



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:53 AM UTC

PDB ID : 1H4I / pdb_00001h4i
Title : Methylobacterium extorquens methanol dehydrogenase
Authors : Ghosh, M.; Anthony, C.; Harlos, K.; Goodwin, M.G.; Blake, C.
Deposited on : 2001-05-11
Resolution : 1.94 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

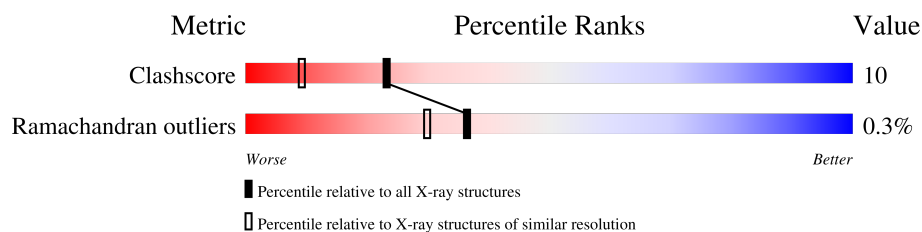
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)

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	599	
1	C	599	
2	B	74	
2	D	74	

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.

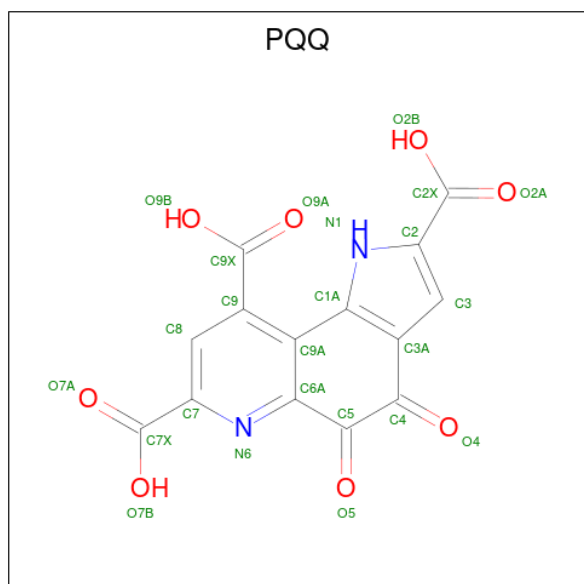
- Molecule 1 is a protein called METHANOL DEHYDROGENASE SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total 4620	C 2947	N 778	O 875	S 20	0	0	0
1	C	595	Total 4620	C 2947	N 778	O 875	S 20	0	0	0

- Molecule 2 is a protein called METHANOL DEHYDROGENASE SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	73	Total 586	C 369	N 103	O 111	S 3	0	0	0
2	D	73	Total 586	C 369	N 103	O 111	S 3	0	0	0

- Molecule 3 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: $C_{14}H_6N_2O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		
3	C	1	Total	C	N	O	0	0
			24	14	2	8		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		



● Molecule 2: METHANOL DEHYDROGENASE SUBUNIT 2



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.16Å 72.19Å 86.17Å 86.21° 76.09° 70.44°	Depositor
Resolution (Å)	20.00 – 1.94	Depositor
% Data completeness (in resolution range)	87.0 (20.00-1.94)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , 0.229	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10462	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: PQQ, CA

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	0.73	3/4750 (0.1%)	1.13	38/6456 (0.6%)
1	C	0.73	3/4750 (0.1%)	1.12	39/6456 (0.6%)
2	B	0.54	0/599	1.02	2/798 (0.3%)
2	D	0.54	0/599	1.01	2/798 (0.3%)
All	All	0.71	6/10698 (0.1%)	1.11	81/14508 (0.6%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	521	MET	SD-CE	-9.11	1.56	1.79
1	A	521	MET	SD-CE	-8.69	1.57	1.79
1	A	16	MET	SD-CE	6.11	1.94	1.79
1	C	16	MET	SD-CE	5.17	1.92	1.79
1	A	334	ILE	CA-CB	5.15	1.60	1.54
1	C	278	MET	SD-CE	-5.07	1.66	1.79

