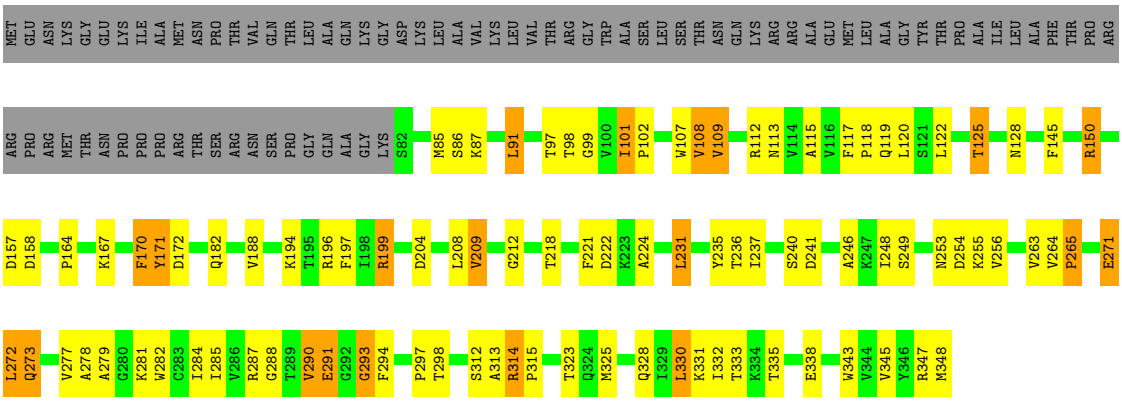
- Molecule 1: Coat protein

Chain A: 48% 23% 6% 23%



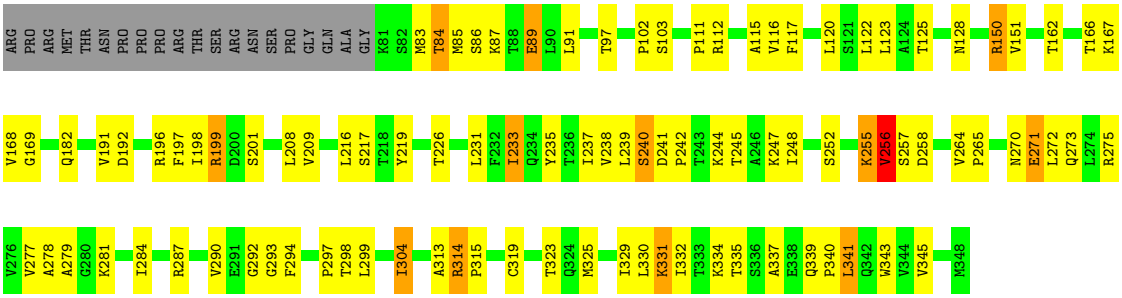
- Molecule 1: Coat protein

Chain B: 49% 22% 6% 23%



- Molecule 1: Coat protein

Chain C: 49% 24% • 23%


ARG PRO ARG MET THR ASN PRO PRO PRO ARG THR SER ARG ASN SER PRO GLY GLN ALA GLY K81 S82 M83 T84 M85 S86 K87 T88 E89 L90 L91 T97 P102 S103 P111 R112 A115 V116 F117 L120 S121 L122 L123 A124 T125 N128 R150 V151 T162 T166 K167
V168 G169 Q182 V191 D192 R196 F197 I198 R199 D200 S201 L208 V209 L216 S217 T218 Y219 T226 L231 F232 I233 Q234 Y235 T236 I237 V238 L239 S240 D241 P242 T243 K244 T245 A246 K247 I248 S252 K255 V256 S257 D258 V264 P265 N270 E271 L272 Q273 L274 R275
V276 V277 A278 A279 G280 K281 I284 R287 V290 E291 G292 G293 F294 P297 T298 L299 I304 A313 R314 P315 C319 T323 Q324 M325 I329 L330 K331 I332 T333 K334 T335 S336 A337 E338 Q339 P340 L341 Q342 W343 V344 V345 M348

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	382.60Å 382.60Å 382.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-3.20)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 2.1	Depositor
R, R_{free}	0.183 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6130	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

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, SO4

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	0.63	0/2074	0.89	1/2823 (0.0%)
1	B	0.61	0/2074	0.86	1/2823 (0.0%)
1	C	0.63	0/2083	0.86	2/2834 (0.1%)
All	All	0.63	0/6231	0.87	4/8480 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	314	ARG	N-CA-C	-6.12	94.48	111.00
1	B	170	PHE	N-CA-C	-5.52	96.11	111.00
1	C	240	SER	N-CA-C	5.47	125.78	111.00
1	A	192	ASP	CB-CG-OD1	5.36	123.13	118.30

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	2035	0	2053	69	0
1	B	2035	0	2053	73	1
1	C	2044	0	2066	56	1
2	A	5	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
3	B	1	0	0	0	0
All	All	6130	0	6172	195	1

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 16.

