



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 05:29 PM UTC

PDB ID : 1D4M / pdb_00001d4m
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 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

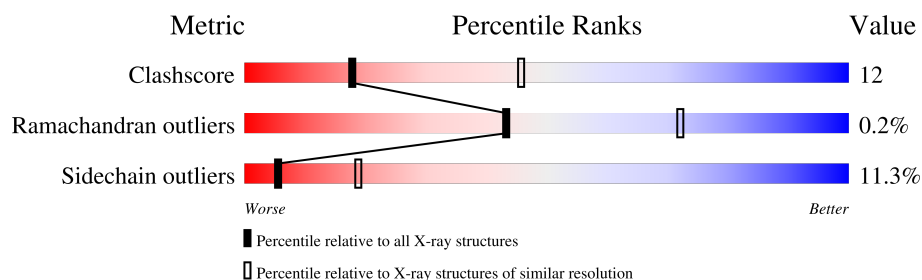
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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	1	299	62% 26% 7% • 5%
2	2	261	76% 16% • • •
3	3	238	76% 16% 6% •
4	4	68	60% 24% 6% 10%

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
5	W71	1	501	-	-	X	-
5	W71	1	502	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7051 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 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			

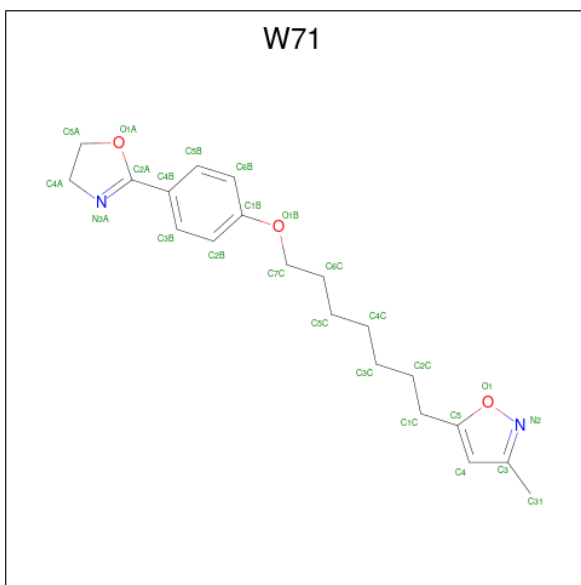
- Molecule 3 is a protein called PROTEIN (COXSACKIEVIRUS A9).

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).

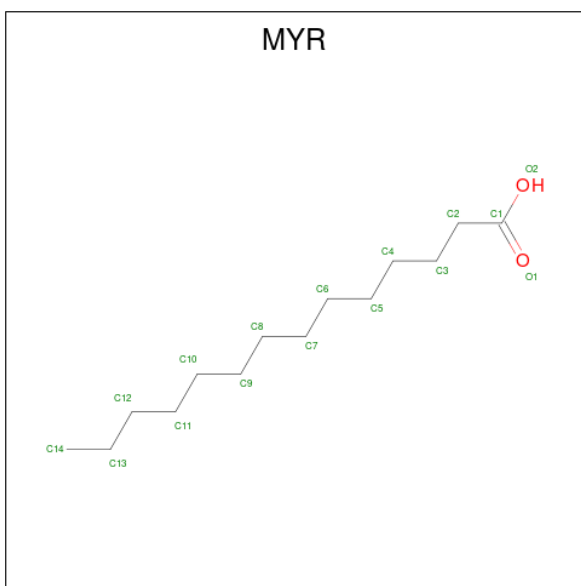
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	4	61	Total	C	N	O	S	0	0	0
			475	294	82	98	1			

- Molecule 5 is 5-(7-(4-(4,5-DIHYDRO-2-OXAZOLYL)PHENOXY)HEPTYL)-3-METHYL ISOXAZOLE (CCD ID: W71) (formula: C₂₀H₂₆N₂O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	1	1	Total 25	C 20	N 2	O 3	0	0
5	1	1	Total 25	C 20	N 2	O 3	0	0

