



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 02:10 PM GMT

PDB ID : 1D4M
Title : THE CRYSTAL STRUCTURE OF COXSACKIEVIRUS A9 TO 2.9 Å RESOLUTION
Authors : Hendry, E.; Hatanaka, H.; Fry, E.; Smyth, M.; Tate, J.; Stanway, G.; Santti, J.; Maaronen, M.; Hyypia, T.; Stuart, D.
Deposited on : 1999-10-04
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

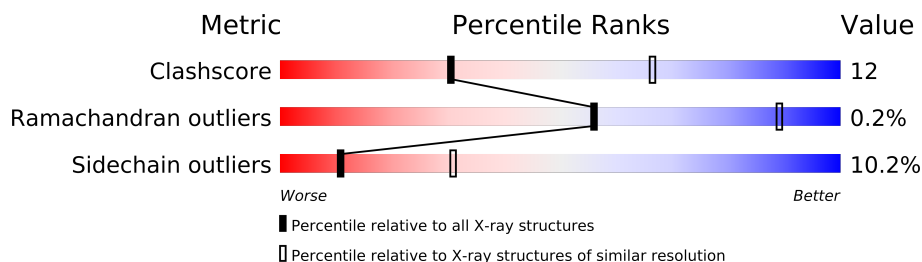
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	299	
2	2	261	
3	3	238	
4	4	68	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7051 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	284	Total	C	N	O	S	0	0	0
			2261	1426	395	428	12			

- Molecule 2 is a protein called PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	252	Total	C	N	O	S	0	0	0
			1959	1239	332	372	16			

- Molecule 3 is a protein called PROTEIN (COXSACKIEVIRUS A9).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	3	238	Total	C	N	O	S	0	0	0
			1843	1173	302	350	18			

- Molecule 4 is a protein called PROTEIN (COXSACKIEVIRUS A9).

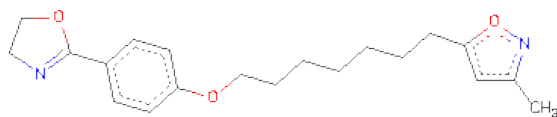
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	61	Total	C	N	O	S	0	0	0
			475	294	82	98	1			

- Molecule 5 is MYRISTIC ACID (three-letter code: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	4	1	Total	C	O	0	0
			15	14	1		

- Molecule 6 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYLISOXAZOLE (three-letter code: W71) (formula: $C_{20}H_{26}N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	1	1	Total	C	N	O	0	0
			25	20	2	3		
6	1	1	Total	C	N	O	0	0
			25	20	2	3		

- Molecule 7 is water.

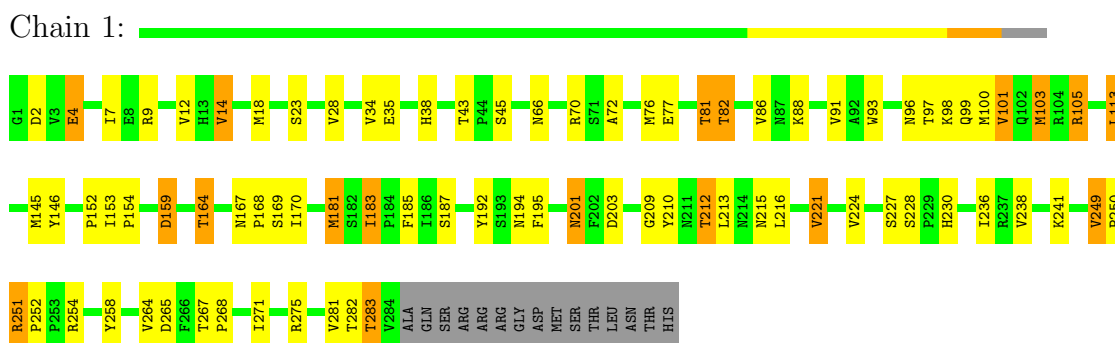
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	1	162	Total 162	O 162	0	0
7	2	146	Total 146	O 146	0	0
7	3	112	Total 112	O 112	0	0
7	4	28	Total 28	O 28	0	0