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	275	LYS	N-CA-C	10.44	124.55	110.35
1	A	275	LYS	N-CA-C	10.38	124.47	110.35
1	C	308	ASN	N-CA-C	8.67	121.52	110.33
1	A	308	ASN	N-CA-C	8.53	121.33	110.33
1	A	110	GLY	N-CA-C	8.30	120.84	110.96
1	C	416	MET	N-CA-C	8.07	120.38	108.60
1	A	416	MET	N-CA-C	7.96	120.22	108.60
1	A	496	LEU	N-CA-C	-7.76	95.86	108.52
1	A	15	VAL	N-CA-C	7.69	123.61	113.07
1	C	277	THR	N-CA-C	-7.65	98.16	110.32
1	A	277	THR	N-CA-C	-7.51	98.38	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	496	LEU	N-CA-C	-7.39	96.47	108.52
1	C	15	VAL	N-CA-C	7.35	123.14	113.07
1	A	114	TRP	CA-C-N	7.17	126.88	119.56
1	A	114	TRP	C-N-CA	7.17	126.88	119.56
1	C	335	VAL	CB-CA-C	-7.13	101.15	110.84
1	A	335	VAL	CB-CA-C	-7.08	101.29	110.98
1	A	588	ASP	N-CA-C	-7.08	95.58	109.10
1	C	91	LYS	CA-C-N	7.06	127.03	119.76
1	C	91	LYS	C-N-CA	7.06	127.03	119.76
1	C	417	ASP	N-CA-C	-7.00	98.82	109.95
1	C	441	GLY	CA-C-N	6.99	127.58	119.47
1	C	441	GLY	C-N-CA	6.99	127.58	119.47
1	A	476	TRP	N-CA-C	-6.99	98.89	109.79
1	C	476	TRP	N-CA-C	-6.98	98.90	109.79
1	C	588	ASP	N-CA-C	-6.87	96.32	108.69
1	A	91	LYS	CA-C-N	6.84	126.81	119.76
1	A	91	LYS	C-N-CA	6.84	126.81	119.76
1	A	441	GLY	CA-C-N	6.83	127.40	119.47
1	A	441	GLY	C-N-CA	6.83	127.40	119.47
1	A	417	ASP	N-CA-C	-6.82	99.11	109.95
1	C	202	GLY	CA-C-N	6.81	126.77	119.76
1	C	202	GLY	C-N-CA	6.81	126.77	119.76
1	A	202	GLY	CA-C-N	6.77	126.74	119.76
1	A	202	GLY	C-N-CA	6.77	126.74	119.76
1	C	114	TRP	CA-C-N	6.75	126.43	119.82
1	C	114	TRP	C-N-CA	6.75	126.43	119.82
1	A	31	GLN	N-CA-C	-6.70	103.91	111.07
1	A	356	ASN	N-CA-C	6.69	125.06	110.80
1	A	109	ARG	N-CA-C	6.66	121.24	113.18
1	C	31	GLN	N-CA-C	-6.63	103.97	111.07
1	A	14	TRP	N-CA-C	-6.59	96.44	107.32
1	C	356	ASN	N-CA-C	6.54	124.73	110.80
1	C	109	ARG	N-CA-C	6.52	121.07	113.18
1	C	14	TRP	N-CA-C	-6.50	96.59	107.32
1	C	324	LYS	N-CA-C	-6.48	97.12	108.20
1	A	37	VAL	CB-CA-C	-6.41	102.23	112.16
1	C	24	ASN	N-CA-C	6.30	118.22	111.36
1	C	37	VAL	CB-CA-C	-6.26	102.45	112.16
1	A	24	ASN	N-CA-C	6.21	118.14	111.36
1	A	324	LYS	N-CA-C	-6.21	97.58	108.20
1	A	282	GLY	N-CA-C	-6.12	98.68	113.18
1	A	220	TYR	N-CA-C	-5.95	105.28	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	70	SER	N-CA-C	-5.93	102.17	110.35
1	C	282	GLY	N-CA-C	-5.85	99.31	113.18
1	A	247	ALA	N-CA-C	-5.85	100.41	109.24
1	C	220	TYR	N-CA-C	-5.76	105.51	112.54
1	A	70	SER	N-CA-C	-5.65	102.55	110.35
1	C	73	ASN	N-CA-C	5.53	117.38	110.91
1	A	535	TYR	N-CA-C	-5.50	100.80	109.50
2	B	19	PHE	CA-C-N	5.49	125.47	120.03
2	B	19	PHE	C-N-CA	5.49	125.47	120.03
1	C	401	ASP	CA-C-N	5.48	125.14	119.05
1	C	401	ASP	C-N-CA	5.48	125.14	119.05
2	D	19	PHE	CA-C-N	5.45	125.43	120.03
2	D	19	PHE	C-N-CA	5.45	125.43	120.03
1	A	275	LYS	O-C-N	5.45	129.51	122.81
1	A	401	ASP	CA-C-N	5.41	125.06	119.05
1	A	401	ASP	C-N-CA	5.41	125.06	119.05
1	C	247	ALA	N-CA-C	-5.40	100.86	109.07
1	A	392	TYR	N-CA-C	-5.31	106.57	113.16
1	C	411	ILE	N-CA-C	5.29	116.94	108.89
1	C	307	VAL	N-CA-C	5.24	118.82	112.80
1	C	275	LYS	O-C-N	5.22	129.24	122.81
1	A	325	LEU	N-CA-C	5.18	117.73	109.81
1	C	458	TYR	N-CA-C	5.17	117.88	109.24
1	C	325	LEU	N-CA-C	5.17	117.71	109.81
1	A	276	TRP	CB-CA-C	5.08	120.05	110.35
1	C	276	TRP	CB-CA-C	5.07	120.04	110.35
1	A	73	ASN	N-CA-C	5.04	116.80	110.91
1	C	124	ILE	N-CA-C	-5.02	101.14	108.17

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	4620	0	4439	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4620	0	4439	98	0
2	B	586	0	584	11	0
2	D	586	0	584	11	0
3	A	24	0	3	2	0
3	C	24	0	3	2	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
All	All	10462	0	10052	212	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 10.

