



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:03 PM UTC

PDB ID : 1OPO / pdb_00001opo
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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

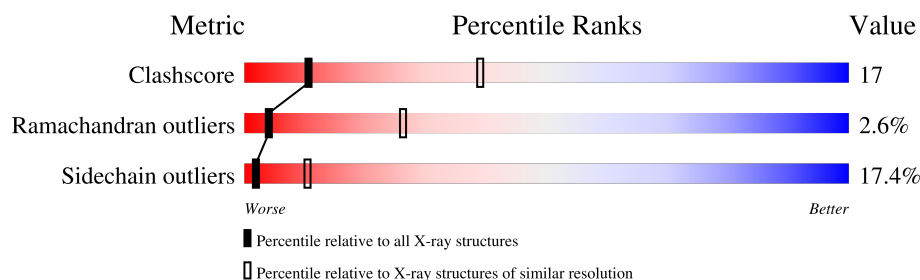
1 Overall quality at a glance

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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	348	42% 26% 9% 23%
1	B	348	46% 23% 7% 23%
1	C	348	45% 25% 7% 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
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 (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: CA) (formula: Ca).

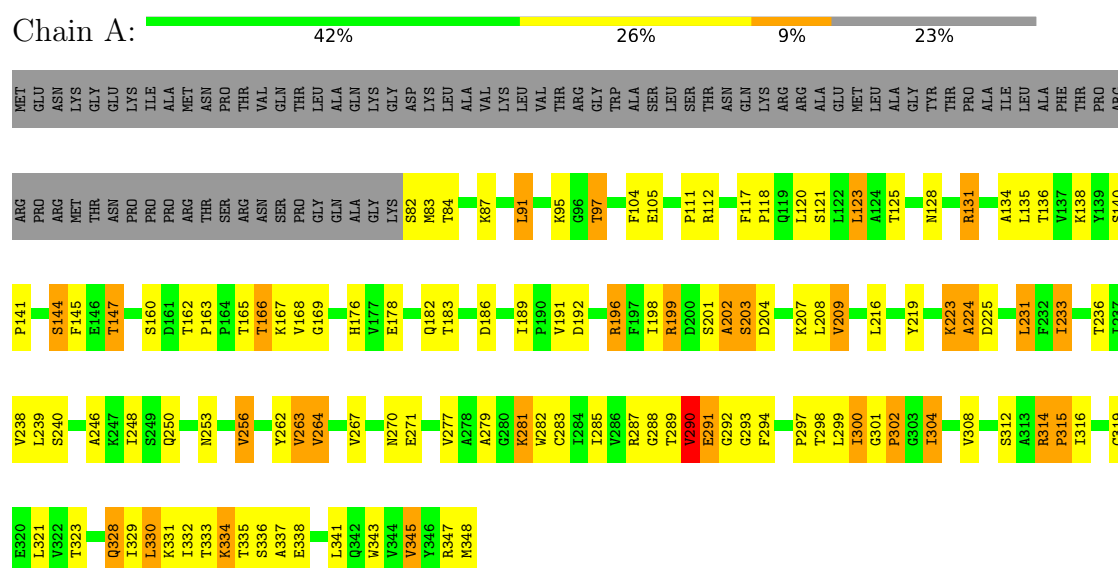
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Ca 1	0	0

3 Residue-property plots

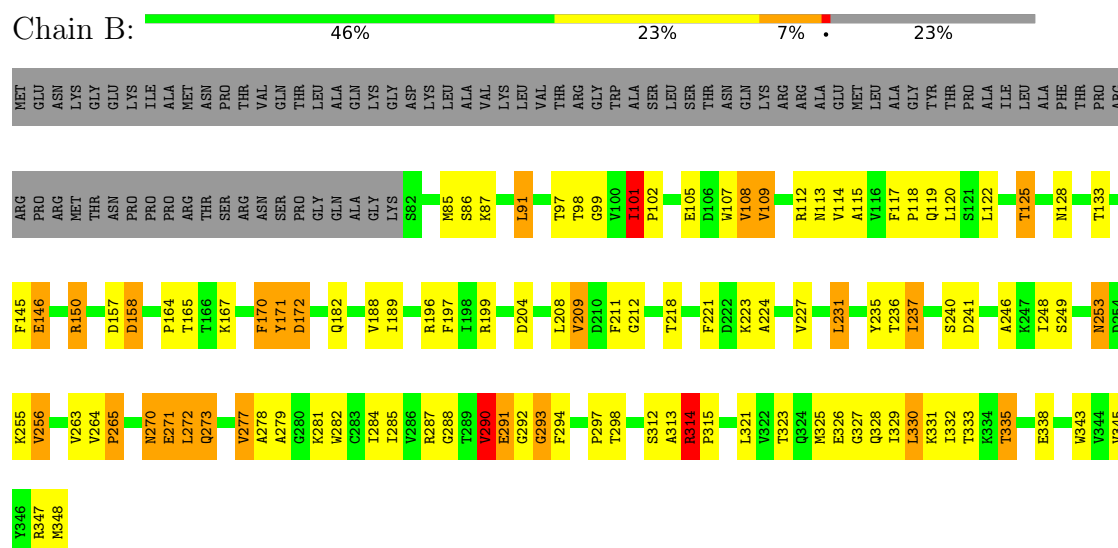
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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