All (195) 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:A:304:ILE:HB	1:A:328:GLN:HG2	1.51	0.93
1:A:279:ALA:HA	1:A:323:THR:HG23	1.50	0.92
1:B:107:TRP:O	1:B:108:VAL:HB	1.74	0.85
1:A:144:SER:O	1:A:147:THR:HG23	1.80	0.81
1:A:145:PHE:HA	1:A:182:GLN:HG2	1.61	0.81
1:C:91:LEU:HD12	1:C:233:ILE:HG12	1.62	0.81
1:A:117:PHE:HB3	1:A:120:LEU:HB3	1.62	0.79
1:B:117:PHE:HB3	1:B:120:LEU:HB3	1.64	0.79
1:A:199:ARG:HB2	1:A:209:VAL:HG11	1.64	0.78
1:A:290:VAL:HG12	1:A:291:GLU:N	1.99	0.77
1:B:279:ALA:HA	1:B:323:THR:HG23	1.66	0.76
1:C:255:LYS:O	1:C:256:VAL:HB	1.84	0.76
1:A:314:ARG:HH11	1:A:314:ARG:CG	2.00	0.75
1:A:250:GLN:HE22	1:A:263:VAL:H	1.33	0.74
1:C:341:LEU:H	1:C:341:LEU:HD12	1.51	0.73
1:B:108:VAL:HG13	1:B:109:VAL:N	2.05	0.71
1:B:125:THR:HG22	1:B:246:ALA:HB3	1.71	0.71
1:B:298:THR:HG23	1:B:331:LYS:HB3	1.73	0.70
1:C:335:THR:HG22	1:C:337:ALA:H	1.55	0.70
1:B:314:ARG:C	1:B:314:ARG:HD3	2.14	0.68
1:B:293:GLY:HA2	1:B:338:GLU:CG	2.24	0.68
1:B:272:LEU:HD22	1:B:273:GLN:N	2.10	0.67
1:B:325:MET:HB3	1:B:328:GLN:HE21	1.59	0.66
1:B:108:VAL:CG1	1:B:109:VAL:N	2.58	0.66
1:C:83:MET:HE1	1:C:123:LEU:HD21	1.77	0.65
1:B:272:LEU:HD22	1:B:273:GLN:H	1.62	0.65
1:A:135:LEU:HD11	1:A:233:ILE:HD11	1.78	0.64
1:A:304:ILE:HB	1:A:328:GLN:CG	2.27	0.64
1:A:138:LYS:HB3	1:A:186:ASP:OD2	1.99	0.63
1:A:270:ASN:HD22	1:A:334:LYS:HG2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PHE:HA	1:B:182:GLN:HG3	1.80	0.63
1:B:108:VAL:O	1:B:109:VAL:HB	1.99	0.62
1:C:323:THR:HG22	1:C:325:MET:O	1.99	0.62
1:A:314:ARG:HH11	1:A:314:ARG:HG2	1.65	0.61
1:B:98:THR:HG22	1:B:99:GLY:H	1.66	0.61
1:C:248:ILE:HG22	1:C:248:ILE:O	2.01	0.61
1:B:150:ARG:HG3	1:B:150:ARG:HH11	1.66	0.60
1:C:117:PHE:HB3	1:C:120:LEU:HB3	1.83	0.60
1:B:218:THR:HG23	1:B:221:PHE:CE2	2.36	0.60
1:C:199:ARG:HD3	1:C:201:SER:O	2.02	0.60
1:A:97:THR:HG22	1:A:219:TYR:HA	1.83	0.60
1:A:289:THR:HG22	1:A:338:GLU:OE1	2.02	0.60
1:B:271:GLU:HG3	1:B:331:LYS:NZ	2.17	0.60
1:A:250:GLN:NE2	1:A:262:TYR:H	2.00	0.60
1:A:290:VAL:CG1	1:A:291:GLU:N	2.65	0.59
1:A:290:VAL:HG12	1:A:291:GLU:H	1.68	0.59
1:C:166:THR:HG22	1:C:168:VAL:H	1.67	0.58
1:C:240:SER:O	1:C:242:PRO:HD3	2.02	0.58