All (212) 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:C:482:THR:HG22	1:C:484:GLY:H	1.35	0.92
1:A:482:THR:HG22	1:A:484:GLY:H	1.33	0.92
1:A:73:ASN:HD22	1:A:94:GLN:HE22	1.22	0.84
1:C:413:HIS:HE1	1:C:443:LYS:H	1.26	0.83
1:C:73:ASN:HD22	1:C:94:GLN:HE22	1.26	0.81
1:C:212:ASP:HB2	1:C:215:ILE:HD12	1.64	0.80
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.17	0.80
1:A:413:HIS:HE1	1:A:443:LYS:H	1.26	0.79
1:A:521:MET:C	1:A:521:MET:HE3	2.07	0.78
1:C:521:MET:C	1:C:521:MET:HE3	2.10	0.76
1:C:114:TRP:CZ3	1:C:116:GLY:HA2	2.20	0.75
1:C:40:LEU:HD22	1:C:578:PHE:HB3	1.69	0.73
1:A:109:ARG:HE	1:A:395:GLN:HG3	1.54	0.73
1:C:109:ARG:HE	1:C:395:GLN:HG3	1.52	0.73
1:A:203:PRO:HB3	1:A:205:LYS:HE2	1.71	0.72
1:C:521:MET:HE1	1:C:523:TYR:CD2	2.25	0.71
1:A:212:ASP:HB2	1:A:215:ILE:HD12	1.71	0.71
1:A:521:MET:HE1	1:A:523:TYR:CD2	2.27	0.70
1:A:521:MET:HE2	1:A:532:ALA:HB3	1.73	0.69
1:C:521:MET:HE2	1:C:532:ALA:HB3	1.73	0.69
1:A:40:LEU:HD22	1:A:578:PHE:HB3	1.73	0.69
1:C:203:PRO:HB3	1:C:205:LYS:HE2	1.75	0.69
1:A:98:ALA:HB1	1:A:129:LEU:HD12	1.76	0.68
1:C:98:ALA:HB1	1:C:129:LEU:HD12	1.75	0.68
1:A:140:THR:OG1	1:A:142:GLU:HG3	1.95	0.67
1:C:140:THR:OG1	1:C:142:GLU:HG3	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ASP:OD2	1:C:525:HIS:HE1	1.78	0.65
1:C:16:MET:HE1	1:C:164:VAL:H	1.60	0.65
1:A:482:THR:HG22	1:A:484:GLY:N	2.09	0.65
1:C:413:HIS:CE1	1:C:443:LYS:H	2.14	0.65
1:A:16:MET:HE1	1:A:164:VAL:H	1.61	0.64
1:C:267:GLU:OE1	1:C:299:HIS:HE1	1.81	0.64
1:C:18:GLY:O	1:C:19:LYS:HB2	1.98	0.63
1:A:81:ASP:OD2	1:A:525:HIS:HE1	1.83	0.62
1:A:18:GLY:O	1:A:19:LYS:HB2	1.99	0.62
1:A:413:HIS:CE1	1:A:443:LYS:H	2.14	0.61
2:D:52:LYS:HA	2:D:52:LYS:HE2	1.80	0.61
1:A:267:GLU:OE1	1:A:299:HIS:HE1	1.83	0.61
1:A:355:VAL:O	1:A:386:CYS:O	2.19	0.61
1:A:200:ALA:O	1:A:276:TRP:HB2	2.01	0.61
1:A:10:SER:HB3	1:A:13:ASN:HD22	1.66	0.61
1:C:205:LYS:HD3	1:C:205:LYS:H	1.66	0.61
1:C:382:ALA:HB1	1:C:385:ILE:HD11	1.82	0.60
1:C:521:MET:HE1	1:C:523:TYR:CE2	2.37	0.60
1:A:404:ARG:HD3	1:A:502:ASP:OD2	2.01	0.60
1:C:404:ARG:HD3	1:C:502:ASP:OD2	2.01	0.60
1:C:482:THR:HG22	1:C:484:GLY:N	2.11	0.60
1:C:355:VAL:O	1:C:386:CYS:O	2.19	0.60
1:C:10:SER:HB3	1:C:13:ASN:HD22	1.67	0.60
1:A:205:LYS:H	1:A:205:LYS:HD3	1.67	0.60
1:C:200:ALA:O	1:C:276:TRP:HB2	2.02	0.60
2:B:52:LYS:HA	2:B:52:LYS:HE2	1.85	0.59
1:A:16:MET:CE	1:A:164:VAL:H	2.16	0.58
1:A:521:MET:HE1	1:A:523:TYR:CE2	2.38	0.58
2:D:71:ILE:O	2:D:72:SER:HB2	2.04	0.58
1:A:382:ALA:HB1	1:A:385:ILE:HD11	1.85	0.58
1:C:276:TRP:HA	1:C:279:THR:HG21	1.86	0.57
1:C:521:MET:HE1	1:C:523:TYR:HD2	1.69	0.57
1:A:29:LEU:O	1:A:482:THR:HG23	2.04	0.56
1:C:3:LYS:HE3	1:C:115:PRO:HB2	1.85	0.56
2:B:71:ILE:O	2:B:72:SER:HB2	2.05	0.56
1:C:16:MET:CE	1:C:164:VAL:H	2.18	0.56
1:A:521:MET:HE1	1:A:523:TYR:HD2	1.71	0.56
2:B:42:ASP:HA	2:B:45:LYS:HE3	1.88	0.56
1:A:276:TRP:HA	1:A:279:THR:HG21	1.88	0.56
2:D:4:THR:HG22	2:D:5:LYS:HD3	1.89	0.55
1:A:9:LYS:HE2	1:A:9:LYS:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:ALA:CB	1:C:385:ILE:HD11	2.36	0.55
1:C:109:ARG:NE	1:C:395:GLN:HG3	2.21	0.54
2:B:4:THR:HG22	2:B:5:LYS:HD3	1.88	0.54
1:C:29:LEU:O	1:C:482:THR:HG23	2.07	0.54
1:A:3:LYS:HE3	1:A:115:PRO:HB2	1.89	0.54