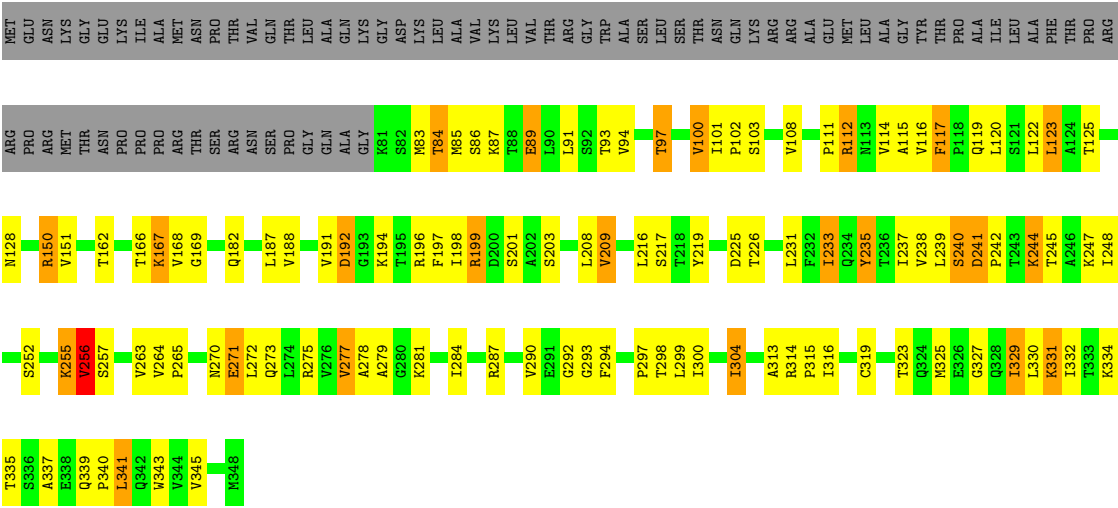


• Molecule 1: Coat protein



• Molecule 1: Coat protein

Chain C: 45% 25% 7% 23%



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, α , β , γ	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 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	0.75	0/2074	1.25	24/2823 (0.9%)
1	B	0.75	0/2074	1.23	15/2823 (0.5%)
1	C	0.77	1/2083 (0.0%)	1.22	22/2834 (0.8%)
All	All	0.76	1/6231 (0.0%)	1.23	61/8480 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	108	VAL	CA-CB	-5.24	1.48	1.54