- Molecule 6 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	4	1	Total	C	O	0	0
			15	14	1		

- 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

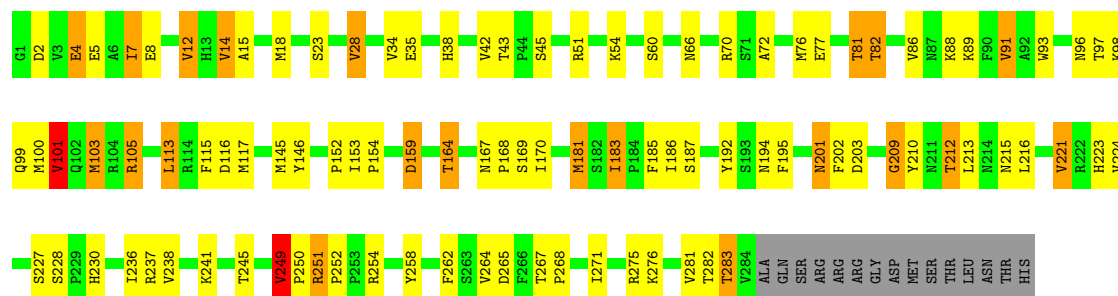
3 Residue-property plots [i](#)

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: PROTEIN (COXSACKIEVIRUS A9)

Chain 1: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	487.30 Å 358.10 Å 305.70 Å 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: W71, MYR

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	0.74	2/2325 (0.1%)	1.16	20/3172 (0.6%)
2	2	0.67	0/2009	1.14	13/2740 (0.5%)
3	3	0.66	0/1892	1.12	12/2581 (0.5%)
4	4	0.89	3/483 (0.6%)	1.34	8/652 (1.2%)
All	All	0.71	5/6709 (0.1%)	1.16	53/9145 (0.6%)

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	7	ILE	CA-CB	7.85	1.63	1.54
1	1	181	MET	SD-CE	-7.62	1.60	1.79
4	4	24	ILE	CA-CB	6.00	1.61	1.54
4	4	62	ILE	CA-CB	5.18	1.60	1.54
4	4	60	VAL	CA-CB	5.14	1.59	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	29	ALA	N-CA-C	-10.27	100.36	108.78
1	1	101	VAL	N-CA-C	9.40	120.23	110.36
1	1	186	ILE	N-CA-C	9.12	120.86	112.29
4	4	44	GLN	N-CA-C	8.36	122.79	112.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	170	ILE	N-CA-C	8.23	119.00	110.36
4	4	51	SER	N-CA-C	7.37	121.53	112.54
1	1	249	VAL	CA-C-N	7.23	127.15	119.85
1	1	249	VAL	C-N-CA	7.23	127.15	119.85
1	1	28	VAL	CA-C-N	7.07	126.90	119.05
1	1	28	VAL	C-N-CA	7.07	126.90	119.05
2	2	55	GLN	CA-C-N	6.91	126.61	119.56
2	2	55	GLN	C-N-CA	6.91	126.61	119.56
3	3	230	PHE	N-CA-C	6.86	121.32	113.15
2	2	125	VAL	CB-CA-C	-6.76	100.27	110.55