1:A:514:SER:HB3	1:A:570:GLN:O	2.08	0.54
1:A:382:ALA:CB	1:A:385:ILE:HD11	2.38	0.54
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.06	0.53
1:A:205:LYS:HD3	1:A:205:LYS:N	2.24	0.53
1:C:296:LYS:NZ	1:C:328:HIS:HE1	2.06	0.53
1:A:296:LYS:HZ1	1:A:306:GLY:HA3	1.73	0.53
1:A:3:LYS:HB3	1:A:115:PRO:HG2	1.91	0.53
1:C:276:TRP:HE3	1:C:279:THR:HG21	1.73	0.53
1:C:296:LYS:HZ1	1:C:306:GLY:HA3	1.74	0.53
1:C:9:LYS:HA	1:C:9:LYS:HE2	1.90	0.53
1:A:109:ARG:NE	1:A:395:GLN:HG3	2.23	0.52
1:A:276:TRP:HE3	1:A:279:THR:HG21	1.74	0.52
1:C:205:LYS:HD3	1:C:205:LYS:N	2.23	0.52
1:A:176:ALA:HB3	3:A:601:PQQ:O7B	2.09	0.52
1:A:414:ILE:HG12	1:A:452:LEU:HD12	1.92	0.52
1:A:426:ARG:HD3	1:A:426:ARG:N	2.25	0.51
1:C:426:ARG:HD3	1:C:426:ARG:N	2.25	0.51
1:C:314:GLU:HG2	1:C:324:LYS:HD3	1.93	0.51
1:C:514:SER:HB3	1:C:570:GLN:O	2.10	0.51
2:D:42:ASP:HA	2:D:45:LYS:HE3	1.93	0.51
1:C:378:MET:HE1	1:C:421:PHE:HA	1.91	0.51
1:A:52:ASN:O	1:A:54:HIS:HD2	1.94	0.50
1:C:127:THR:HG23	1:C:162:PRO:HG3	1.94	0.50
1:C:207:LEU:O	1:C:283:ARG:NH2	2.45	0.50
1:A:207:LEU:O	1:A:283:ARG:NH2	2.45	0.50
1:C:148:GLU:OE2	2:D:50:ARG:NH1	2.45	0.50
1:A:68:HIS:CE1	1:A:534:TYR:HE1	2.29	0.50
1:C:103:CYS:SG	1:C:104:CYS:N	2.85	0.49
1:C:3:LYS:HB3	1:C:115:PRO:HG2	1.94	0.49
2:D:23:ILE:HD12	2:D:30:PRO:HD3	1.93	0.49
1:A:103:CYS:SG	1:A:104:CYS:N	2.85	0.49
1:A:378:MET:HE1	1:A:421:PHE:HA	1.93	0.49
1:C:212:ASP:CB	1:C:215:ILE:HD12	2.39	0.49
1:C:278:MET:HE1	1:C:304:TYR:C	2.37	0.49
1:C:399:SER:OG	1:C:479:THR:HG22	2.12	0.49
1:C:68:HIS:CE1	1:C:534:TYR:HE1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:MET:HE1	1:A:304:TYR:C	2.38	0.49
1:C:335:VAL:HG22	1:C:351:LEU:CD2	2.42	0.49
1:A:594:TRP:HB2	1:C:472:ARG:HB2	1.95	0.48
2:B:23:ILE:HD12	2:B:30:PRO:HD3	1.96	0.48
1:C:37:VAL:O	1:C:40:LEU:HB2	2.13	0.48
1:C:1:ASN:O	1:C:5:VAL:HG23	2.14	0.48
1:A:127:THR:HG23	1:A:162:PRO:HG3	1.95	0.48
1:A:399:SER:OG	1:A:479:THR:HG22	2.13	0.48
1:C:205:LYS:H	1:C:205:LYS:CD	2.23	0.48
1:A:1:ASN:O	1:A:5:VAL:HG23	2.13	0.48
2:D:56:GLU:O	2:D:60:LYS:HG3	2.14	0.48
1:A:314:GLU:HG2	1:A:324:LYS:HD3	1.96	0.47
1:A:335:VAL:HG22	1:A:351:LEU:CD2	2.43	0.47
1:A:364:LYS:CD	1:A:364:LYS:C	2.87	0.47
1:C:52:ASN:O	1:C:54:HIS:HD2	1.98	0.47
1:A:18:GLY:O	1:A:19:LYS:CB	2.63	0.47
1:C:176:ALA:HB3	3:C:601:PQQ:O7B	2.15	0.47
2:B:56:GLU:O	2:B:60:LYS:HG3	2.15	0.47
1:A:15:VAL:O	1:A:16:MET:HG2	2.15	0.47
1:A:364:LYS:C	1:A:364:LYS:HD3	2.40	0.46
1:C:51:LEU:O	1:C:52:ASN:HB2	2.15	0.46
1:A:521:MET:HE3	1:A:522:THR:N	2.29	0.46
1:C:15:VAL:O	1:C:16:MET:HG2	2.15	0.46
1:A:148:GLU:OE2	2:B:50:ARG:NH1	2.48	0.46
1:A:208:LEU:CD2	1:A:289:GLU:HG2	2.45	0.46
1:C:1:ASN:H1	1:C:166:LYS:H	1.63	0.46
1:C:18:GLY:O	1:C:19:LYS:CB	2.62	0.46
1:C:414:ILE:HG12	1:C:452:LEU:HD12	1.96	0.46
1:A:243:TRP:CZ2	3:A:601:PQQ:C6A	2.99	0.46
1:C:425:TYR:C	1:C:426:ARG:HD3	2.41	0.45
1:A:205:LYS:H	1:A:205:LYS:CD	2.23	0.45
1:A:540:TRP:N	1:A:541:PRO:HD2	2.31	0.45
1:C:424:PRO:O	1:C:426:ARG:NH1	2.49	0.45
1:A:452:LEU:HB2	1:A:473:PHE:HA	1.98	0.45
1:C:476:TRP:CZ2	1:C:541:PRO:HD3	2.52	0.45
1:A:37:VAL:O	1:A:40:LEU:HB2	2.17	0.45
1:C:238:GLY:O	1:C:262:PRO:HA	2.17	0.45
1:C:296:LYS:HZ3	1:C:328:HIS:HE1	1.64	0.45
1:A:424:PRO:O	1:A:426:ARG:NH1	2.50	0.44
1:A:3:LYS:HB2	1:A:3:LYS:HE2	1.76	0.44
