



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 01:37 pm GMT

PDB ID : 1OPO  
Title : THE STRUCTURE OF CARNATION MOTTLE VIRUS  
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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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

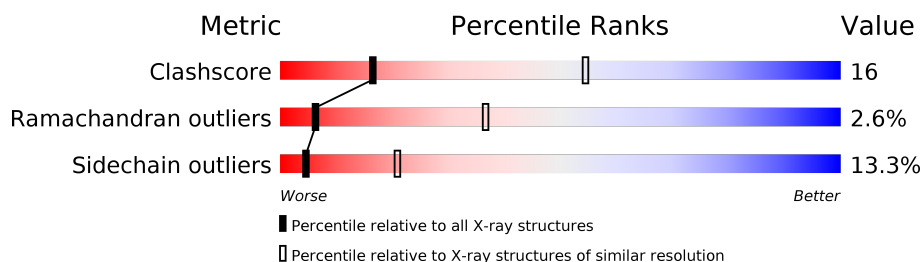
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	
1	C	348	

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](#)

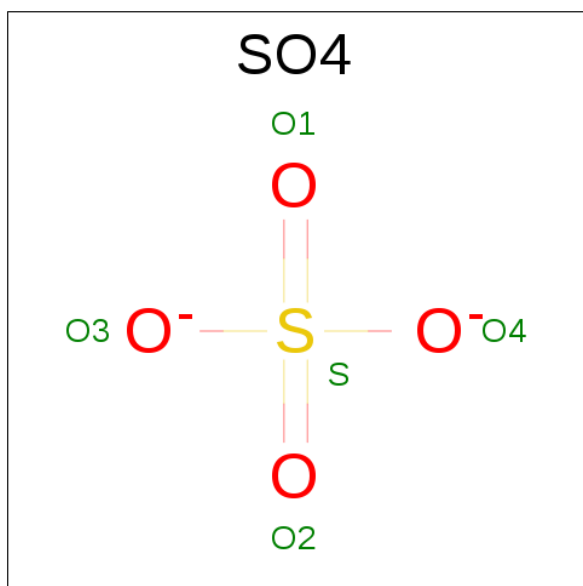
There are 3 unique types of molecules in this entry. The entry contains 6130 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

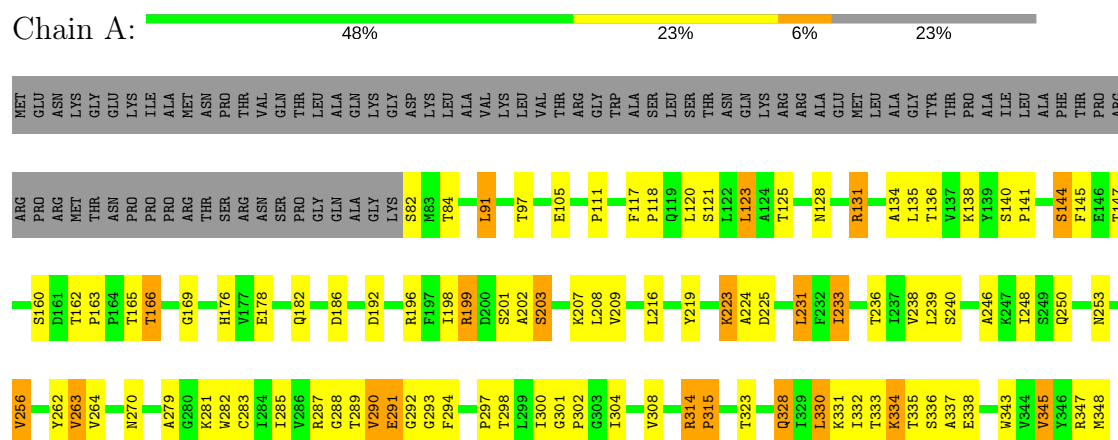
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0

### 3 Residue-property plots

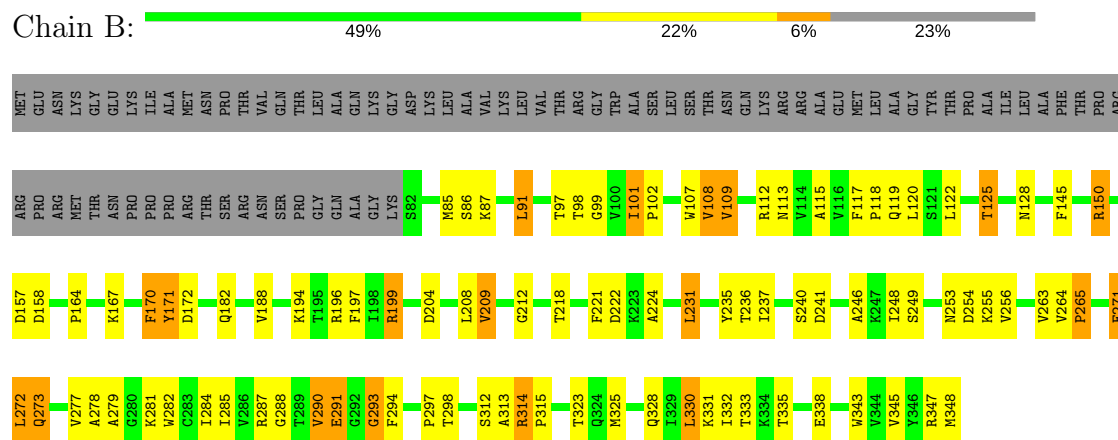
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