3 Residue-property plots

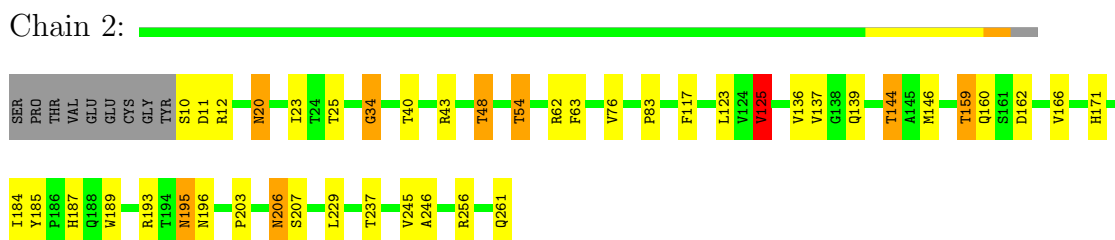
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

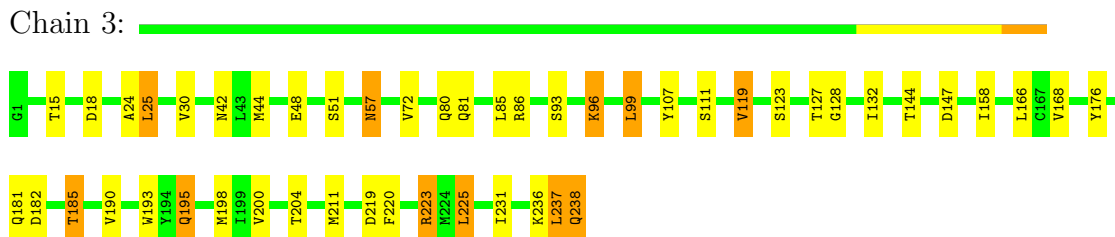
• Molecule 1: PROTEIN (COXSACKIEVIRUS A9)



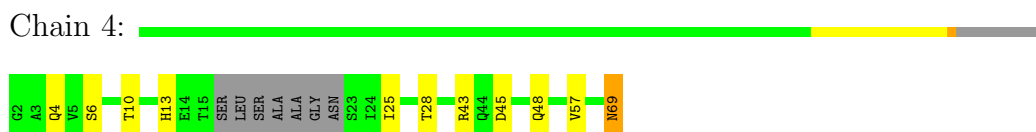
• Molecule 2: PROTEIN (COXSACKIEVIRUS A9)



• Molecule 3: PROTEIN (COXSACKIEVIRUS A9)



• Molecule 4: PROTEIN (COXSACKIEVIRUS A9)



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	487.30Å 358.10Å 305.70Å 90.00° 128.10° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	41.0 (20.00-2.90)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.169 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7051	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: MYR, W71