1:A:364:LYS:HD3	1:A:365:THR:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:TRP:CZ2	3:C:601:PQQ:C6A	3.00	0.44
1:A:129:LEU:HD13	1:A:129:LEU:O	2.17	0.44
1:C:521:MET:HE3	1:C:522:THR:N	2.31	0.44
1:C:364:LYS:C	1:C:364:LYS:CD	2.91	0.44
1:C:29:LEU:HD13	1:C:529:GLN:HG3	1.99	0.44
1:C:208:LEU:HD22	1:C:289:GLU:HG2	2.00	0.44
1:A:476:TRP:CZ2	1:A:541:PRO:HD3	2.52	0.44
1:C:243:TRP:CE2	1:C:307:VAL:HG21	2.53	0.44
1:C:193:GLU:HB2	2:D:55:VAL:HG11	2.00	0.43
1:A:153:LYS:HA	1:A:153:LYS:HE2	2.00	0.43
1:C:148:GLU:CD	2:D:50:ARG:NH1	2.76	0.43
1:C:540:TRP:N	1:C:541:PRO:HD2	2.34	0.43
2:B:47:MET:HG2	2:B:50:ARG:HH12	1.84	0.43
1:A:208:LEU:HD22	1:A:289:GLU:HG2	2.00	0.43
1:A:378:MET:HA	1:A:420:PRO:HG2	2.01	0.43
1:A:243:TRP:CE2	1:A:307:VAL:HG21	2.53	0.43
1:C:153:LYS:HE2	1:C:153:LYS:HA	2.00	0.43
1:C:423:LEU:HD21	1:C:431:PHE:HA	2.01	0.43
1:C:117:ASP:OD2	1:C:118:GLY:N	2.52	0.43
1:C:208:LEU:CD2	1:C:289:GLU:HG2	2.49	0.42
1:C:454:GLN:HE21	1:C:470:MET:HE1	1.84	0.42
1:A:447:GLN:H	1:A:447:GLN:NE2	2.17	0.42
1:C:129:LEU:HD13	1:C:129:LEU:O	2.18	0.42
1:A:212:ASP:CB	1:A:215:ILE:HD12	2.45	0.42
1:A:425:TYR:C	1:A:426:ARG:HD3	2.44	0.42
1:C:73:ASN:ND2	1:C:129:LEU:H	2.16	0.42
1:C:452:LEU:HB2	1:C:473:PHE:HA	2.01	0.42
1:A:117:ASP:OD2	1:A:118:GLY:N	2.52	0.42
2:B:67:ASP:HB3	2:B:70:LYS:HZ3	1.84	0.42
1:C:364:LYS:C	1:C:364:LYS:HD3	2.45	0.42
1:C:378:MET:HA	1:C:420:PRO:HG2	2.00	0.42
1:A:423:LEU:HD21	1:A:431:PHE:HA	2.01	0.42
1:A:15:VAL:HG12	1:A:61:VAL:HG22	2.02	0.42
1:A:238:GLY:O	1:A:262:PRO:HA	2.19	0.42
1:A:413:HIS:CE1	1:A:443:LYS:HB2	2.55	0.42
1:A:473:PHE:HB3	1:A:492:LEU:HD12	2.01	0.42
1:C:276:TRP:C	1:C:279:THR:HG23	2.45	0.42
2:B:67:ASP:HB3	2:B:70:LYS:NZ	2.35	0.42
1:A:51:LEU:O	1:A:52:ASN:HB2	2.19	0.42
1:A:329:PRO:HA	1:A:335:VAL:HA	2.02	0.42
1:A:48:THR:OG1	1:A:54:HIS:CE1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ASN:ND2	1:A:474:ALA:HB1	2.35	0.42
1:A:521:MET:HE3	1:A:521:MET:O	2.20	0.42
2:D:47:MET:HG2	2:D:50:ARG:HH12	1.84	0.42
1:C:329:PRO:HA	1:C:335:VAL:HA	2.02	0.41
1:C:521:MET:HE2	1:C:532:ALA:CB	2.48	0.41
1:A:276:TRP:C	1:A:279:THR:HG23	2.45	0.41
1:A:304:TYR:O	1:A:305:ALA:C	2.63	0.41
1:A:73:ASN:ND2	1:A:129:LEU:H	2.19	0.41
1:A:472:ARG:HB2	1:C:594:TRP:HB2	2.03	0.41
1:C:3:LYS:HB2	1:C:3:LYS:HE2	1.75	0.41
1:C:15:VAL:C	1:C:16:MET:HG2	2.46	0.41
1:C:48:THR:OG1	1:C:54:HIS:CE1	2.74	0.41
1:A:535:TYR:CD2	1:A:576:VAL:HG23	2.56	0.41
1:C:473:PHE:HB3	1:C:492:LEU:HD12	2.03	0.41
2:B:6:CYS:HA	2:B:12:CYS:HA	2.02	0.40
1:C:423:LEU:HA	1:C:424:PRO:HD3	1.91	0.40
1:A:447:GLN:CD	1:A:447:GLN:N	2.79	0.40
2:D:67:ASP:HB3	2:D:70:LYS:NZ	2.36	0.40
1:A:335:VAL:HG22	1:A:351:LEU:HD21	2.04	0.40
1:C:10:SER:HB3	1:C:13:ASN:ND2	2.34	0.40
1:C:326:LEU:O	1:C:337:THR:HA	2.21	0.40
1:A:296:LYS:HZ3	1:A:328:HIS:HE1	1.69	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	A	429/599 (72%)	404 (94%)	25 (6%)	0	100	100
1	C	593/599 (99%)	555 (94%)	37 (6%)	1 (0%)	43	37
2	B	71/74 (96%)	70 (99%)	0	1 (1%)	9	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	71/74 (96%)	70 (99%)	0	1 (1%)	9	2
All	All	1164/1346 (86%)	1099 (94%)	62 (5%)	3 (0%)	36	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	72	SER
2	D	72	SER
1	C	19	LYS