1:B:293:GLY:HA2	1:B:338:GLU:HG2	1.84	0.58
1:B:282:TRP:HE1	1:B:323:THR:CG2	2.15	0.58
1:B:107:TRP:O	1:B:108:VAL:CB	2.50	0.58
1:B:158:ASP:HB3	1:C:197:PHE:CE1	2.38	0.58
1:B:290:VAL:HG12	1:B:291:GLU:N	2.19	0.58
1:B:98:THR:HG22	1:B:99:GLY:N	2.19	0.58
1:A:166:THR:HB	1:A:169:GLY:H	1.68	0.57
1:A:290:VAL:HG12	1:A:292:GLY:H	1.70	0.57
1:C:122:LEU:O	1:C:125:THR:HG22	2.05	0.57
1:A:302:PRO:O	1:A:328:GLN:NE2	2.38	0.57
1:B:108:VAL:HG12	1:B:113:ASN:HD22	1.70	0.56
1:C:237:ILE:HG22	1:C:238:VAL:N	2.19	0.56
1:B:288:GLY:CA	1:B:315:PRO:HG2	2.35	0.56
1:B:285:ILE:O	1:B:343:TRP:HA	2.05	0.56
1:A:297:PRO:HB3	1:A:332:ILE:HG12	1.88	0.56
1:B:108:VAL:O	1:B:212:GLY:O	2.23	0.56
1:A:131:ARG:HB3	1:A:131:ARG:HH11	1.70	0.55
1:A:250:GLN:HB3	1:A:345:VAL:HG13	1.88	0.55
1:C:339:GLN:HB3	1:C:340:PRO:HD2	1.88	0.55
1:B:253:ASN:H	1:B:253:ASN:ND2	2.04	0.55
1:A:105:GLU:HB2	1:A:216:LEU:HB3	1.89	0.55
1:C:116:VAL:HG13	1:C:233:ILE:HD13	1.89	0.55
1:A:131:ARG:HH11	1:A:131:ARG:CB	2.19	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:HIS:ND1	1:A:178:GLU:OE1	2.41	0.54
1:A:199:ARG:HB2	1:A:209:VAL:CG1	2.35	0.54
1:B:85:MET:O	1:B:236:THR:HA	2.08	0.54
1:A:314:ARG:CG	1:A:314:ARG:NH1	2.68	0.53
1:C:97:THR:HG22	1:C:219:TYR:HA	1.88	0.53
1:C:252:SER:HB3	1:C:343:TRP:CE2	2.43	0.53
1:B:91:LEU:HD13	1:B:231:LEU:HD13	1.91	0.52
1:A:250:GLN:HE22	1:A:263:VAL:N	2.04	0.52
1:C:197:PHE:O	1:C:209:VAL:HG13	2.09	0.52
1:A:270:ASN:HD21	1:A:336:SER:HA	1.74	0.51
1:B:288:GLY:HA3	1:B:315:PRO:HG2	1.92	0.51
1:C:297:PRO:HB3	1:C:332:ILE:HG12	1.92	0.51
1:B:108:VAL:O	1:B:109:VAL:CB	2.57	0.51
1:A:162:THR:HG22	1:A:163:PRO:O	2.11	0.51
1:B:293:GLY:HA2	1:B:338:GLU:HG3	1.93	0.51
1:C:265:PRO:HA	1:C:273:GLN:O	2.10	0.51
1:A:335:THR:HG22	1:A:337:ALA:H	1.76	0.51
1:B:170:PHE:O	1:B:171:TYR:HB2	2.10	0.51
1:B:297:PRO:HB3	1:B:332:ILE:HG13	1.92	0.51
1:A:165:THR:HB	2:A:500:SO4:O2	2.11	0.50
1:C:84:THR:HB	1:C:238:VAL:HG22	1.94	0.50
1:A:201:SER:HB2	1:A:256:VAL:O	2.12	0.50
1:B:328:GLN:OE1	1:B:328:GLN:HA	2.11	0.50
1:A:169:GLY:HA3	2:A:500:SO4:O3	2.12	0.49
1:B:291:GLU:CG	1:B:313:ALA:HA	2.42	0.49
1:C:112:ARG:HD3	1:C:198:ILE:HG21	1.93	0.49
1:C:199:ARG:CB	1:C:209:VAL:HG11	2.41	0.49