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	1	0.58	0/2325	0.81	0/3172
2	2	0.55	0/2009	0.81	2/2740 (0.1%)
3	3	0.55	0/1892	0.80	0/2581
4	4	0.60	0/483	0.88	0/652
All	All	0.56	0/6709	0.81	2/9145 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	125	VAL	CB-CA-C	-5.86	100.27	111.40
2	2	195	ASN	CB-CA-C	-5.75	98.91	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	195	ASN	Mainchain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2261	0	2192	75	0
2	2	1959	0	1878	39	0
3	3	1843	0	1802	46	0
4	4	475	0	456	8	0
5	4	15	0	27	1	0
6	1	50	0	52	22	0
7	1	162	0	0	18	0
7	2	146	0	0	7	0
7	3	112	0	0	4	0
7	4	28	0	0	3	0
All	All	7051	0	6407	155	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (155) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:97:THR:H	6:1:502:W71:H313	1.16	1.04
6:1:501:W71:H312	6:1:502:W71:H2C2	1.43	1.00
1:1:82:THR:HB	7:1:617:HOH:O	1.60	0.99
1:1:4:GLU:HG2	4:4:4:GLN:HG2	1.50	0.92
1:1:97:THR:N	6:1:502:W71:H313	1.92	0.83
6:1:501:W71:H312	6:1:502:W71:C2C	2.08	0.83
1:1:215:ASN:HB3	6:1:502:W71:H5B	1.60	0.82
1:1:96:ASN:HD21	1:1:99:GLN:HE21	1.27	0.81
1:1:145:MET:SD	1:1:164:THR:HG23	2.20	0.81
1:1:209:GLY:O	1:1:212:THR:HG23	1.81	0.80
3:3:195:GLN:HE21	3:3:195:GLN:HA	1.46	0.79
3:3:42:ASN:HD22	3:3:44:MET:H	1.31	0.78
1:1:14:VAL:HG13	3:3:219:ASP:HA	1.69	0.73
2:2:184:ILE:HG23	3:3:99:LEU:HD21	1.70	0.72
1:1:181:MET:HE3	3:3:24:ALA:HB2	1.70	0.72
1:1:96:ASN:HD21	1:1:99:GLN:NE2	1.88	0.71
6:1:502:W71:H6C2	6:1:502:W71:H2B	1.71	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:268:PRO:HG2	2:2:159:THR:HB	1.72	0.71
3:3:107:TYR:CE2	3:3:225:LEU:HD13	2.26	0.70
3:3:15:THR:HB	7:3:323:HOH:O	1.91	0.70
1:1:181:MET:HE1	1:1:183:ILE:HD11	1.73	0.70
3:3:57:ASN:H	3:3:57:ASN:HD22	1.39	0.69
2:2:117:PHE:HD2	3:3:204:THR:HG22	1.57	0.68
1:1:164:THR:HG21	1:1:169:SER:OG	1.93	0.68
1:1:215:ASN:HB2	6:1:502:W71:O1A	1.94	0.68
3:3:144:THR:HG23	3:3:147:ASP:H	1.60	0.67
1:1:81:THR:HG21	1:1:228:SER:OG	1.93	0.67
2:2:160:GLN:HE21	2:2:162:ASP:H	1.43	0.66
1:1:252:PRO:HD3	2:2:184:ILE:HD11	1.76	0.66
1:1:187:SER:OG	6:1:502:W71:H6C1	1.96	0.66
1:1:251:ARG:HB3	2:2:185:TYR:OH	1.96	0.66
1:1:192:TYR:HA	6:1:502:W71:H5C1	1.77	0.65
1:1:275:ARG:HE	3:3:57:ASN:HD21	1.44	0.65
2:2:123:LEU:HG	2:2:125:VAL:HG22	1.79	0.64
6:1:501:W71:H312	6:1:502:W71:C3C	2.28	0.64
1:1:7:ILE:HG22	4:4:6:SER:HA	1.79	0.64
2:2:25:THR:HB	7:2:318:HOH:O	1.96	0.64
1:1:164:THR:HG22	1:1:167:ASN:HB2	1.82	0.62
4:4:43:ARG:HG3	4:4:43:ARG:HH11	1.64	0.61
1:1:81:THR:CG2	1:1:82:THR:HG22	2.30	0.61