1	1	12	VAL	N-CA-C	6.67	118.19	109.58
2	2	50	GLU	N-CA-C	6.53	120.98	112.89
3	3	200	VAL	N-CA-CB	-6.50	104.68	111.64
1	1	223	HIS	N-CA-C	-6.50	100.86	110.48
2	2	168	THR	N-CA-C	6.43	120.99	113.20
2	2	195	ASN	CB-CA-C	-6.35	98.91	111.60
3	3	96	LYS	N-CA-C	6.30	119.82	111.75
4	4	63	LYS	N-CA-C	6.28	118.93	111.33
1	1	5	GLU	N-CA-C	6.18	120.02	111.55
2	2	105	GLY	N-CA-C	-6.12	101.99	112.64
1	1	116	ASP	N-CA-C	-6.03	101.59	110.52
1	1	276	LYS	N-CA-C	6.02	117.51	111.07
1	1	262	PHE	N-CA-C	6.01	120.19	112.26
4	4	25	ILE	N-CA-C	5.88	121.57	109.34
1	1	51	ARG	N-CA-C	-5.80	101.88	110.46
1	1	245	THR	N-CA-C	5.79	119.52	110.32
3	3	236	LYS	N-CA-C	-5.69	102.61	110.35
4	4	55	GLU	N-CA-C	5.67	116.93	108.76
2	2	154	GLU	N-CA-C	5.63	118.57	109.40
3	3	168	VAL	CA-C-N	5.58	125.55	120.03
3	3	168	VAL	C-N-CA	5.58	125.55	120.03
1	1	202	PHE	CA-C-N	5.42	129.27	120.60
1	1	202	PHE	C-N-CA	5.42	129.27	120.60
1	1	15	ALA	N-CA-C	5.39	118.05	110.23
1	1	209	GLY	N-CA-C	5.39	118.85	112.33
1	1	60	SER	N-CA-C	5.36	117.12	111.28
2	2	213	MET	N-CA-C	5.31	119.61	113.18
1	1	89	LYS	N-CA-C	5.30	119.44	112.92
4	4	61	MET	N-CA-C	5.25	117.21	108.02
3	3	181	GLN	N-CA-C	5.20	117.57	110.24
3	3	140	ASN	N-CA-C	5.15	118.38	108.45
3	3	165	VAL	N-CA-C	5.15	115.26	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	48	THR	N-CA-C	-5.14	106.14	112.72
4	4	52	LYS	N-CA-C	-5.14	105.80	111.71
4	4	10	THR	N-CA-C	5.13	117.47	110.24
2	2	54	THR	CB-CA-C	-5.12	100.87	109.48
3	3	179	VAL	N-CA-C	-5.10	105.57	110.72
3	3	59	GLN	N-CA-C	5.08	119.75	111.37
3	3	138	GLY	N-CA-C	-5.06	102.16	110.56