1:C:279:ALA:HA	1:C:323:THR:HB	1.93	0.49
1:A:314:ARG:HG2	1:A:314:ARG:NH1	2.25	0.49
1:B:87:LYS:NZ	1:B:119:GLN:HE22	2.10	0.49
1:C:199:ARG:CA	1:C:209:VAL:HG11	2.43	0.49
1:C:299:LEU:HB3	1:C:304:ILE:HG12	1.95	0.49
1:C:115:ALA:HA	1:C:278:ALA:HB2	1.94	0.48
1:A:134:ALA:HB3	1:A:236:THR:HB	1.94	0.48
1:B:125:THR:CG2	1:B:246:ALA:HB3	2.42	0.48
1:A:294:PHE:CE1	1:A:315:PRO:HB2	2.49	0.48
1:C:216:LEU:HD12	1:C:217:SER:H	1.79	0.48
1:C:255:LYS:HA	1:C:255:LYS:CE	2.44	0.48
1:C:87:LYS:HE3	1:C:89:GLU:OE2	2.14	0.48
1:C:115:ALA:HB2	1:C:277:VAL:HG12	1.96	0.48
1:C:271:GLU:HG3	1:C:331:LYS:NZ	2.29	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:SER:HB2	1:A:239:LEU:O	2.13	0.47
1:A:288:GLY:CA	1:A:315:PRO:HG2	2.44	0.47
1:A:300:ILE:HD12	1:A:300:ILE:N	2.28	0.47
1:B:170:PHE:O	1:B:171:TYR:CB	2.62	0.47
1:B:282:TRP:HE1	1:B:323:THR:HG22	1.77	0.47
1:C:111:PRO:HG2	1:C:198:ILE:HG23	1.95	0.47
1:A:111:PRO:O	1:A:121:SER:HA	2.14	0.47
1:B:291:GLU:HG3	1:B:313:ALA:HA	1.96	0.47
1:B:108:VAL:CG1	1:B:109:VAL:H	2.27	0.47
1:C:272:LEU:HD12	1:C:273:GLN:H	1.80	0.47
1:A:279:ALA:CA	1:A:323:THR:HG23	2.34	0.47
1:A:289:THR:O	1:A:290:VAL:HG23	2.15	0.47
1:B:279:ALA:CA	1:B:323:THR:HG23	2.41	0.47
1:B:101:ILE:HD12	1:B:101:ILE:H	1.79	0.46
1:B:120:LEU:HD21	1:B:237:ILE:HD11	1.96	0.46
1:B:265:PRO:HA	1:B:273:GLN:O	2.16	0.46
1:B:150:ARG:HH11	1:B:150:ARG:CG	2.29	0.46
1:B:271:GLU:HG3	1:B:331:LYS:HZ1	1.80	0.46
1:A:118:PRO:O	1:A:347:ARG:NH2	2.48	0.46
1:B:271:GLU:HG3	1:B:331:LYS:HZ3	1.81	0.46
1:A:285:ILE:O	1:A:343:TRP:HA	2.16	0.45
1:A:223:LYS:HE3	1:A:223:LYS:HB3	1.81	0.45
1:A:91:LEU:HD13	1:A:231:LEU:HD13	1.97	0.45
1:C:248:ILE:O	1:C:248:ILE:CG2	2.64	0.45
1:C:272:LEU:HD12	1:C:273:GLN:N	2.32	0.45
1:C:294:PHE:CD1	1:C:341:LEU:HD23	2.51	0.45
1:B:199:ARG:NH2	1:B:204:ASP:O	2.49	0.45
1:A:160:SER:HB2	1:A:207:LYS:NZ	2.32	0.45
1:B:248:ILE:O	1:B:248:ILE:CG2	2.65	0.45
1:C:102:PRO:HA	1:C:219:TYR:HB3	1.98	0.45
1:B:167:LYS:O	1:B:170:PHE:O	2.34	0.45
1:A:82:SER:HB2	1:A:240:SER:HA	1.99	0.44
1:A:202:ALA:O	1:A:203:SER:CB	2.66	0.44
1:C:86:SER:HA	1:C:235:TYR:O	2.18	0.44
1:C:237:ILE:CG2	1:C:238:VAL:N	2.80	0.44
1:C:150:ARG:HG3	1:C:151:VAL:N	2.32	0.44