1:1:81:THR:HG22	1:1:82:THR:HG22	1.83	0.61
1:1:282:THR:HB	7:1:657:HOH:O	2.02	0.60
3:3:132:ILE:HG22	3:3:166:LEU:HD22	1.84	0.60
4:4:57:VAL:HG13	7:4:90:HOH:O	2.02	0.59
2:2:117:PHE:CD2	3:3:204:THR:HG22	2.38	0.59
1:1:230:HIS:HB3	7:1:523:HOH:O	2.01	0.59
3:3:237:LEU:O	3:3:238:GLN:HB2	2.03	0.58
3:3:81:GLN:HB2	3:3:193:TRP:CZ3	2.39	0.58
1:1:201:ASN:HD22	1:1:201:ASN:N	2.01	0.58
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.49	0.58
5:4:1:MYR:H42	5:4:1:MYR:O1	2.03	0.58
1:1:101:VAL:HG22	1:1:258:TYR:HD2	1.68	0.58
2:2:48:THR:HG23	7:2:270:HOH:O	2.04	0.58
1:1:72:ALA:HB3	1:1:103:MET:HG2	1.85	0.57
2:2:159:THR:HG22	7:2:365:HOH:O	2.04	0.57
3:3:182:ASP:OD2	3:3:185:THR:HB	2.05	0.57
2:2:144:THR:HB	7:2:395:HOH:O	2.03	0.57
1:1:227:SER:HA	7:1:617:HOH:O	2.04	0.57
6:1:502:W71:H6C2	6:1:502:W71:C2B	2.35	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:93:TRP:HE1	1:1:99:GLN:HE22	1.53	0.56
3:3:85:LEU:CD1	3:3:190:VAL:HB	2.35	0.56
1:1:70:ARG:NH2	7:1:590:HOH:O	2.38	0.56
3:3:93:SER:HA	3:3:96:LYS:HG2	1.88	0.56
1:1:91:VAL:HG13	1:1:221:VAL:HG13	1.88	0.56
1:1:113:LEU:HD22	1:1:194:ASN:HD21	1.71	0.56
2:2:136:VAL:HG22	2:2:139:GLN:HB2	1.86	0.55
1:1:170:ILE:HD11	1:1:181:MET:HG2	1.89	0.55
1:1:35:GLU:HA	2:2:189:TRP:HB2	1.90	0.54
1:1:105:ARG:NH1	1:1:254:ARG:O	2.39	0.54
1:1:98:LYS:HE3	1:1:210:TYR:CE2	2.42	0.54
1:1:70:ARG:NH1	7:1:664:HOH:O	2.38	0.53
2:2:54:THR:HG21	7:2:274:HOH:O	2.07	0.53
3:3:25:LEU:HG	7:3:272:HOH:O	2.08	0.53
3:3:51:SER:HB3	3:3:99:LEU:HD22	1.90	0.53
6:1:501:W71:N2	6:1:502:W71:H311	2.24	0.53
7:1:650:HOH:O	2:2:184:ILE:CG2	2.57	0.53
2:2:193:ARG:NH2	3:3:158:ILE:HG23	2.24	0.52
1:1:181:MET:CE	3:3:24:ALA:HB2	2.40	0.52
1:1:271:ILE:HD11	2:2:171:HIS:HB2	1.91	0.52
1:1:185:PHE:CZ	1:1:187:SER:HB3	2.45	0.52
1:1:101:VAL:HG22	1:1:258:TYR:CD2	2.44	0.52
3:3:85:LEU:HD11	3:3:190:VAL:HB	1.90	0.52
1:1:43:THR:HB	7:1:663:HOH:O	2.09	0.52
7:1:650:HOH:O	2:2:184:ILE:HG21	2.08	0.52
1:1:275:ARG:HE	3:3:57:ASN:ND2	2.07	0.51
3:3:195:GLN:NE2	3:3:195:GLN:HA	2.20	0.51
6:1:501:W71:C31	6:1:502:W71:H4C2	2.40	0.51
2:2:40:THR:HG23	7:2:372:HOH:O	2.10	0.51
2:2:206:ASN:ND2	2:2:207:SER:H	2.09	0.50
1:1:72:ALA:CB	1:1:103:MET:HG2	2.41	0.50
1:1:81:THR:CG2	1:1:228:SER:OG	2.60	0.49
1:1:181:MET:CE	1:1:183:ILE:HD11	2.40	0.49
3:3:238:GLN:NE2	7:3:315:HOH:O	2.45	0.49
1:1:93:TRP:HE1	1:1:99:GLN:NE2	2.11	0.48
1:1:215:ASN:CB	6:1:502:W71:H5B	2.39	0.48
3:3:144:THR:HG22	3:3:147:ASP:CG	2.34	0.48
1:1:77:GLU:HG2	7:1:616:HOH:O	2.14	0.48