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	195	ASN	Mainchain

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	1	2261	0	2192	77	0
2	2	1959	0	1878	41	0
3	3	1843	0	1802	47	0
4	4	475	0	456	8	0
5	1	50	0	52	22	0
6	4	15	0	27	1	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	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (160) 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)
1:1:97:THR:H	5:1:502:W71:H313	1.16	1.04
5:1:501:W71:H312	5:1:502:W71:H2C2	1.43	1.00
1:1:82:THR:HB	7:1:617:HOH:O	1.60	0.99
1:1:181:MET:HE1	1:1:183:ILE:HD11	1.47	0.94
1:1:4:GLU:HG2	4:4:4:GLN:HG2	1.50	0.92
1:1:97:THR:N	5:1:502:W71:H313	1.92	0.83
5:1:501:W71:H312	5:1:502:W71:C2C	2.08	0.83
1:1:215:ASN:HB3	5:1:502: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:HE1	1:1:183:ILE:CD1	2.18	0.72
1:1:96:ASN:HD21	1:1:99:GLN:NE2	1.88	0.71
5:1:502:W71:H2B	5:1:502:W71:H6C2	1.71	0.71
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
3:3:57:ASN:HD22	3:3:57:ASN:H	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	5:1:502: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
2:2:64:TYR:HB3	2:2:89:MET:HE2	1.76	0.66
1:1:252:PRO:HD3	2:2:184:ILE:HD11	1.76	0.66
1:1:187:SER:OG	5:1:502: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	5:1:502: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
1:1:7:ILE:HG22	4:4:6:SER:HA	1.79	0.64
5:1:501:W71:H312	5:1:502:W71:C3C	2.28	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:HH11	4:4:43:ARG:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:1:181:MET:HE3	3:3:24:ALA:HB2	1.84	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
1:1:201:ASN:HD22	1:1:201:ASN:N	2.01	0.58
3:3:81:GLN:HB2	3:3:193:TRP:CZ3	2.39	0.58
2:2:20:ASN:HD21	2:2:62:ARG:HE	1.49	0.58
6:4:1:MYR:H42	6:4:1: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
5:1:502:W71:H6C2	5:1:502:W71:C2B	2.35	0.56
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
5:1:501:W71:N2	5:1:502: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
1:1:101:VAL:HG22	1:1:258:TYR:CD2	2.44	0.52
1:1:185:PHE:CZ	1:1:187:SER:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:85:LEU:HD11	3:3:190:VAL:HB	1.90	0.52
3:3:144:THR:HG22	3:3:147:ASP:CG	2.34	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:HA	3:3:195:GLN:NE2	2.20	0.51
5:1:501:W71:C31	5:1:502: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
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	5:1:502:W71:H5B	2.39	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
1:1:227:SER:CA	7:1:617:HOH:O	2.59	0.47
5:1:501:W71:C31	5:1:502:W71:H2C2	2.30	0.47
2:2:193:ARG:NH1	3:3:123:SER:O	2.47	0.47
1:1:115:PHE:HE1	1:1:117:MET:HE2	1.79	0.47
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	5:1:502: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
5:1:501:W71:H312	5:1:502:W71:C4C	2.45	0.46
3:3:18:ASP:HB2	4:4:43:ARG:HH12	1.79	0.46
2:2:10:SER:HB3	2:2:12:ARG:HG2	1.97	0.46
2:2:206:ASN:HD22	2:2:207:SER:H	1.64	0.46
1:1:249:VAL:HA	1:1:250:PRO:HD2	1.70	0.46
2:2:20:ASN:HD21	2:2:62:ARG:HH21	1.63	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	5:1:502:W71:H4A2	2.16	0.45
1:1:282:THR:HG22	1:1:283:THR:H	1.81	0.45
1:1:28:VAL:HG23	1:1:28:VAL:O	2.16	0.45
1:1:152:PRO:HD2	7:1:635:HOH:O	2.17	0.45
2:2:193:ARG:NH2	3:3:158:ILE:CG2	2.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:115:PHE:CE1	1:1:117:MET:HE2	2.52	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
2:2:12:ARG:HD3	4:4:69:ASN:H	1.82	0.44
3:3:83:PHE:C	3:3:83:PHE:CD1	2.95	0.44
5:1:502:W71:H2B	7:1:533:HOH:O	2.18	0.43
5:1:501:W71:H313	5:1:502: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:HD22	2:2:20:ASN:N	2.15	0.43
3:3:111:SER:O	3:3:220:PHE:HA	2.19	0.43
1:1:146:TYR:HB3	1:1:168:PRO:HG2	1.99	0.43
2:2:34:GLY:HA3	2:2:203:PRO:HD3	2.00	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
2:2:33:VAL:O	2:2:34:GLY:C	2.62	0.42
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
1:1:100:MET:HE2	3:3:236:LYS:HG2	2.01	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	5:1:502:W71:H2C1	2.01	0.42
1:1:195:PHE:CE1	1:1:251:ARG:HD2	2.55	0.41
5:1:501:W71:H313	5:1:502:W71:H312	2.02	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
1:1:153:ILE:HA	1:1:154:PRO:HD3	1.95	0.41
1:1:164:THR:HG21	1:1:169:SER:HG	1.83	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 [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	1	282/299 (94%)	264 (94%)	17 (6%)	1 (0%)	30	59
2	2	250/261 (96%)	227 (91%)	22 (9%)	1 (0%)	30	59
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%)	43	72

All (2) Ramachandran outliers are listed below:

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

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	1	254/267 (95%)	219 (86%)	35 (14%)	3	12
2	2	209/217 (96%)	189 (90%)	20 (10%)	8	26
3	3	211/211 (100%)	191 (90%)	20 (10%)	8	26
4	4	53/57 (93%)	46 (87%)	7 (13%)	4	13
All	All	727/752 (97%)	645 (89%)	82 (11%)	5	19