1:B:120:LEU:HD21	1:B:237:ILE:CD1	2.48	0.44
1:B:97:THR:HB	1:B:218:THR:HG22	2.00	0.44
1:A:288:GLY:HA3	1:A:315:PRO:HG2	1.99	0.43
1:C:115:ALA:HB2	1:C:277:VAL:CG1	2.47	0.43
1:C:128:ASN:N	1:C:241:ASP:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:VAL:HG12	1:C:192:ASP:O	2.18	0.43
1:C:199:ARG:HB2	1:C:209:VAL:HG11	1.99	0.43
1:B:284:ILE:HG12	1:B:345:VAL:HG22	2.00	0.43
1:B:278:ALA:O	1:B:323:THR:HG21	2.19	0.43
1:C:290:VAL:HG12	1:C:292:GLY:H	1.83	0.43
1:A:125:THR:HB	1:A:246:ALA:HB3	2.01	0.43
1:B:158:ASP:HB3	1:C:197:PHE:CZ	2.53	0.43
1:B:294:PHE:CE1	1:B:315:PRO:HB2	2.54	0.43
1:B:288:GLY:C	1:B:315:PRO:HG2	2.39	0.42
1:A:199:ARG:CB	1:A:209:VAL:HG11	2.41	0.42
1:B:253:ASN:ND2	1:B:253:ASN:N	2.67	0.42
1:A:282:TRP:HE1	1:A:323:THR:CG2	2.32	0.42
1:A:289:THR:O	1:A:289:THR:HG23	2.19	0.42
1:B:115:ALA:HB2	1:B:277:VAL:CG1	2.50	0.42
1:B:314:ARG:HH11	1:B:314:ARG:HG3	1.85	0.42
1:C:122:LEU:O	1:C:125:THR:CG2	2.67	0.42
1:A:301:GLY:O	1:A:304:ILE:HG22	2.20	0.42
1:A:314:ARG:HH11	1:A:314:ARG:HG3	1.80	0.42
1:B:330:LEU:HD23	1:B:330:LEU:HA	1.70	0.42
1:A:330:LEU:HD23	1:A:330:LEU:HA	1.83	0.42
1:A:270:ASN:ND2	1:A:334:LYS:HG2	2.33	0.42
1:A:123:LEU:HD12	1:A:123:LEU:HA	1.89	0.42
1:B:101:ILE:HG22	1:B:102:PRO:HD2	2.01	0.42
1:B:86:SER:HA	1:B:235:TYR:O	2.20	0.41
1:B:122:LEU:O	1:B:125:THR:OG1	2.35	0.41
1:B:240:SER:O	1:B:241:ASP:HB3	2.20	0.41
1:C:231:LEU:HD23	1:C:231:LEU:HA	1.76	0.41
1:B:150:ARG:CG	1:B:150:ARG:NH1	2.83	0.41
1:C:125:THR:HG23	1:C:245:THR:HG23	2.02	0.41
1:B:117:PHE:CB	1:B:120:LEU:HB3	2.45	0.41
1:B:164:PRO:HA	1:C:244:LYS:HE3	2.02	0.41
1:A:140:SER:HA	1:A:141:PRO:HD3	1.92	0.41
1:A:297:PRO:HG2	1:A:308:VAL:HG11	2.03	0.41
1:A:298:THR:HG23	1:A:331:LYS:HB3	2.03	0.41
1:C:284:ILE:HG12	1:C:345:VAL:HG22	2.03	0.41
1:A:281:LYS:HB3	1:A:348:MET:HB3	2.04	0.40
1:C:166:THR:HB	1:C:169:GLY:H	1.86	0.40
1:C:275:ARG:HG3	1:C:329:ILE:HG12	2.03	0.40
1:A:283:CYS:HB2	1:A:348:MET:CE	2.51	0.40
1:A:282:TRP:HE1	1:A:323:THR:HG22	1.86	0.40
1:B:197:PHE:O	1:B:209:VAL:HG22	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LEU:HD23	1:C:239:LEU:HA	1.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASP:OD2	1:C:89:GLU:OE2[2_555]	2.12	0.08