7:1:650:HOH:O	2:2:184:ILE:HB	2.13	0.47
6:1:501:W71:C31	6:1:502:W71:H2C2	2.30	0.47
1:1:227:SER:CA	7:1:617:HOH:O	2.59	0.47
2:2:193:ARG:NH1	3:3:123:SER:O	2.47	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:100:MET:CE	3:3:236:LYS:HG2	2.46	0.46
2:2:20:ASN:HD21	2:2:62:ARG:NE	2.13	0.46
1:1:215:ASN:HB3	6:1:502:W71:C5B	2.37	0.46
3:3:44:MET:O	3:3:48:GLU:HG3	2.15	0.46
3:3:182:ASP:H	3:3:185:THR:HG22	1.79	0.46
6:1:501:W71:H312	6:1:502:W71:C4C	2.45	0.46
3:3:18:ASP:HB2	4:4:43:ARG:HH12	1.79	0.46
2:2:206:ASN:HD22	2:2:207:SER:H	1.64	0.46
2:2:10:SER:HB3	2:2:12:ARG:HG2	1.97	0.46
2:2:20:ASN:HD21	2:2:62:ARG:HH21	1.63	0.46
1:1:249:VAL:HA	1:1:250:PRO:HD2	1.70	0.46
3:3:158:ILE:HD13	7:3:337:HOH:O	2.16	0.46
2:2:83:PRO:HD2	7:2:314:HOH:O	2.16	0.45
1:1:212:THR:O	6:1:502:W71:H4A2	2.16	0.45
1:1:282:THR:HG22	1:1:283:THR:H	1.81	0.45
2:2:193:ARG:NH2	3:3:158:ILE:CG2	2.80	0.45
1:1:152:PRO:HD2	7:1:635:HOH:O	2.17	0.45
1:1:28:VAL:HG23	1:1:28:VAL:O	2.16	0.45
1:1:4:GLU:HG2	4:4:4:GLN:CG	2.35	0.45
1:1:66:ASN:HB3	7:1:613:HOH:O	2.17	0.45
2:2:20:ASN:H	2:2:20:ASN:HD22	1.64	0.44
3:3:176:TYR:CZ	3:3:223:ARG:HD3	2.52	0.44
4:4:45:ASP:HB3	7:4:95:HOH:O	2.18	0.44
1:1:100:MET:HE2	3:3:236:LYS:HG2	1.99	0.44
2:2:12:ARG:HD3	4:4:69:ASN:H	1.82	0.44
6:1:502:W71:H2B	7:1:533:HOH:O	2.18	0.43
6:1:501:W71:H313	6:1:502:W71:C31	2.48	0.43
2:2:184:ILE:HG23	3:3:99:LEU:CD2	2.45	0.43
1:1:252:PRO:CD	2:2:184:ILE:HD11	2.47	0.43
2:2:20:ASN:N	2:2:20:ASN:HD22	2.15	0.43
3:3:111:SER:O	3:3:220:PHE:HA	2.19	0.43
2:2:34:GLY:HA3	2:2:203:PRO:HD3	2.00	0.43
1:1:146:TYR:HB3	1:1:168:PRO:HG2	1.99	0.43
7:1:569:HOH:O	3:3:223:ARG:HG2	2.18	0.43
1:1:86:VAL:HG13	7:1:621:HOH:O	2.19	0.43
3:3:127:THR:HG22	3:3:128:GLY:N	2.34	0.43
3:3:181:GLN:HG2	3:3:185:THR:CG2	2.48	0.42
1:1:18:MET:HE3	7:1:580:HOH:O	2.18	0.42
3:3:119:VAL:HG13	3:3:211:MET:HB2	2.00	0.42
1:1:154:PRO:HA	1:1:159:ASP:OD1	2.20	0.42
1:1:213:LEU:HB2	6:1:502:W71:H2C1	2.01	0.42
6:1:501:W71:H313	6:1:502:W71:H312	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:1:195:PHE:CE1	1:1:251:ARG:HD2	2.55	0.41
3:3:127:THR:O	3:3:198:MET:HA	2.19	0.41
1:1:76:MET:HA	1:1:236:ILE:O	2.20	0.41
3:3:107:TYR:CZ	3:3:225:LEU:HD13	2.54	0.41
2:2:125:VAL:HG13	2:2:187:HIS:HB3	2.03	0.41
1:1:164:THR:HG21	1:1:169:SER:HG	1.83	0.41
1:1:153:ILE:HA	1:1:154:PRO:HD3	1.95	0.41
1:1:38:HIS:HB2	7:4:90:HOH:O	2.20	0.41
3:3:85:LEU:HD12	3:3:190:VAL:HB	2.02	0.41
3:3:231:ILE:HD12	3:3:231:ILE:HA	1.96	0.40
1:1:265:ASP:HB3	2:2:137:VAL:HB	2.04	0.40
2:2:63:PHE:CD1	2:2:246:ALA:HB2	2.56	0.40