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	2	ASP
1	1	4	GLU
1	1	8	GLU
1	1	12	VAL
1	1	14	VAL
1	1	23	SER
1	1	34	VAL
1	1	42	VAL
1	1	45	SER
1	1	54	LYS
1	1	81	THR
1	1	82	THR
1	1	88	LYS
1	1	91	VAL
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	183	ILE
1	1	201	ASN
1	1	203	ASP
1	1	212	THR
1	1	216	LEU
1	1	221	VAL
1	1	237	ARG
1	1	238	VAL
1	1	241	LYS
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

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Mol	Chain	Res	Type
2	2	136	VAL
2	2	137	VAL
2	2	144	THR
2	2	146	MET
2	2	159	THR
2	2	166	VAL
2	2	184	ILE
2	2	196	ASN
2	2	229	LEU
2	2	237	THR
2	2	245	VAL
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	158	ILE
3	3	168	VAL
3	3	181	GLN
3	3	185	THR
3	3	195	GLN
3	3	200	VAL
3	3	204	THR
3	3	223	ARG
3	3	225	LEU
3	3	237	LEU
3	3	238	GLN
4	4	10	THR
4	4	13	HIS
4	4	25	ILE
4	4	28	THR
4	4	48	GLN
4	4	63	LYS
4	4	69	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	49	GLN
1	1	87	ASN
1	1	99	GLN
1	1	194	ASN
1	1	201	ASN
1	1	204	GLN
1	1	214	ASN
2	2	20	ASN
2	2	94	GLN
2	2	95	ASN
2	2	119	GLN
2	2	160	GLN
2	2	206	ASN
3	3	35	ASN
3	3	42	ASN
3	3	57	ASN
3	3	140	ASN
3	3	195	GLN
3	3	206	ASN
4	4	4	GLN
4	4	8	GLN
4	4	29	ASN
4	4	44	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 oligosaccharides 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
5	W71	1	501	-	27,27,27	2.42	7 (25%)	33,34,34	4.18	11 (33%)
5	W71	1	502	-	27,27,27	2.36	8 (29%)	33,34,34	4.16	10 (30%)
6	MYR	4	1	4	13,14,15	0.45	0	12,13,15	0.60	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
5	W71	1	501	-	-	8/15/22/22	0/3/3/3
5	W71	1	502	-	-	6/15/22/22	0/3/3/3
6	MYR	4	1	4	-	8/12/12/13	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	1	501	W71	O1-C5	6.67	1.45	1.35
5	1	502	W71	O1-C5	6.22	1.44	1.35
5	1	502	W71	C2A-N3A	6.03	1.34	1.27
5	1	501	W71	C2A-N3A	4.96	1.33	1.27
5	1	502	W71	O1A-C2A	4.11	1.42	1.36
5	1	501	W71	C4-C3	-4.02	1.33	1.40
5	1	501	W71	O1-N2	-3.68	1.35	1.42
5	1	501	W71	O1A-C2A	3.63	1.41	1.36
5	1	501	W71	C3-N2	3.50	1.36	1.30
5	1	501	W71	C4B-C2A	-3.27	1.40	1.47
5	1	502	W71	C4-C3	-3.00	1.35	1.40
5	1	502	W71	O1-N2	-2.86	1.37	1.42
5	1	502	W71	C3-N2	2.83	1.35	1.30
5	1	502	W71	C5B-C4B	2.51	1.43	1.39
5	1	502	W71	C6B-C1B	2.38	1.43	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1	502	W71	O1A-C2A-N3A	-11.59	108.23	118.25
5	1	501	W71	O1-C5-C1C	11.33	133.13	115.87
5	1	501	W71	O1A-C2A-N3A	-10.64	109.05	118.25
5	1	502	W71	O1-C5-C1C	10.57	131.97	115.87
5	1	502	W71	O1A-C2A-C4B	10.33	128.90	115.85
5	1	501	W71	O1A-C2A-C4B	9.46	127.81	115.85
5	1	502	W71	O1-C5-C4	-8.54	101.80	109.73
5	1	501	W71	O1-C5-C4	-7.75	102.53	109.73
5	1	501	W71	C31-C3-N2	7.37	126.01	119.97
5	1	502	W71	C4A-N3A-C2A	6.12	112.18	106.75
5	1	501	W71	C4A-N3A-C2A	6.07	112.14	106.75
5	1	502	W71	C31-C3-N2	6.01	124.89	119.97
5	1	501	W71	C4-C3-N2	-5.58	107.48	111.54
5	1	502	W71	C4-C3-N2	-5.40	107.61	111.54
5	1	501	W71	C5-O1-N2	-3.87	105.39	108.30
5	1	501	W71	C1C-C5-C4	-3.84	124.06	134.03
5	1	501	W71	C2C-C1C-C5	-3.53	106.25	113.49
5	1	502	W71	C5-O1-N2	-3.22	105.88	108.30
5	1	502	W71	C1C-C5-C4	-3.03	126.15	134.03
5	1	501	W71	C5A-C4A-N3A	-2.25	99.50	104.42
5	1	502	W71	C5A-C4A-N3A	-2.17	99.70	104.42