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	VAL	N-CA-C	9.94	120.36	111.81
1	B	329	ILE	N-CA-C	9.70	122.91	108.46
1	B	292	GLY	N-CA-C	-9.52	102.86	114.66
1	A	277	VAL	N-CA-C	9.32	120.14	110.36
1	B	170	PHE	N-CA-C	-9.17	96.11	109.59
1	A	329	ILE	N-CA-C	8.49	121.11	108.46
1	C	277	VAL	N-CA-C	8.19	118.96	110.36
1	A	264	VAL	CA-C-N	8.15	128.09	119.85
1	A	264	VAL	C-N-CA	8.15	128.09	119.85
1	A	209	VAL	N-CA-C	7.88	118.28	111.90
1	C	314	ARG	N-CA-C	-7.81	94.48	108.47
1	A	189	ILE	CB-CA-C	-7.69	103.47	111.00
1	B	211	PHE	N-CA-C	7.30	120.67	111.69
1	A	341	LEU	N-CA-C	7.21	119.87	110.43
1	C	327	GLY	N-CA-C	7.12	124.84	114.10
1	C	240	SER	N-CA-C	7.03	125.78	110.80
1	B	327	GLY	N-CA-C	6.97	123.66	113.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	189	ILE	CA-C-N	6.92	126.88	120.03
1	B	189	ILE	C-N-CA	6.92	126.88	120.03
1	B	277	VAL	N-CA-C	6.87	118.45	110.62
1	B	172	ASP	N-CA-C	-6.81	104.97	113.28
1	C	100	VAL	CA-C-N	-6.57	117.86	122.59
1	C	100	VAL	C-N-CA	-6.57	117.86	122.59
1	A	183	THR	N-CA-C	6.31	119.01	108.73
1	A	202	ALA	N-CA-C	-6.26	100.39	109.59
1	C	329	ILE	N-CA-C	6.06	117.49	108.46
1	C	316	ILE	N-CA-C	6.02	115.77	108.06
1	A	302	PRO	N-CA-C	-5.95	101.75	111.68
1	A	104	PHE	N-CA-C	5.92	119.20	109.85
1	C	241	ASP	CB-CA-C	5.87	115.72	110.44
1	A	304	ILE	N-CA-C	-5.79	99.88	108.45
1	A	192	ASP	N-CA-C	-5.75	100.92	110.17
1	B	321	LEU	N-CA-C	5.73	119.02	110.14
1	A	167	LYS	N-CA-C	-5.67	105.17	111.36
1	A	300	ILE	N-CA-C	5.61	116.02	108.17
1	B	158	ASP	N-CA-C	5.60	117.65	108.52
1	A	321	LEU	N-CA-C	5.60	118.82	110.14
1	A	191	VAL	N-CA-C	5.59	116.53	108.48
1	A	316	ILE	N-CA-C	5.53	115.66	108.35
1	A	204	ASP	N-CA-C	-5.51	102.74	110.50
1	A	199	ARG	N-CA-C	5.47	118.41	110.42
1	C	192	ASP	N-CA-C	-5.46	102.38	110.46
1	C	101	ILE	CA-C-O	5.43	122.36	119.15
1	A	224	ALA	N-CA-C	5.40	122.31	110.80
1	A	196	ARG	N-CA-C	5.32	117.28	109.24
1	C	117	PHE	CA-C-N	5.30	126.47	119.84
1	C	117	PHE	C-N-CA	5.30	126.47	119.84
1	C	235	TYR	N-CA-C	5.29	117.02	109.14
1	C	167	LYS	N-CA-C	-5.27	104.79	111.11
1	C	194	LYS	N-CA-C	5.27	117.86	109.96
1	B	101	ILE	CA-C-N	5.25	125.18	119.78
1	B	101	ILE	C-N-CA	5.25	125.18	119.78
1	B	314	ARG	N-CA-C	-5.24	98.23	109.81
1	B	290	VAL	N-CA-C	5.24	120.24	109.34
1	C	187	LEU	CA-C-N	-5.20	116.12	122.93
1	C	187	LEU	C-N-CA	-5.20	116.12	122.93
1	C	101	ILE	N-CA-C	5.15	112.97	107.76
1	C	94	VAL	N-CA-C	5.15	116.11	108.23
1	A	168	VAL	CB-CA-C	-5.13	105.14	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	ILE	N-CA-C	5.13	113.79	109.02
1	C	225	ASP	N-CA-C	5.09	117.66	107.62

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	73	0
1	B	2035	0	2053	76	1
1	C	2044	0	2066	61	1
2	A	5	0	0	2	0
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	207	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 17.

All (207) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:283:CYS:HB2	1:A:348:MET:HE3	1.68	0.75
1:A:250:GLN:HE22	1:A:263:VAL:H	1.33	0.74
1:B:314:ARG:C	1:B:314:ARG:HD3	2.14	0.73
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: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: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
1:B:145:PHE:HA	1:B:182:GLN:HG3	1.80	0.63
1:C:323:THR:HG22	1:C:325:MET:O	1.99	0.62
1:B:108:VAL:O	1:B:109:VAL:HB	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:288:GLY:C	1:B:315:PRO:HG2	2.39	0.48
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:C:83:MET:HE1	1:C:123:LEU:HD21	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:314:ARG:C	1:B:314:ARG:CD	2.89	0.45
1:A:314:ARG:C	1:A:314:ARG:CD	2.90	0.44
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:A:314:ARG:C	1:A:314:ARG:HD2	2.42	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:299:LEU:C	1:C:300:ILE:HD12	2.43	0.43
1:C:128:ASN:N	1:C:241:ASP:O	2.51	0.43
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:331:LYS:C	1:C:332:ILE:HG13	2.43	0.43
1:B:146:GLU:N	1:B:146:GLU:CD	2.76	0.43
1:C:83:MET:CE	1:C:123:LEU:HD21	2.49	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:270:ASN:HD21	1:B:335:THR:C	2.26	0.43
1:B:294:PHE:CE1	1:B:315:PRO:HB2	2.54	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:299:LEU:C	1:A:300:ILE:HD12	2.45	0.41
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:331:LYS:C	1:A:332:ILE:HG13	2.46	0.40
1:C:235:TYR:CD1	1:C:235:TYR:C	3.00	0.40
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:C:325:MET:HE2	1:C:325:MET:HB3	1.86	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
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