There are no symmetry-related clashes.

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	1	282/299 (94%)	264 (94%)	17 (6%)	1 (0%)	43	82
2	2	250/261 (96%)	227 (91%)	22 (9%)	1 (0%)	43	82
3	3	236/238 (99%)	228 (97%)	8 (3%)	0	100	100
4	4	57/68 (84%)	55 (96%)	2 (4%)	0	100	100
All	All	825/866 (95%)	774 (94%)	49 (6%)	2 (0%)	56	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	224	VAL
2	2	34	GLY

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	1	254/267 (95%)	222 (87%)	32 (13%)	7 18
2	2	209/217 (96%)	190 (91%)	19 (9%)	14 38
3	3	211/211 (100%)	194 (92%)	17 (8%)	17 45
4	4	53/57 (93%)	47 (89%)	6 (11%)	9 25
All	All	727/752 (97%)	653 (90%)	74 (10%)	11 31

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	ASP
1	1	4	GLU
1	1	9	ARG
1	1	12	VAL
1	1	14	VAL
1	1	23	SER
1	1	34	VAL
1	1	45	SER
1	1	81	THR
1	1	82	THR
1	1	88	LYS
1	1	101	VAL
1	1	103	MET
1	1	105	ARG
1	1	113	LEU
1	1	159	ASP
1	1	164	THR
1	1	181	MET
1	1	183	ILE
1	1	201	ASN
1	1	203	ASP
1	1	212	THR
1	1	216	LEU
1	1	221	VAL
1	1	238	VAL
1	1	241	LYS

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Mol	Chain	Res	Type
1	1	249	VAL
1	1	251	ARG
1	1	264	VAL
1	1	267	THR
1	1	281	VAL
1	1	283	THR
2	2	11	ASP
2	2	20	ASN
2	2	23	ILE
2	2	43	ARG
2	2	48	THR
2	2	54	THR
2	2	76	VAL
2	2	125	VAL
2	2	144	THR
2	2	146	MET
2	2	159	THR
2	2	166	VAL
2	2	196	ASN
2	2	206	ASN
2	2	229	LEU
2	2	237	THR
2	2	245	VAL
2	2	256	ARG
2	2	261	GLN
3	3	25	LEU
3	3	30	VAL
3	3	57	ASN
3	3	72	VAL
3	3	80	GLN
3	3	86	ARG
3	3	96	LYS
3	3	99	LEU
3	3	119	VAL
3	3	168	VAL
3	3	185	THR
3	3	195	GLN
3	3	200	VAL
3	3	223	ARG
3	3	225	LEU
3	3	237	LEU
3	3	238	GLN