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	1	501	W71	C2C-C1C-C5-C4
6	4	1	MYR	O1-C1-C2-C3
5	1	501	W71	C2B-C1B-O1B-C7C
5	1	501	W71	C6B-C1B-O1B-C7C
5	1	502	W71	C6B-C1B-O1B-C7C
5	1	502	W71	C4C-C5C-C6C-C7C
5	1	502	W71	C2B-C1B-O1B-C7C
5	1	501	W71	C1C-C2C-C3C-C4C
6	4	1	MYR	C4-C5-C6-C7
6	4	1	MYR	C11-C10-C9-C8
5	1	501	W71	C5-C1C-C2C-C3C
5	1	502	W71	C5-C1C-C2C-C3C
5	1	501	W71	C3C-C4C-C5C-C6C
5	1	501	W71	C4C-C5C-C6C-C7C
6	4	1	MYR	C5-C6-C7-C8
6	4	1	MYR	C2-C3-C4-C5
6	4	1	MYR	C6-C7-C8-C9

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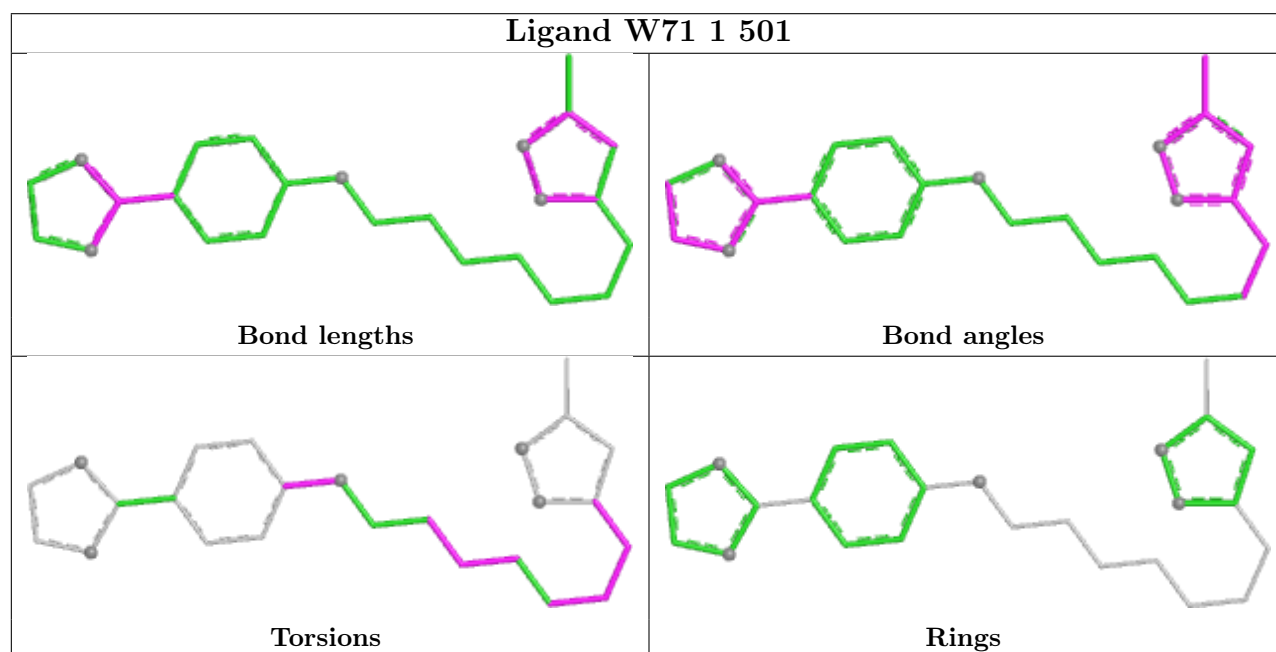
Mol	Chain	Res	Type	Atoms
6	4	1	MYR	C10-C11-C12-C13
5	1	501	W71	C2C-C1C-C5-O1
6	4	1	MYR	C1-C2-C3-C4
5	1	502	W71	C2C-C3C-C4C-C5C
5	1	502	W71	C3C-C4C-C5C-C6C