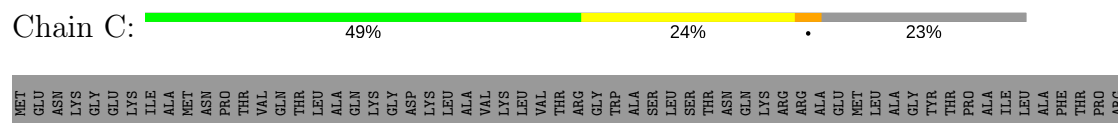
#### • Molecule 1: Coat protein



#### • Molecule 1: Coat protein



#### • Molecule 1: Coat protein



ARG	PRO	ARG	ARG	THR	ASN	PRO	PRO	PRO	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	T238	Q234	Y235	T236	I237	V238	L239	S240	D241	P242	T243	K244	T245	A246	K247	I248	S252	K255	L256	S257	D258	V264	P265	N270	E271	L272	Q273	L274	R275
V276	V277	A278	A279	G280	K281	T284	R287	V290	F291	G292	G293	F294	P297	T298	L299	I304	A313	R314	P315	C319	T323	Q324	N325	I329	L330	K331	I332	T333	K334	T335	S336	A337	E338	Q339	F340	L341	Q342	V343	V344	V345	N348								

## 4 Data and refinement statistics

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, $\alpha$ , $\beta$ , $\gamma$	382.60 Å   382.60 Å   382.60 Å 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 <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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(°)	Ideal(°)
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

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

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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:CG	1:A:314:ARG:HH11	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

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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:HG2	1:A:314:ARG:HH11	1.65	0.61
1:B:98:THR:HG22	1:B:99:GLY:H	1.66	0.61
1:C:248:ILE:O	1:C:248:ILE:HG22	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:289:THR:HG22	1:A:338:GLU:OE1	2.02	0.60
1:A:97:THR:HG22	1:A:219:TYR:HA	1.83	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:HH11	1:A:131:ARG:HB3	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:ND2	1:B:253:ASN:H	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

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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:HA	1:B:328:GLN:OE1	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:CE	1:C:255:LYS:HA	2.44	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
1:C:87:LYS:HE3	1:C:89:GLU:OE2	2.14	0.48

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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:N	1:A:300:ILE:HD12	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:289:THR:O	1:A:290:VAL:HG23	2.15	0.47
1:A:279:ALA:CA	1:A:323:THR:HG23	2.34	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:202:ALA:O	1:A:203:SER:CB	2.66	0.44
1:A:82:SER:HB2	1:A:240:SER:HA	1.99	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:191:VAL:HG12	1:C:192:ASP:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ARG:HB2	1:C:209:VAL:HG11	1.99	0.43
1:C:128:ASN:N	1:C:241:ASP:O	2.51	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:N	1:B:253:ASN:ND2	2.67	0.42
1:A:289:THR:HG23	1:A:289:THR:O	2.19	0.42
1:A:282:TRP:HE1	1:A:323:THR:CG2	2.32	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:HA	1:B:330:LEU:HD23	1.70	0.42
1:A:330:LEU:HA	1:A:330:LEU:HD23	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:122:LEU:O	1:B:125:THR:OG1	2.35	0.41
1:B:86:SER:HA	1:B:235:TYR:O	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LEU:HA	1:C:239:LEU:HD23	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%)	5	32
1	B	265/348 (76%)	244 (92%)	12 (4%)	9 (3%)	4	28
1	C	266/348 (76%)	245 (92%)	17 (6%)	4 (2%)	12	51
All	All	796/1044 (76%)	738 (93%)	37 (5%)	21 (3%)	6	36

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

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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 ⓘ

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%)	6	27
1	B	228/294 (78%)	195 (86%)	33 (14%)	4	17
1	C	229/294 (78%)	198 (86%)	31 (14%)	4	20
All	All	685/882 (78%)	594 (87%)	91 (13%)	4	21

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

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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

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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

Some 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

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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 carbohydrates 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	A	500	-	4,4,4	0.21	0	6,6,6	1.34	1 (16%)
2	SO4	B	501	-	4,4,4	0.42	0	6,6,6	2.56	4 (66%)
2	SO4	C	502	-	4,4,4	0.43	0	6,6,6	1.92	2 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	500	-	-	0/0/0/0	0/0/0/0
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	SO4	O4-S-O2	-3.73	88.70	109.26
2	C	502	SO4	O3-S-O2	-3.31	91.00	109.26
2	B	501	SO4	O4-S-O1	-2.48	95.60	109.26
2	A	500	SO4	O2-S-O1	-2.21	94.18	109.64
2	C	502	SO4	O2-S-O1	2.43	126.64	109.64
2	B	501	SO4	O3-S-O1	2.49	123.00	109.26
2	B	501	SO4	O4-S-O3	3.41	124.31	108.96

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 ⓘ

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

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.