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
3	PQQ	C	601	4	26,26,26	2.48	8 (30%)	34,40,40	2.34	10 (29%)
3	PQQ	A	601	4	26,26,26	2.49	8 (30%)	34,40,40	2.33	10 (29%)

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
3	PQQ	C	601	4	-	0/12/28/28	0/3/3/3
3	PQQ	A	601	4	-	0/12/28/28	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PQQ	C5-C4	-7.72	1.43	1.54
3	C	601	PQQ	C5-C4	-7.71	1.43	1.54
3	A	601	PQQ	O9B-C9X	-4.60	1.16	1.30
3	C	601	PQQ	O9B-C9X	-4.59	1.16	1.30
3	A	601	PQQ	O4-C4	-3.91	1.14	1.23
3	C	601	PQQ	O4-C4	-3.91	1.14	1.23
3	C	601	PQQ	O2A-C2X	3.79	1.31	1.22
3	A	601	PQQ	O2A-C2X	3.78	1.31	1.22
3	C	601	PQQ	O7B-C7X	-3.43	1.20	1.30
3	A	601	PQQ	O7B-C7X	-3.41	1.20	1.30
3	A	601	PQQ	O2B-C2X	-3.33	1.21	1.30
3	C	601	PQQ	O2B-C2X	-3.32	1.21	1.30
3	C	601	PQQ	O7A-C7X	2.82	1.30	1.22
3	A	601	PQQ	O7A-C7X	2.82	1.30	1.22
3	A	601	PQQ	C6A-C5	2.58	1.53	1.50
3	C	601	PQQ	C6A-C5	2.58	1.53	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	PQQ	O5-C5-C6A	4.82	127.27	121.76
3	A	601	PQQ	O5-C5-C6A	4.80	127.24	121.76
3	C	601	PQQ	O4-C4-C5	-4.76	112.51	118.37
3	A	601	PQQ	O4-C4-C5	-4.75	112.52	118.37
3	A	601	PQQ	O7B-C7X-C7	4.40	125.15	114.71
3	C	601	PQQ	O7B-C7X-C7	4.38	125.11	114.71
3	A	601	PQQ	O2A-C2X-C2	-4.00	112.89	121.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	PQQ	O9B-C9X-C9	4.00	126.65	115.28
3	C	601	PQQ	O9B-C9X-C9	4.00	126.65	115.28
3	C	601	PQQ	O2A-C2X-C2	-3.99	112.92	121.01
3	C	601	PQQ	O9B-C9X-O9A	-3.73	115.34	123.35
3	A	601	PQQ	O9B-C9X-O9A	-3.72	115.36	123.35
3	C	601	PQQ	O7A-C7X-C7	-3.70	113.86	121.30
3	A	601	PQQ	O7A-C7X-C7	-3.69	113.88	121.30
3	A	601	PQQ	O2B-C2X-C2	3.49	121.80	114.27
3	C	601	PQQ	O2B-C2X-C2	3.49	121.79	114.27
3	C	601	PQQ	C3A-C4-C5	3.33	120.80	117.03
3	A	601	PQQ	C3A-C4-C5	3.31	120.78	117.03
3	C	601	PQQ	C1A-C3A-C4	-2.64	120.11	122.33
3	A	601	PQQ	C1A-C3A-C4	-2.61	120.14	122.33