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Mol	Chain	Res	Type
4	4	10	THR
4	4	13	HIS
4	4	25	ILE
4	4	28	THR
4	4	48	GLN
4	4	69	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	52	HIS
1	1	99	GLN
1	1	201	ASN
1	1	204	GLN
1	1	214	ASN
2	2	20	ASN
2	2	97	GLN
2	2	119	GLN
2	2	160	GLN
2	2	163	GLN
2	2	206	ASN
2	2	218	ASN
3	3	35	ASN
3	3	42	ASN
3	3	56	ASN
3	3	57	ASN
3	3	195	GLN
3	3	206	ASN
4	4	4	GLN
4	4	44	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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$
6	W71	1	501	-	27,27,27	2.33	6 (22%)	34,34,34	5.48	9 (26%)
6	W71	1	502	-	27,27,27	2.15	7 (25%)	34,34,34	5.26	7 (20%)
5	MYR	4	1	4	14,14,15	4.53	1 (7%)	11,13,15	0.52	0

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
6	W71	1	501	-	-	0/14/22/22	0/3/3/3
6	W71	1	502	-	-	0/14/22/22	0/3/3/3
5	MYR	4	1	4	-	0/11/12/13	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	1	MYR	O1-C1	16.81	1.23	1.11
6	1	501	W71	O1-N2	-8.42	1.35	1.42
6	1	502	W71	O1-N2	-6.58	1.37	1.42
6	1	502	W71	C2A-N3A	5.47	1.34	1.27
6	1	501	W71	C2A-N3A	4.54	1.33	1.27
6	1	502	W71	O1A-C2A	3.84	1.42	1.36
6	1	501	W71	O1A-C2A	3.38	1.41	1.36
6	1	501	W71	C4B-C2A	-3.06	1.40	1.47
6	1	501	W71	C4-C3	-2.96	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1	501	W71	O1-C5	2.49	1.45	1.38
6	1	502	W71	C5B-C4B	2.28	1.43	1.39
6	1	502	W71	O1-C5	2.26	1.44	1.38
6	1	502	W71	C6B-C1B	2.18	1.43	1.38
6	1	502	W71	C4-C3	-2.14	1.35	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1	501	W71	O1-C5-C1C	25.63	133.13	116.70
6	1	502	W71	O1-C5-C1C	23.82	131.97	116.70
6	1	502	W71	O1A-C2A-C4B	12.73	128.90	115.61
6	1	501	W71	O1A-C2A-C4B	11.68	127.81	115.61
6	1	502	W71	O1A-C2A-N3A	-10.68	108.23	118.38
6	1	501	W71	O1A-C2A-N3A	-9.81	109.05	118.38
6	1	501	W71	C5-O1-N2	-6.98	105.39	107.66
6	1	502	W71	C4A-N3A-C2A	5.55	112.18	106.68
6	1	501	W71	C4A-N3A-C2A	5.50	112.14	106.68
6	1	502	W71	C5-O1-N2	-5.49	105.88	107.66
6	1	501	W71	C2C-C1C-C5	-3.31	106.25	113.89
6	1	501	W71	C31-C3-N2	3.03	126.01	120.05
6	1	502	W71	O1-C5-C4	-2.98	101.80	112.67
6	1	501	W71	O1-C5-C4	-2.78	102.53	112.67
6	1	502	W71	C31-C3-N2	2.46	124.89	120.05
6	1	501	W71	C1C-C5-C4	-2.04	124.06	128.51

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.