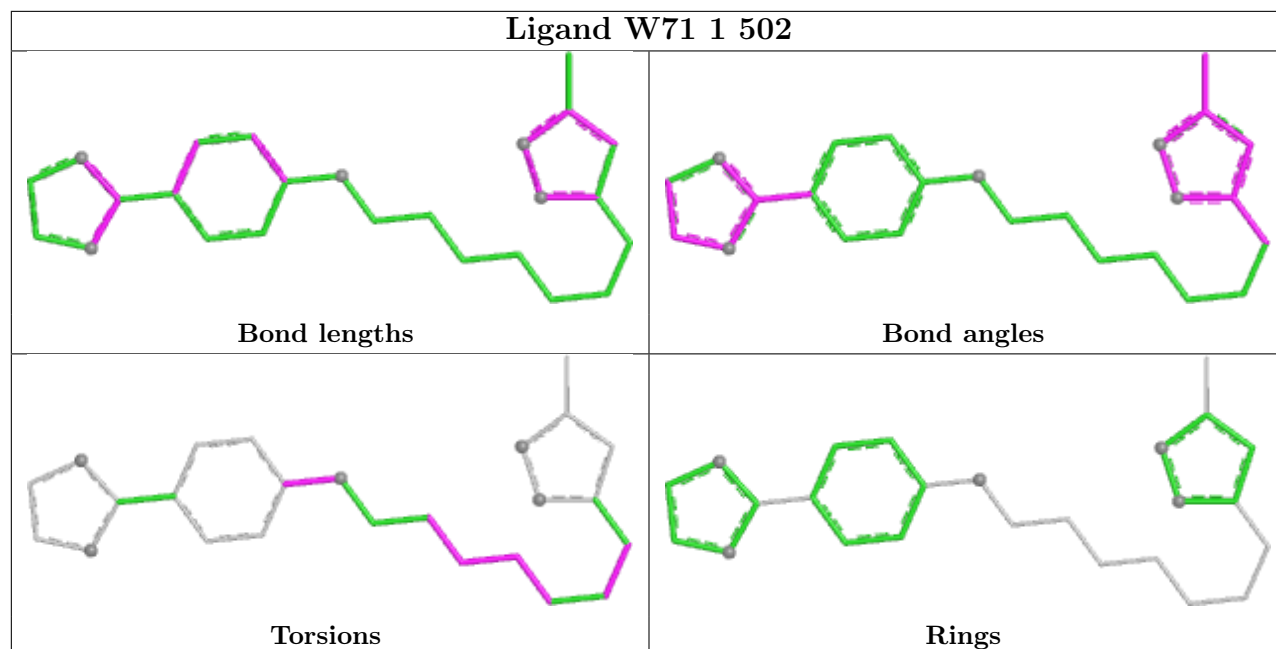
There are no ring outliers.

3 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	1	501	W71	9	0
5	1	502	W71	22	0
6	4	1	MYR	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.