There are no chirality outliers.

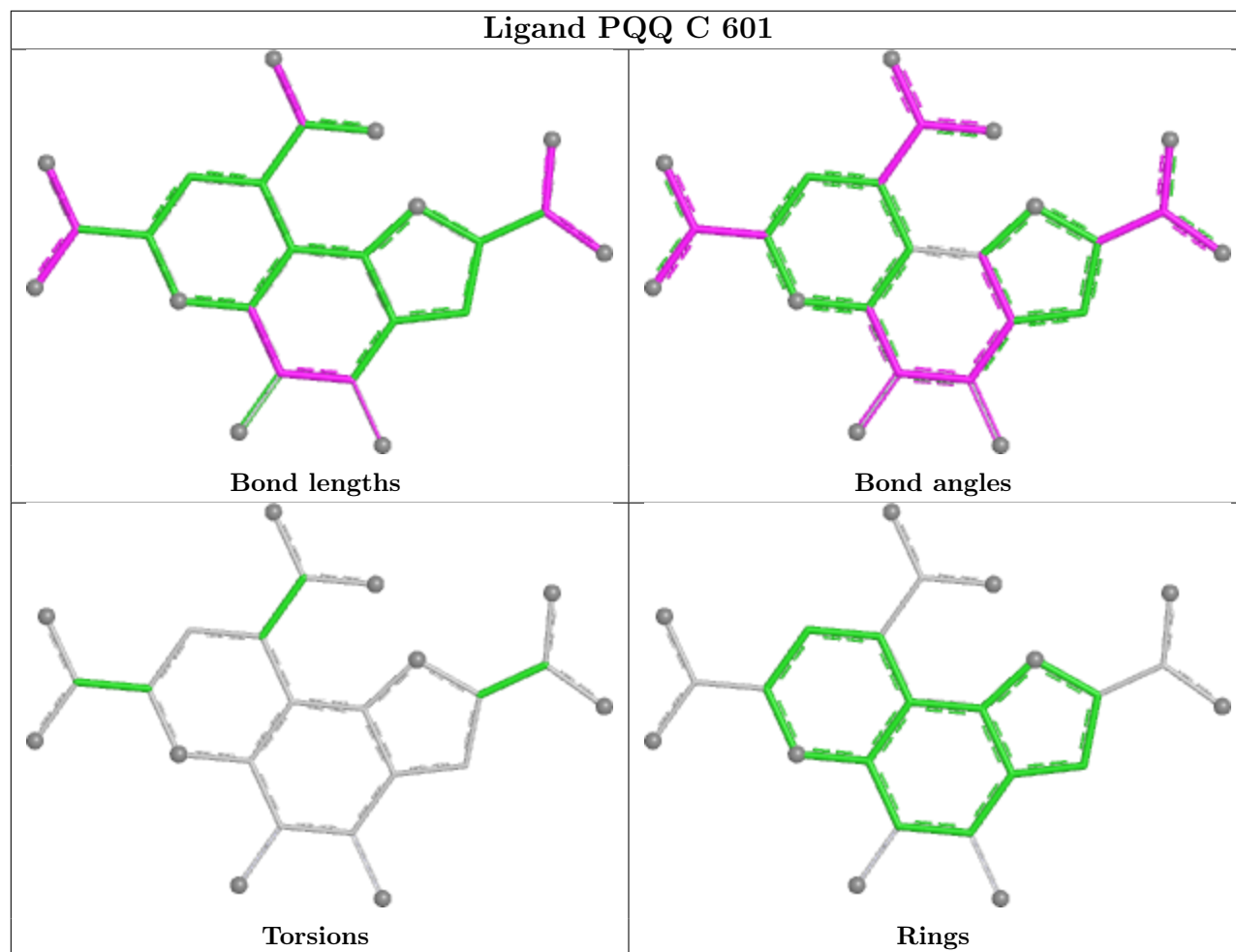
There are no torsion outliers.