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	265/348 (76%)	249 (94%)	8 (3%)	8 (3%)	4 28
1	B	265/348 (76%)	244 (92%)	12 (4%)	9 (3%)	3 24
1	C	266/348 (76%)	245 (92%)	17 (6%)	4 (2%)	10 44
All	All	796/1044 (76%)	738 (93%)	37 (5%)	21 (3%)	5 31

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	SER
1	A	224	ALA
1	B	108	VAL
1	B	224	ALA
1	B	290	VAL
1	B	293	GLY
1	C	293	GLY
1	A	290	VAL
1	A	291	GLU
1	A	293	GLY
1	B	171	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291	GLU
1	C	256	VAL
1	C	313	ALA
1	A	225	ASP
1	B	109	VAL
1	B	118	PRO
1	C	315	PRO
1	A	256	VAL
1	A	315	PRO
1	B	256	VAL

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	228/294 (78%)	201 (88%)	27 (12%)	5 23
1	B	228/294 (78%)	195 (86%)	33 (14%)	3 15
1	C	229/294 (78%)	198 (86%)	31 (14%)	4 18
All	All	685/882 (78%)	594 (87%)	91 (13%)	4 18

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	THR
1	A	91	LEU
1	A	123	LEU
1	A	128	ASN
1	A	131	ARG
1	A	136	THR
1	A	144	SER
1	A	166	THR
1	A	196	ARG
1	A	198	ILE
1	A	199	ARG
1	A	208	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	223	LYS
1	A	231	LEU
1	A	233	ILE
1	A	238	VAL
1	A	248	ILE
1	A	253	ASN
1	A	263	VAL
1	A	264	VAL
1	A	287	ARG
1	A	314	ARG
1	A	328	GLN
1	A	330	LEU
1	A	333	THR
1	A	334	LYS
1	A	345	VAL
1	B	91	LEU
1	B	101	ILE
1	B	112	ARG
1	B	125	THR
1	B	128	ASN
1	B	150	ARG
1	B	157	ASP
1	B	188	VAL
1	B	194	LYS
1	B	196	ARG
1	B	199	ARG
1	B	208	LEU
1	B	209	VAL
1	B	222	ASP
1	B	231	LEU
1	B	249	SER
1	B	254	ASP
1	B	255	LYS
1	B	263	VAL
1	B	264	VAL
1	B	265	PRO
1	B	271	GLU
1	B	272	LEU
1	B	273	GLN
1	B	281	LYS
1	B	287	ARG
1	B	312	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	314	ARG
1	B	330	LEU
1	B	333	THR
1	B	335	THR
1	B	347	ARG
1	B	348	MET
1	C	84	THR
1	C	85	MET
1	C	89	GLU
1	C	103	SER
1	C	150	ARG
1	C	162	THR
1	C	167	LYS
1	C	182	GLN
1	C	196	ARG
1	C	199	ARG
1	C	208	LEU
1	C	226	THR
1	C	233	ILE
1	C	247	LYS
1	C	255	LYS
1	C	256	VAL
1	C	257	SER
1	C	258	ASP
1	C	264	VAL
1	C	270	ASN
1	C	271	GLU
1	C	281	LYS
1	C	287	ARG
1	C	298	THR
1	C	304	ILE
1	C	314	ARG
1	C	319	CYS
1	C	330	LEU
1	C	331	LYS
1	C	334	LYS
1	C	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126	ASN
1	A	128	ASN
1	A	148	ASN
1	A	250	GLN
1	A	270	ASN
1	A	342	GLN
1	B	119	GLN
1	B	128	ASN
1	B	253	ASN
1	B	270	ASN
1	B	273	GLN
1	B	328	GLN
1	B	342	GLN
1	C	119	GLN
1	C	148	ASN
1	C	273	GLN
1	C	324	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 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	501	-	4,4,4	0.48	0	6,6,6	2.69	4 (66%)
2	SO4	C	502	-	4,4,4	0.42	0	6,6,6	1.98	2 (33%)
2	SO4	A	500	-	4,4,4	0.23	0	6,6,6	1.35	1 (16%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	SO4	O4-S-O2	-3.95	88.70	109.31
2	B	501	SO4	O4-S-O3	3.57	124.31	109.06
2	C	502	SO4	O3-S-O2	-3.51	91.00	109.31
2	B	501	SO4	O4-S-O1	-2.63	95.60	109.31
2	B	501	SO4	O3-S-O1	2.62	123.00	109.31
2	C	502	SO4	O2-S-O1	2.33	126.64	109.43
2	A	500	SO4	O2-S-O1	-2.06	94.18	109.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	SO4	2	0

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 was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.