5.3.1 Protein backbone

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%)	3	23
1	B	265/348 (76%)	244 (92%)	12 (4%)	9 (3%)	3	20
1	C	266/348 (76%)	245 (92%)	17 (6%)	4 (2%)	8	37
All	All	796/1044 (76%)	738 (93%)	37 (5%)	21 (3%)	4	26

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
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%)	190 (83%)	38 (17%)	2	11
1	B	228/294 (78%)	187 (82%)	41 (18%)	2	9
1	C	229/294 (78%)	189 (82%)	40 (18%)	2	10
All	All	685/882 (78%)	566 (83%)	119 (17%)	2	10

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	MET
1	A	84	THR
1	A	87	LYS
1	A	91	LEU
1	A	95	LYS
1	A	97	THR
1	A	112	ARG
1	A	123	LEU
1	A	128	ASN
1	A	131	ARG
1	A	136	THR
1	A	144	SER
1	A	147	THR
1	A	166	THR
1	A	196	ARG
1	A	198	ILE
1	A	208	LEU
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	267	VAL

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Mol	Chain	Res	Type
1	A	271	GLU
1	A	281	LYS
1	A	287	ARG
1	A	290	VAL
1	A	312	SER
1	A	314	ARG
1	A	319	CYS
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	105	GLU
1	B	112	ARG
1	B	114	VAL
1	B	125	THR
1	B	128	ASN
1	B	133	THR
1	B	146	GLU
1	B	150	ARG
1	B	157	ASP
1	B	165	THR
1	B	188	VAL
1	B	196	ARG
1	B	208	LEU
1	B	209	VAL
1	B	223	LYS
1	B	227	VAL
1	B	231	LEU
1	B	237	ILE
1	B	249	SER
1	B	253	ASN
1	B	255	LYS
1	B	256	VAL
1	B	263	VAL
1	B	264	VAL
1	B	265	PRO
1	B	270	ASN
1	B	271	GLU
1	B	272	LEU

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Mol	Chain	Res	Type
1	B	273	GLN
1	B	281	LYS
1	B	287	ARG
1	B	312	SER
1	B	314	ARG
1	B	326	GLU
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	93	THR
1	C	97	THR
1	C	100	VAL
1	C	103	SER
1	C	112	ARG
1	C	114	VAL
1	C	119	GLN
1	C	123	LEU
1	C	150	ARG
1	C	162	THR
1	C	167	LYS
1	C	182	GLN
1	C	188	VAL
1	C	196	ARG
1	C	199	ARG
1	C	203	SER
1	C	208	LEU
1	C	226	THR
1	C	233	ILE
1	C	244	LYS
1	C	247	LYS
1	C	255	LYS
1	C	256	VAL
1	C	257	SER
1	C	263	VAL
1	C	264	VAL
1	C	270	ASN
1	C	271	GLU

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Mol	Chain	Res	Type
1	C	281	LYS
1	C	287	ARG
1	C	298	THR
1	C	304	ILE
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 (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	126	ASN
1	A	128	ASN
1	A	148	ASN
1	A	250	GLN
1	A	253	ASN
1	A	270	ASN
1	A	342	GLN
1	B	119	GLN
1	B	128	ASN
1	B	148	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 ⓘ

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 oligosaccharides 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	C	502	-	4,4,4	0.49	0	6,6,6	1.99	2 (33%)
2	SO4	B	501	-	4,4,4	0.40	0	6,6,6	2.55	4 (66%)
2	SO4	A	500	-	4,4,4	0.30	0	6,6,6	1.30	1 (16%)

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	-3.99	88.70	109.56
2	C	502	SO4	O3-S-O2	-3.55	91.00	109.56
2	B	501	SO4	O4-S-O3	2.86	124.31	108.54
2	B	501	SO4	O4-S-O1	-2.67	95.60	109.56
2	B	501	SO4	O3-S-O1	2.57	123.00	109.56
2	C	502	SO4	O2-S-O1	2.50	126.64	109.06
2	A	500	SO4	O2-S-O1	-2.11	94.18	109.06

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

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.