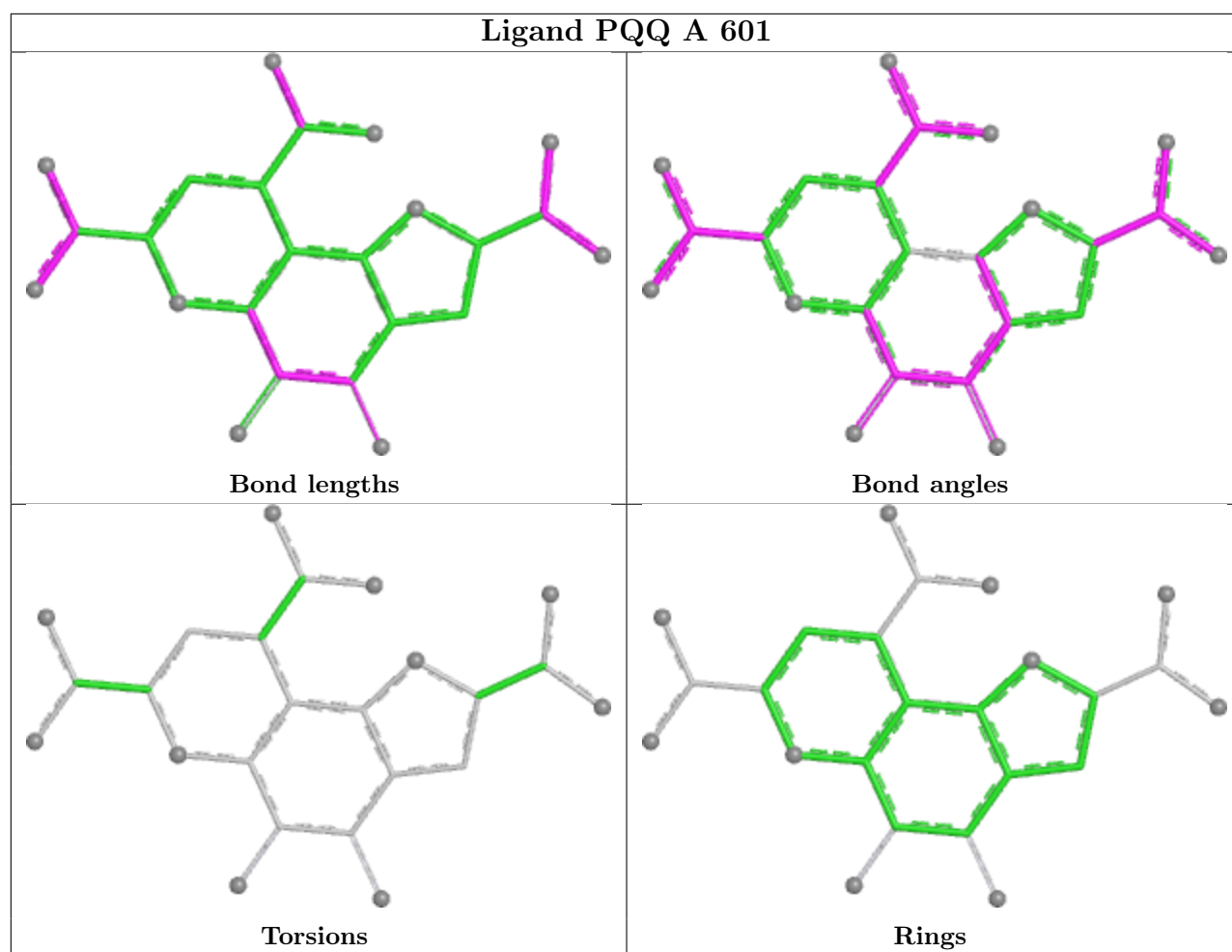
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	601	PQQ	2	0
3	A	601	PQQ	2	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.